AN ASSESSMENT OF THE DISPERSION MODELS IN THE MARSS SYSTEM USED AT THE KENNEDY SPACE CENTER

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ABSTRACT

This report is an assessment by NOAA's Air Resources Laboratory of the Ocean Breeze/Dry Gulch (OB/DG) and Local Meteorological Puff (LOMPUFF) dispersion models presently available for use within the Meteorological and Range Safety Support (MARSS) system at NASA's Kennedy Space Center (KSC). Improvements in the modeling of both regional scale wind fields and effluent dispersion, combined with recent rapid advances in computer technology, have brought about the need to re-evaluate the use of the OB/DG dispersion model, especially since other launch facilities have switched or are switching to newer models. The key question is whether significant improvements (better accuracy, applicability over a wider range of effluent and atmospheric conditions) are possible, given the present state of dispersion modeling.

The review team considered the source and wind characteristics at KSC, and the dispersion data available. It then examined KSC capabilities for regional scale modeling (present and near-future), and meteorological data collection. The various components of the dispersion models (OB/DG and Lompuff) available at KSC were studied in detail, to identify strengths and weaknesses. Possible alternate models were discussed briefly, and recommendations for future modeling and model testing at KSC were provided.

The review team believes that the OB/DG model is both limited in applicability and outdated, and recommends that it be replaced with a more capable model. In addition, a comprehensive transport and dispersion experiment is recommended, to replace the limited OB data set with data obtained over a much wider range of time, meteorological conditions, and source locations, so that the new model (and expected future improved models) can be properly tested. At NASA's request, a comprehensive "strawman" experimental plan and cost estimate was developed during the review process as an Appendix to this report.
1.0 INTRODUCTION

This report is an assessment of the Ocean Breeze/Dry Gulch (OB/DG) and Local Meteorological Puff (LOMPUFF) dispersion models presently available for use at NASA’s Kennedy Space Center (KSC). Dispersion modeling capabilities are needed at KSC because of the risk of releases of airborne contaminants associated with a variety of activities. Site operations such as liquid fuel and oxidizer storage and transfer, and the exhaust plumes from rocket engines (the Rocket Exhaust Effluent Diffusion Model, REEDM, is used for this latter case) result in more-or-less routine operational releases that must be assessed for on- and off-site safety and health issues. There are also occasional accidental releases due to operational errors, or to equipment failures or damage; assessments must be performed for these as well. The assessments must generally be provided quickly, in near-real-time for the accidental releases, so site managers can make informed decisions about continuing operations, or take steps to protect workers and spectators in the event of accidental releases.

NOAA’s Air Resources Laboratory was asked to review the present dispersion modeling capabilities within the Meteorological and Range Safety Support (MARSS) system at KSC. Improvements over the last decade or so in the modeling of both regional scale wind fields and effluent dispersion, combined with recent rapid advances in computer technology, have brought about the need to re-evaluate the use of the OB/DG dispersion model, especially since other launch facilities, including Vandenberg AFB, have switched or are switching to newer models (often AFTOX, a USAF-developed code). The key question is whether significant improvements (better accuracy, applicability over a wider range of effluent and atmospheric conditions) are possible, given the present state of dispersion modeling. This report attempts to examine the requirements for such a model, the difficulties facing it, and the data available to drive it, and offers recommendations for future modeling and model testing at KSC.

The review team has tried to take a fairly broad view of the problem. We have recognized the complexity of the wind patterns along the Florida east coast, and have examined existing and/or pending abilities to measure and model these flows. We have also considered some of the more likely effluent sources, and the ability of dispersion models to deal with such sources. The adequacy of the existing meteorological data collection system has been considered, especially as it relates to evaluating transport and dispersion conditions in the coastal environment. The adequacy of the existing computer system used for dispersion modeling was discussed. Finally, we considered the likely availability of additional information (such as winds and temperatures aloft, from newly emerging remote sensing systems) and its implications for driving a new generation of transport and dispersion models that might be better suited to coping with complex release scenarios. At NASA’s request, we specifically addressed the following points:

- The validity of the predictions of the models for parameters such as safe distance, spilled fluid pool thickness and evaporation rate, and exposure levels.
- Whether the OB/DG and LOMPUFF models should be tested with a full field test of the evaporative source and diffusion models.
- Guidance on the nature and timing of model verification tests, including any tests of submodels such as those for spilled fluid pool thickness and evaporation rate.
- Whether there are more appropriate models that would better characterize dispersion at KSC.
Section 2 of this report provides some background on dispersion modeling, in terms of the general categories of dispersion models presently available. Section 3 briefly discusses some of the effluent source characteristics and chemicals that are important at KSC. Section 4 describes the unusual wind characteristics of the Cape Canaveral area, ranging from synoptic influences through the localized sea breeze and river breeze effects observed at KSC, to site-specific influences on dispersion such as large paved regions and building wakes. Section 5 reviews the tracer dispersion data known to be available for KSC, and discusses their advantages and shortcomings. Section 6 reviews some of the regional scale modeling work that has been accomplished for the area, with particular attention to the sea breeze and its impact on wind patterns. The RAMS model, now being added to the existing capabilities at KSC, is considered at some length, because it shows considerable promise (despite some limitations) in elucidating these complex regional scale flows that impact local dispersion. Section 7 discusses the extensive (but mostly) surface-based meteorological data collection capabilities in place around KSC that can provide information for use in dispersion models. Section 8 considers the OB/DG and LOMPUFF models presently available on the MARSS system at KSC, including the submodels used to generate the required source term, and details their strengths and weaknesses. Section 9 discusses several alternative source models for effluent spills, while Section 10 describes a number of alternative dispersion models with attractive characteristics for possible use at KSC. Section 11 provides conclusions about the existing dispersion modeling capabilities at KSC, and recommendations for possible improvements to those capabilities. At NASA's request, Appendix A was added to the report during the review process; it provides a tentative design for a comprehensive flow and dispersion experiment to replace the OB/DG data set, as an aid to developing and testing improved transport and dispersion models for the Cape area.

### 2.0 BACKGROUND

Mathematical dispersion models are important components in emergency response or planning systems that deal with hazardous atmospheric contaminants. The most appropriate modeling technique for a particular emergency response system depends on the model's purpose. Some models simulate dispersion on quite large (even global) scales, while others deal only with near-field dispersion out to a few kilometres from the effluent source. Models can often be classified as simple, computationally efficient "Class A" models, which provide real-time (or near real-time) estimates of transport and diffusion during accidental releases, and slower, more complex "Class B" models which simulate releases in more detail. Class B models are frequently useful for planning and for detailed post-accident assessments. The diffusion modeling techniques that have been developed for passive contaminants (i.e., gaseous materials which are approximately the density of ambient air, and so do not alter the local wind, turbulence, and temperature fields) generally fall into four categories: (a) solutions of the diffusion equation; (b) stochastic modeling; (c) assumed concentration distribution methods; and (d) statistical models. These categories are reviewed briefly below; for more extensive discussions, see Eckman and Dobosy, 1989, and Drake et al., 1979.

The diffusion equation for a contaminant of concentration $C$ in a turbulent fluid with mean velocity components $u_i$ ($i = 1,2,3$) in the direction $x_i$ is given by:
where $t$ is time, $S$ is the net source/sink for the contaminant, and a prime indicates a fluctuating quantity. Repeated indices indicate summation. The mean of the product $u_i' C'$ is the turbulent flux of the contaminant in the $x_i$ direction. The difficulty in solving this equation is that the turbulent fluxes are unknown quantities; this is the well known "closure problem". Additional equations or assumptions are needed to provide a soluble system. First-order closure assumes that the turbulent fluxes are proportional to the components of the mean concentration gradient; this hypothesis was heavily explored in the past because it permits analytical solutions (e.g., Sutton, 1953), but it is generally unrealistic (see Pasquill and Smith, 1983). Second-order closure schemes (Donaldson, 1973) introduce additional equations for the turbulent fluxes, but also introduce unknown third moments, which are generally assumed to depend on the first and second moments to close the system. The solutions obtained in this way are more realistic than those from first-order closure schemes, but require considerable computational effort.

Stochastic techniques treat the turbulent velocity fluctuations of a fluid particle as a Markov process, so that the fluctuating velocity at some time $t + \tau$ is related to its value at the earlier time $t$ through a Lagrangian velocity correlation $R_{ij}(\tau)$, and to a random contribution selected from a given statistical distribution (see Smith, 1968):

$$u_i'(t + \tau) = R_{ij}(\tau) u_j'(t) + u_i''(t)$$

The equation is applied to the motion of a large number of fluid particles, and the resulting particle distribution represents the time-averaged diffusion of a contaminant in the fluid. For homogeneous turbulence, the random term $u_i''(t)$ is sampled from a Gaussian distribution with a constant variance; for inhomogeneous turbulence, it is taken from more complex distributions (e.g., see Thomson, 1984).

The assumed-distribution method assumes that the concentration distribution within a contaminant cloud has a known, specific mathematical form. Probably the best known member of this family is the Gaussian plume formula (e.g., Hanna et al. 1982) for a continuous emission:

$$C = \frac{q}{2\pi U \sigma_2 \sigma_3} \exp\left[ -\frac{1}{2} \left( \frac{x_2}{\sigma_2} \right)^2 \right] \left\{ \exp\left[ -\frac{1}{2} \left( \frac{x_3 - h}{\sigma_3} \right)^2 \right] + \exp\left[ -\frac{1}{2} \left( \frac{x_3 + h}{\sigma_3} \right)^2 \right] \right\}$$

where $q$ is the effluent emission rate (mass/time); $U$ is the spatially-invariant mean wind speed, taken to be along the $x_1$ direction; $\sigma_2$ and $\sigma_3$ are the standard deviations of the effluent concentration distribution in the $x_2$ (crosswind) and $x_3$ (vertical) directions; and $h$ is the effective effluent release height.

An assumed-distribution that is generally more appropriate for complex terrain is the puff model (see, e.g., Ludwig et al., 1977; Mikkelsen et al., 1984), wherein a (usually Gaussian) puff of contaminant is moved about by the spatially-variable mean wind field, and is diffused steadily by the turbulence. The Gaussian puff equation is:
\[ C = \frac{Q}{(2\pi)^{3/2} \sigma_1 \sigma_2 \sigma_3} \exp \left\{ \frac{1}{2} \left[ \left( \frac{y_1}{\sigma_1} \right)^2 + \left( \frac{y_2}{\sigma_2} \right)^2 + \left( \frac{y_3}{\sigma_3} \right)^2 \right] \right\} \]  

(2.4)

where \( Q \) is the total mass of material in the puff, and the \( y \) give distances from the puff’s center.

**Statistical models** establish quantitative empirical relationships between concentrations and emissions by exploring the dependence of the predictions on combinations of key physical and meteorological variables. Often a certain amount of theoretical understanding of the relevant processes is assumed, to help select the appropriate variables for inclusion. Multi-variable regressions or other statistical tools are then used to develop an equation with empirically-based coefficients and exponents. Once the particular method is calibrated to a particular site, it can be used for predictions. One advantage of the method is that it may elucidate the relative importance of different variables. However, significant changes in source configuration (height, release rate, effluent temperature or other characteristics, etc.) or in meteorological conditions beyond the conditions and data used to derive the predictive expression invalidate its use, making the estimates unreliable. Drake et al. (1979) are blunt: "A statistical model is not applicable beyond the range of conditions included in the data used in its development and optimization."

Table 2.1 shows some of the advantages and disadvantages of the various modeling techniques described in this section. The OB/DG model used at KSC is a typical statistical model, while the LOMPUFF model is a puff model characteristic of the assumed-distribution class.

The modeling techniques described so far are intended to simulate the dispersion of passive contaminants. However, many hazardous materials are denser than air and/or are stored at low temperatures, and thus are strongly affected by gravity during the initial stages of the dispersion. The modeling of dense-contaminant releases is less developed than that for passive releases. Most of the practical techniques for dense-contaminant dispersion fall into the assumed-distribution category discussed above (see Eckman, 1990). These techniques assume that instantaneous releases of dense contaminant are cylindrical in shape, whereas continuous releases are treated as rectangular slabs. Initially, the dense clouds in these models flatten out on the ground (slump) as a result of the negative buoyancy. Later, the clouds become dilute enough to be treated as passive clouds, and in fact, most of the dense-contaminant models simulate the later passive phases of the diffusion with a Gaussian plume or puff model. Neither the OB/DG model nor the LOMPUFF model has the capability to simulate dense-contaminant releases.

### 3.0 SOURCE CHARACTERISTICS TYPICAL OF KSC

A convenient and comprehensive listing of source locations, characteristics, and quantities of potential effluents was not found by the NOAA team within the MARSS documentation. However, examination of the MARSS Program Maintenance Manual (Wiley et al., 1988) indicates that 44 sites have been identified on the KSC/CCAFS area as potential sources. These are summarized in Table 3.1. Although the map coordinates for each site are specified, no information was found in the MARSS documentation about the probable height above ground of the source(s) at that site.
Table 2.1. Advantages and disadvantages of various diffusion techniques discussed in text (modified from Eckman and Dobosy, 1989).

<table>
<thead>
<tr>
<th>TECHNIQUE</th>
<th>ADVANTAGES</th>
<th>DISADVANTAGES</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diffusion-equation</td>
<td>Easy to introduce inhomogeneous turbulence and chemical reactions.</td>
<td>Closure problem.</td>
</tr>
<tr>
<td>techniques</td>
<td>Analytical solutions possible in simple situations.</td>
<td>Grid resolution problem.</td>
</tr>
<tr>
<td>Stochastic techniques</td>
<td>Relatively simple to install on a computer.</td>
<td>Must be repeated for many particles.</td>
</tr>
<tr>
<td></td>
<td>Can introduce inhomogeneous turbulence.</td>
<td>Results often similar to those of simpler techniques.</td>
</tr>
<tr>
<td>Gaussian plume model</td>
<td>Simplicity.</td>
<td>Not appropriate for complex terrain or nonstationary conditions.</td>
</tr>
<tr>
<td></td>
<td>Limited input requirements.</td>
<td>Not appropriate for light winds.</td>
</tr>
<tr>
<td>Puff models</td>
<td>Relatively simple.</td>
<td>Utility decreases if puffs become too large.</td>
</tr>
<tr>
<td></td>
<td>Can cope with complex terrain and light winds.</td>
<td>Computation time rapidly increases with number of puffs.</td>
</tr>
<tr>
<td></td>
<td>Can introduce inhomogeneous turbulence to a limited extent.</td>
<td></td>
</tr>
<tr>
<td>Statistical models</td>
<td>Simple to use.</td>
<td>Transfer to other sites unreliable.</td>
</tr>
<tr>
<td></td>
<td>Based on site-specific data.</td>
<td>Use for conditions or scales beyond initial derivation is risky.</td>
</tr>
<tr>
<td></td>
<td>Limited data requirements.</td>
<td></td>
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<tr>
<td>Sites listed in MARSS system as potential effluent release locations within KSC/CCAFS area</td>
<td></td>
<td></td>
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<tr>
<td>--------------------------------------------------------------------------------------------</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Astrotech</td>
<td>LC-40</td>
<td></td>
</tr>
<tr>
<td>Cargo Hazardous Servicing</td>
<td>LC-41</td>
<td></td>
</tr>
<tr>
<td>Castor IV</td>
<td>LC-46</td>
<td></td>
</tr>
<tr>
<td>CCAFS Industrial Area</td>
<td>MAB Area</td>
<td></td>
</tr>
<tr>
<td>CCF-39 (Propellant Storage)</td>
<td>OPF</td>
<td></td>
</tr>
<tr>
<td>Contr. Rd - Rail Car Siding</td>
<td>Ordnance Storage Area 3</td>
<td></td>
</tr>
<tr>
<td>Delta HPF</td>
<td>Poseidon Wharf</td>
<td></td>
</tr>
<tr>
<td>Delta Spin Test Facility</td>
<td>Prototype Lab</td>
<td></td>
</tr>
<tr>
<td>ESA-60A: Propellant Lab</td>
<td>S&amp;A Building</td>
<td></td>
</tr>
<tr>
<td>Fire Training Area</td>
<td>SAEF-II</td>
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<tr>
<td>Fuel Farm 1</td>
<td>Second Stage Buildup</td>
<td></td>
</tr>
<tr>
<td>HMF Area (M7-961)</td>
<td>SLF</td>
<td></td>
</tr>
<tr>
<td>HMF Area (M7-1212)</td>
<td>SMAB/SPIF</td>
<td></td>
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<tr>
<td>Hypergol Payload Test</td>
<td>SRB Hot Fire Area East</td>
<td></td>
</tr>
<tr>
<td>ITL Railcar Storage</td>
<td>SRB Hot Fire Area West</td>
<td></td>
</tr>
<tr>
<td>KSC Industrial Area</td>
<td>SRB Recovery Area</td>
<td></td>
</tr>
<tr>
<td>LC-14</td>
<td>SRB Refurb Facility</td>
<td></td>
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<tr>
<td>LC-17</td>
<td>Suspect Rail Car Siding</td>
<td></td>
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<tr>
<td>LC-36A</td>
<td>Titan III ITL Area</td>
<td></td>
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<tr>
<td>LC-36B</td>
<td>Trident Wharf</td>
<td></td>
</tr>
<tr>
<td>LC-39A</td>
<td>VAB</td>
<td></td>
</tr>
<tr>
<td>LC-39B</td>
<td>VPF</td>
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</table>
A wide variety of actual (generally under appropriate controls) and potential release scenarios exist at KSC. Routine releases include venting of materials from storage tanks, or during transfer operations such as filling or emptying launch vehicle fuel tanks. Other operational effluent releases occur during launches -- principally the emission of combustion products; these latter are dealt with by the REEDM code (see Boyd and Bowman, 1986), and are not considered here. Accidental releases are associated with tank or piping failures, fuel handling accidents, launch failures, or fires. REEDM is also used to deal with catastrophic post-launch accidents and the resulting cloud. There is a potential for radiological releases produced by payload destruction during a catastrophic launch accident; this apparently has been handled by the EMERGE code, and is also not treated here.

Discussions with NASA, USAF, and ENSCO personnel at KSC indicate that NASA uses the OB/DG model to deal with both operational and emergency effluent releases, while the USAF uses OB/DG only for emergencies. Some effluent vent locations (e.g., for space shuttle fueling) were described as being 60 to 200 ft above ground level (AGL); this is significant because the OB/DG model was developed and is valid only for a ground level source. Releases from such elevated sources are treated as being at ground level. Some accidental releases (especially those involving hypergolic materials) have the potential to be "hot spills" involving fire or explosion; neither OB/DG nor LOMPUFF can deal with these. Large, rapid spills of N₂O₄ will tend to behave as a dense gas release until enough air entrainment and N₂O₄ dissociation have occurred to allow the cloud to behave as a passive gas. Again, neither OB/DG or LOMPUFF can deal with this aspect of a release.

The principal chemicals of concern at KSC are included in a data base in the MARSS code, together with their significant characteristics such as boiling point; critical temperature, pressure, and volume; molecular weight; short- and long-term exposure limits; and so on. The main chemicals of interest are discussed further in Section 8.2.1, and shown in Table 8.1 there, as part of a discussion of the source strength evaluation.

4.0 WINDS AT KSC

The KSC, because of its location on what is virtually a barrier island off the east coast of Florida, is subject to very complicated wind flow patterns, on large (synoptic), regional, and local scales. Fortunately a good deal of work has been devoted to the study of the area, and considerable understanding and predictive ability have been developed in recent years. This capability is continuing to improve, partly because of the recent improvements in regional scale modeling discussed in Section 6, and partly because of improved observational capabilities and coastline studies at other sites.

Siler (1980) has examined the synoptic weather patterns that influence wind conditions along the east coast of Florida, using the National Weather Service surface analyses for 79 days in 1965. He found that nine basic weather patterns make up more than 98% of the observed cases. These cases are largely tied to the location and strength of the subtropical anticyclone and its associated east-west ridge of high pressure, which in turn determine general flow directions and strengths. Using Siler's notation, the basic patterns and their annual average percentage frequency of occurrence are:
A1: subtropical ridge lying north of Cape Canaveral, 20.5%
A2: subtropical ridge lying very close to Cape Canaveral, 13.7%
A3: subtropical ridge lying south of Cape Canaveral, 9.2%
D1: cold front approaching from the north or northwest, 9.6%
D2: cold front over southern Florida, 7.6%
B: high pressure centered over eastern third of the U. S., 15.2%
GH: high pressure in the Gulf of Mexico, 7.9%
E: low pressure in the Gulf of Mexico, 3.7%
LV: weak pressure gradient within 278 km (150 naut. mi.) of KSC, 11.4%

Patterns A1, A2, and B have a combined annual probability of occurrence of nearly 50%. The occurrence of the particular patterns varies strongly with the season. Examination of current and forecast weather maps thus allows a reasonable estimate of what the large-scale wind patterns are or will be like. Siler's (1980) emphasis was on the frequency of onshore flows and the probability of precipitation associated with the identified weather patterns, because these phenomena affect dispersion and deposition of toxic materials. For example, on an annual basis, there is a 91% probability that a type A1 weather pattern will produce onshore or alongshore winds (winds coming from roughly NW through E to S directions). In descending order of probability, for similar wind directions, the annual average values are 86% (type B), 51% (type E), 47% (type A2), 45% (type LV), 21% (type GH), 12% (type D2), 8% (type A3), and 7% (type D1). Such information might be quite helpful in a probabilistic approach to dispersion modeling for a specified range of release scenarios.

On a regional scale, the meteorological situation at KSC is quite complex. Kennedy Space Center lies on Cape Canaveral and Merritt Island, on the Florida east coast, separated from the mainland by the Indian River, with the Banana River splitting the land mass to the south. During the day, the incoming solar radiation warms the land considerably, setting up a thermally driven circulation from the cooler ocean waters toward the land (the well-known sea breeze effect). A similar but somewhat weaker effect is produced by the Indian River, and perhaps by the Banana River (Taylor et al., 1990). In the evening, as the land cools below the water temperatures, a thermal circulation directed toward the water occurs (the land breeze). Both of these flow systems are actually circulations, with a layer of moderate breeze near the ground, and a weak return flow aloft. Interactions with the synoptic flow and the Coriolis effect due to planetary rotation combine to produce very complicated near-coast flow patterns and effluent trajectories. The daytime sea breeze provides a zone of convergence and uplift over the land; the resulting updrafts quite often are sufficient to produce convective showers or even thunderstorms by late afternoon, particularly during the summer months. These convective rainstorms can produce very complicated flows before their passage. Lyons and Fisher (1988) have shown the potential dispersion pattern of a toxic gas within a seabreeze along which a thunderstorm mesosystem occurred. Their climatological analysis of St. Lucie, FL, revealed the potential for complex, frequently shifting winds associated with a stable boundary layer caused by a mesohigh ahead of the thunderstorm's rain shaft.

Taylor et al. (1990) have described their observations of the local wind patterns at three different times of the year during the Kennedy Space Center Atmospheric Boundary Layer Experiment (KABLE). During mid-autumn, 1988, a sea breeze or its influence was observed on 7 of 12 experimental days. The sea breeze usually began between 0900 and 1100 EST. The difference between overland and overwater temperatures was as little as 1°C. The main sea breeze front moved inland at a speed of 1 to 3 m/s on most days, and the maximum depth of the sea breeze layer was between 400 m and 800 m. The sea breeze was observed to reach more than 40 km
inland. The Indian River breeze was also observed on all sea breeze days; it began at about
the same time as the main sea breeze, and was about 50 m to 200 m deep. It was most
prevalent in the Indian River area south of Titusville. It retarded the movement of the sea breeze
across Merritt Island, and altered the PBL winds for several km around the river. The turbulence
level in the PBL (as indicated by measurements of the standard deviation of wind direction, $\sigma_{uv}$
and of the fluctuations of the vertical wind component, $\sigma_w$) increased during the day until the
sea or river breeze passed through, and then decreased; $\sigma_u$ values were found to be a good
indicator of the sea breeze passage, attaining peak values just prior to the front's passage,
which was followed by a change in wind direction.

In late spring of 1989, 13 of 19 experimental days had an identifiable sea breeze. The sea
breeze usually began about 1000 to 1100 EST, but this seemed (not surprisingly) to be affected
by the strength of the wind component perpendicular to the coastline; earlier onset times
occurred for weaker offshore winds. The sea breeze layer was about 600 to 800 m deep on the
average, but ranged between 200 and more than 1000 m; this too may be related to the
strength of the gradient winds normal to the coast. River breezes from the Indian and Banana
Rivers were observed on most days, with onset times similar to those of the sea breeze. The
sea breeze circulation was found to be asymmetric, and this asymmetry increased with the
strength of the gradient wind normal to the coast.

On a local scale, typical of the launch facility itself, or of its components, one expects other
phenomena to influence dispersion, although these do not seem to have been documented.
For example, the large structures and paved areas of the launch complex should be thermally
adequate to produce a weak heat island effect (for an introduction to this phenomenon, see
Oke, 1982; Vukovich and King, 1980). These effects should be most pronounced at night under
light wind, clear sky conditions, and may be observable only as a perturbation of the land
breeze. If the synoptic winds are calm and no land breeze exists, a typical heat island
circulation (radially inward flow near the surface) could occur. The very large buildings at KSC
(e.g., the VAB) will generate proportionally large aerodynamic wakes, especially under strong
wind conditions, and these wakes will perturb the initial plume dimensions, path, and dispersion
rate for materials released within the wake influence zone. This zone may reach several
characteristic dimensions (e.g., the building width or height) downwind, which may be several
hundred feet or more for large buildings. These perturbations may be difficult to incorporate
realistically into an operational dispersion model because of the already complex flow patterns
at KSC, although the wake influences may be very significant in determining near-field (on-site)
concentrations. The literature provides guidance for wake dispersion modeling only in less
complicated incident flows (e.g., Hosker, 1984), with rather simple parameterizations (e.g., virtual
source treatments) that may sometimes be adequate to describe effects beyond the near-wake
region. Strong daytime convection due to solar heating in this sub-tropical area is expected to
obscure the picture further.

5.0 Dispersion Data Available for KSC

5.1 Introductory Comments

Dispersion measurements have been performed in coastal environments at a number of
locations in the U. S. over the last 40 years. Most of those data were collected along the
southern California coast, although limited measurements have been made along the Atlantic
and Gulf coasts. Summaries addressing dispersion and dispersion coefficients for coastal
regions were prepared in the early 1980s for use by the U. S. Nuclear Regulatory Commission (MacRae et al., 1983; Shearer and Kaleel, 1982; Kaleel et al., 1983).

Prior to the mid-1970s, the tracer materials used in these (and most other dispersion) tests were predominantly fluorescent particles (FP; e.g., zinc sulfide). Since 1974, gaseous tracers such as sulfur hexafluoride ($\text{SF}_6$) and various fluorocarbons have become popular for diffusion measurements. However, only FP tracers are known to have been utilized in studies of the KSC/Cape Canaveral area. The only dispersion measurements identified as being performed near KSC and Cape Canaveral are the Ocean Breeze (OB) measurements (Haugen and Taylor, 1963).

The Ocean Breeze dispersion experiments were part of a much larger set of studies performed in the late 1950s and early 1960s which included the Green Glow, Series 30, and Dry Gulch measurement programs, in a variety of settings. The Ocean Breeze and Dry Gulch (OB/DG) data are believed to be the most complete tracer data sets presently available to assess dispersion in a coastal environment. However, the tests were performed prior to the advent of the newer gaseous tracer technologies, and have some shortcomings as a result.

Perhaps the most important of these shortcomings is the uncertainty in the measured concentrations introduced by dry deposition of the FP on to vegetation between the source and the receptor point. There is disagreement in the literature regarding the quantitative significance of this phenomenon. Simpson (1961) found very high deposition of FP to desert vegetation, with 80% or more of the airborne mass being scavenged within 3.2 km of the ground level source, under very stable nocturnal conditions, whereas Leighton et al. (1965) suggested that only 10% or less of the material would be deposited under unstable daytime conditions during the first few miles of travel. Kamada et al. (1991) and Skupniewicz et al. (1992) have discussed the significance of deposition losses from the Mountain Iron zinc sulfide tracer releases near Vandenberg AFB in the 1960s; Kamada (1992, personal communication) suggests that regression equations based on zinc sulfide tracer studies may significantly underpredict dosages at ranges beyond a few kilometres. There is also a tendency of fluorescent particles to lose their fluorescent capability (and hence become non-detectable) after exposure to strong sunlight and high humidity (Leighton et al., 1965); the amount of degradation seemed to vary by manufacturer's lot. Corrections to the data for these effects are uncertain, and therefore limit the accuracy of empirical techniques (such as the OB/DG equation discussed in Section 8.3, below) based on those data. However, both effects are such that the tracer observations will increasingly underestimate the amount of airborne material far downwind; a model "tuned" to fit those data will therefore tend to underpredict airborne concentrations far from the source.

While the Ocean Breeze site-specific measurements are very relevant to the KSC setting, it is also important to briefly review the character and scope of the experiments. As with any program, there were certain points of focus and also limits of applicability. The primary objective of the OB/DG program was to obtain data to formulate a site-specific dispersion equation. The initial role of this equation was to provide a somewhat qualitative, somewhat quantitative estimate of basic atmospheric dispersion conditions at the Cape Canaveral test range, to assist range safety assessments for pending operations. Later applications followed, to extend the equation for use as a more quantitative method for predicting airborne concentrations.

The OB data were collected over the flat but heavily vegetated terrain of Cape Canaveral. All of the tests were conducted during daylight hours, mostly during the afternoon and early
evening. As a result, the bulk of the data were collected during convectively unstable atmospheric conditions, with on-shore winds of variable strengths. The OB tracer data set consisted of 76 separate diffusion measurement cases. Each tracer test used a continuous, 30 minute duration, ground level release of zinc sulfide fluorescent particles (FP) from an aerosol fog generator. The FP releases and sampling were performed within the 10 m layer of air immediately above ground level. The releases of FP were made near the shoreline. Samples were collected on the land at three concentric arcs about 1.2 km, 2.4 km, and 4.8 km from the release point.

A lateral spreading parameter, \( \sigma_y \), was derived from the near-surface samples of tracer distributions on each sampling arc. The apparent \( \sigma_z \) value was then calculated from the measured tracer concentrations, although the mass conservation and vertical distributions of FP were not measured. The above comments concerning the deposition of FP and its possible degradation in sunlight and high humidity are pertinent here.

5.2 OB/DG Tracer Dispersion Data Set Strengths/Weaknesses

The Ocean Breeze data were collected near KSC, and are clearly relevant to dispersion at the KSC complex for atmospheric conditions similar to those sampled during the field measurements. It is important to recognize that, because not all possible meteorological situations were covered by the OB test periods, atmospheric conditions not explicitly included in the test group may be poorly described by OB dispersion results.

Strengths

- Near-surface releases of small particulate effluents may be represented by the observations of the FP tracer behavior.
- The OB tracer data were collected under on-shore flow situations, which are a common occurrence at KSC.
- The OB/DG equation was developed from one-half of the OB/DG data set. The resulting statistical (empirical) equation was tested against the balance of the data with quite good results.
- The OB/DG equation does quite well for those situations which fall within the range of atmospheric conditions covered by the measurement program.

Weaknesses

- Dispersion was measured only for near-surface releases; elevated releases may behave differently, especially at night.
- Deposition and other non-conservative processes were not measured along with the tracer concentrations.
- FP tracer cases relate to mostly steady-state atmospheric conditions, for short travel times and distances.
FP releases were 30 minutes in duration, somewhere between a short puff and a continuous plume; this complicates the analysis, because puff and plume diffusion theories are different.

Vertical diffusion was calculated from the ground level FP "footprint", without aid of measurements of FP deposition, or of vertical FP mass distributions.

The influences of convection and sea breeze convergence on vertical plume displacements and recirculations were not determined.

Dense gas plumes or vapors from liquid spills with temperatures and densities far different from ambient atmospheric density and temperature will disperse differently than the FP used for the OB data set.

The portion of the data set used for checking the statistical predictive equation was not truly independent of the data set used to develop the equation. Some correlations between the two data sets are expected.

In summary, the FP-developed descriptions of dispersion at KSC are useful, but lack generality and completeness. Important aspects of atmospheric transport and rates of diffusion were not covered by the OB program. Diffusion at and immediately downwind of the land/water and water/land interfaces and diffusion at short distances from sources have not been addressed. Diffusion in the lee of large structures has also not been addressed, but other dispersion programs may provide some limited guidance on this issue.

6.0 REGIONAL MODELING CAPABILITIES AT KSC

6.1 Introductory Comments

Transport and dispersion of effluents on local scales are influenced by larger scale wind patterns. At KSC, for example, the complex flows described in Section 4 strongly affect the overall trajectory of a release. The ability to model transport and dispersion is thus at least partially dependent on the ability to predict these regional scale flow fields. A 1981 Department of Energy Model Validation Workshop at Savannah River Lab concluded that significant improvement in the accuracy of air quality model forecasts can be obtained by using more realistic wind field analysis. The following discussion reviews both past and current mesoscale numerical weather prediction (NWP) modeling efforts in Florida. The applicability of these models for driving air quality models over the KSC region will also be evaluated.

6.2 Previous Florida Modeling Studies

Numerical modeling of the Florida region was first begun in the 1970s. These models predicted mesoscale circulations on the order of 50 km or greater. The model grid spacing was usually about 10 km, with a total domain size of 400 km by 400 km; a dry hydrostatic model was generally used. About the same time, work also began on simulating individual cloud scale patterns using non-hydrostatic models with explicit prognostic equations for cloud water and ice. Horizontal grid spacings for these latter models were about 1 km, with a domain size of about 50 km by 50 km. Both types of modeling studies focused mainly on predicting the mesoscale sea breeze pattern and its forcing of cloud scale processes during synoptically
undisturbed days. While much of this early work did not focus on air quality, its relevance to pollutant transport and dispersion is significant because the accurate prediction of meteorological processes is crucial. Coupling of the separate mesoscale and cloud models into a single two-way interactive model could not be accomplished until recently, with the advent of more powerful supercomputers.

One of the first modeling simulations of Florida-area mesoscale weather patterns was conducted by Pielke (1974). He utilized a dry hydrostatic mesoscale model to study Florida sea breeze circulations using an 11 km grid spacing over a 330 km by 360 km domain. Cotton et al. (1976) later used a three-dimensional dry mesoscale sea breeze model to obtain sea breeze-perturbed soundings, which were then used to initialize a one-dimensional cloud model. Pielke and Mahrer (1978) incorporated a surface energy budget and a radiation parameterization into the original Pielke model. Their results indicated that the surface characteristics could modify the position and timing of the predicted sea breeze circulation and convection. Gannon (1978) and McCumber and Pielke (1981) modified Pielke's model to include the effects of soil and vegetation coverage, and the variation of incoming solar radiation due to clouds. They found all these factors to be important in determining the location and intensity of the sea breeze circulations. Work by McQueen and Pielke (1985) and Michaels et al. (1987) using Pielke's model with soil and vegetation parameterizations verified the importance of surface characteristics on the regional flow fields.

Using a sophisticated three-dimensional cloud model, Tripoli and Cotton (1980) ran experiments to explore some of the factors which account for deep convective cloud development over Florida. Cooper et al. (1982) and Cunning et al. (1982) simulated thunderstorm cloud activity using the three-dimensional cloud modeling approach. They found that while cloud initiation was caused primarily by mesoscale forcings, later development was controlled mainly by cloudscale (1 to 10 km) processes. These studies implied that a linking of the two scales was necessary to adequately predict meteorological patterns over Florida.

6.3 Recent Regional Models Applied to KSC

Recent attempts to model the Florida area regional weather have therefore tried to predict both mesoscale and cloud-scale circulations. The latest modeling activities have also stressed prediction of local circulations such as river and island breezes, and modifications to circulations due to land use patterns.

Lyons et al. (1986, 1987, 1988, 1992a) used Pielke's hydrostatic mesoscale model with 7.5 km grid spacing coupled with a diagnostic cloud scheme to forecast sea breeze-induced thunderstorms at Cape Kennedy for synoptically undisturbed events. This simplified approach was the first attempt to run a mesoscale model in real time at KSC. Forecasts using this technique were fairly successful in predicting thunderstorm occurrence at KSC; however, the results could only be used on synoptically undisturbed days. Lyons et al. (1992a) found that this typically occurs on only 20% to 30% of days at KSC. This approach also could not predict some significant small scale weather patterns such as the Merritt Island thunderstorm described by Nicholson et al. (1988), river breezes induced by the Banana and Indian Rivers (Taylor et al., 1989), and heat island convergence zones at Merritt Island and the Cape Canaveral land masses.

Lyons and Pielke (1990), Lyons et al. (1992b), Pielke et al. (1990), and Nicholls et al. (1991) have used the Regional Atmospheric Modeling System (RAMS) to simulate regional circulations
in Florida on a very fine scale. RAMS, developed at Colorado State University, couples a non-hydrostatic prognostic cloud model described by Tripoli and Cotton (1982) with two hydrostatic mesoscale models (Tremback et al., 1985; Mahrer and Pielke, 1977). The model employs a two-way nested-grid scheme to allow for feedbacks between the local scale circulations and the mesoscale and synoptic scale flows. Non-hydrostatic physics and the explicit cloud model equations allow the finest mesh resolution to be very high; grid spacing on the order of 1 km has been applied by the above authors for Florida area simulations. Currently RAMS is the only nested-grid non-hydrostatic model to be applied to the flow over KSC.

Results using RAMS to simulate pollutant transport over KSC reported by Lyons and Pielke (1990) have shown the ability of the model to resolve the unique fine scale flow fields in and around the Cape. Figure 6.1 shows predicted streamlines and stability indices for KSC for a hindcast simulation on 7 November, 1988. A full three-dimensional nested-grid structure was employed, with a 1 km inner mesh. The vertical cross-section shows three distinct circulations associated with the east coast sea breeze and the Merritt Island and Cape Canaveral heat island effects. The authors concluded that vertical transport would be significant, and that any resultant pollutant transport would be substantially different than would be predicted by a two-dimensional diagnostic wind field model driven by the MARRS surface-layer meteorological tower network. However, these simulations did not use the RAMS cloud model, and any effect on dispersion due to deep convection could not be assessed.

Nicholls et al. (1991) used the two-dimensional RAMS model with explicit cloud microphysics parameterizations turned on to simulate the interaction between the Florida sea breezes and the ensuing moist convection. They found that sea breeze-induced deep convection can generate very deep horizontally propagating gravity waves. These gravity waves can then alter the larger scale flow fields and initiate new convection.

Because current regional modeling work at KSC has been done mainly with the RAMS model, and because a version (A•RAMS) of the RAMS code is to be delivered soon to KSC for use on a computer workstation, the following section looks closely at the RAMS strengths and weaknesses as they may affect dispersion simulations at KSC.

6.4 RAMS Model Description

6.4.1 Grid structure

RAMS utilizes a grid stagger technique to reduce finite differencing error. Standard cartesian or stereographic grids can be specified. A two-way interactive multiple nested-grid scheme is provided, to allow scale interactions. The nested-grid approach allows a fine mesh to resolve local-scale circulations in the area of interest, and a coarser mesh elsewhere. This procedure can be computationally efficient. Grid sizes used for KSC have covered 1, 3, 9, and 12 km. Grid domains of the finest mesh have ranged from 50 km to 400 km in either direction, depending on the grid spacing. The model can be run in one, two, or three dimensions. Recent studies by Lyons et al. (1992a,b) have shown that 3 km grid resolution may be adequate to predict the flow fields properly at KSC.

The model vertical surfaces follow a terrain-following height coordinate system. Typically the vertical domain extends to 15 km AGL, but higher levels are included if deep convection is simulated. This coordinate system is much like the sigma surfaces used in other mesoscale models which are on terrain-following pressure-type surfaces.
Figure 6.1: (a) ARAMS-predicted surface wind streamlines at 1700 GMT, 7 November 1966. TIX is the Titusville Airport and X68 is the Shuttle landing strip; (b) ARAMS-predicted Pasquill-Gifford stability class based on the temperature lapse rates in the lowest 30 meters at 1700 GMT, 7 November 1966, 1 = A through 7 = G; (c) Streamlines of the u and w components of the ARAMS-generated winds at 1700 GMT in a 40 km wide east-west plane through TIX, surface to 3000 m AGL at 1700 GMT, 7 November 1966. (From Pielke et al., 1990.)
6.4.2 Initialization and data assimilation

The RAMS model can be initialized from spatially inhomogeneous meteorological observations. Therefore, simulations are not limited to synoptically undisturbed cases, as were earlier versions of the Pielke model. NOAA/ National Meteorological Center (NMC) model-gridded data and surface and rawinsonde sites are objectively analyzed to isentropic surfaces before being interpolated to the model grid. The objective analysis follows the widely used Barnes approach. Currently, the model is configured to use NMC model data on a 2.5° latitude-longitude horizontal grid and mandatory pressure levels.

Special surface or upper air data sets such as high temporal and spatial resolution data can also be ingested to enhance the initialized fields. Information on spatially-varying surface variables such as soil moisture, soil and vegetation types, surface temperature and water content, terrain height, land roughness, land percentage, and water surface temperature can be ingested. A simple data assimilation technique is available in RAMS to "nudge" the model simulation at sites where special data may exist, but the scheme has not been widely used.

6.4.3 RAMS model physics

The RAMS model contains a full set of non-hydrostatic compressible dynamic equations, a thermodynamic equation, and a set of cloud microphysics equations for water- and ice-phase clouds and precipitation. Numerous options exist for parameterizations representing the planetary boundary layer, cloud, and radiation effects. The discussion here concentrates on the most frequently used options, and those applicable to modeling at KSC.

The surface parameterization of vertical heat, water vapor, and momentum fluxes is computed as a function of ground surface temperature derived from a surface energy balance (Mahrer and Pielke, 1977). Soil temperature and moisture are predicted from a prognostic soil model (McCumber and Pielke, 1981) modified for RAMS by Tremback and Kessler (1985). RAMS currently treats 12 different soil types. The soil model usually extends 50 cm to 75 cm beneath the surface.

Smagorinsky-type vertical eddy viscosity mixing with Richardson-number dependence is normally used to mix variables in the boundary layer. This method utilizes a first-order closure vertical diffusion coefficient profile, and is valid for model grid spacings greater than 1 or 2 km. A second-order closure scheme in which turbulent kinetic energy is explicitly predicted is a RAMS option, but it is only realistic for large eddy simulations where the horizontal and vertical grid spacings are similar. The second-order closure scheme is based on Deardorff's (1980) work. The McNider stable boundary layer parameterizations can produce unrealistic mixing profiles, and are not recommended by the Colorado State University modeling group.

A longwave and shortwave radiation parameterization (Chen and Cotton, 1983) is used when clouds are included in a RAMS simulation. The longwave technique accounts for both clear and cloudy air absorption. In clear air, the effects of both water vapor and carbon dioxide absorption are predicted. Cloud effects on both short and longwave radiation are based on Stephens' (1978 a,b) empirical scheme. This scheme is computationally intensive, but when clouds are not present, the Mahrer and Pielke (1977) radiation parameterization can be used. The latter scheme does not include the effects of liquid water and ice.
RAMS includes both an explicit cloud microphysics scheme and a convective cloud parameterization. The most realistic (but computationally intensive) option includes the conversion and growth of aggregates, ice melting, evaporation, and sedimentation and a prognostic nucleation model. The cloud model is described in detail by Cotton et al. (1982, 1986). A cloud parameterization based on the Fritch-Chappell approach can be specified instead of the cloud microphysics codes, but this scheme is valid only on coarse grids of 20 km or greater. The explicit cloud microphysics model runs at resolutions of about 2 km or less. RAMS currently has no satisfactory scheme to simulate cloud effects for model grid spacings between 2 km and 20 km.

6.4.4 Numerics

RAMS is normally used with the non-hydrostatic time-split compressible primitive equations in one, two, or three dimensions. Non-hydrostatic physics allows for the high resolution grid spacings needed to simulate deep convection or flow over complex terrain. The complex differencing scheme is described in detail by Tremback et al. (1987). Lateral boundary conditions can be treated in several ways; the only upper boundary condition that seems to work well with the non-hydrostatic option is a simple rigid lid approach.

6.4.5 Operational capabilities

RAMS has not been used operationally for real-time air quality dispersion forecasts. Lyons et al. (1992a) summarized work in forecasting thunderstorm potential over Cape Canaveral using the Pielke model, a RAMS predecessor. However, their simulations used the dry hydrostatic model, and were therefore not applicable when synoptic disturbances were nearby or when moist convection was present. To our knowledge, no other regional model has been applied at the Cape to forecast mesoscale circulations in real-time.

6.5 RAMS Model Strengths/Weaknesses and Recommendations

Strengths

RAMS has been applied successfully at KSC in a hindcast mode and this is one of its greatest strengths. Other strengths include:

- The ability to predict three-dimensional wind fields over a high resolution domain, to simulate horizontal and vertical transport. The model can predict the state of the atmosphere at offshore locations where meteorological towers are not available.
- Non-hydrostatic physics allow realistic prediction of the atmosphere over a limited domain at very high spatial resolution. This capability is essential for modeling at KSC, where very high resolution grids are needed to predict the local scale flow fields.
- The effects of vegetation and soil variations on atmospheric flows are parameterized realistically. These effects have been shown to be significant in the Florida area.
- A two-way nested-grid capability provides for scale interactions and savings in computational time and memory.
- Various levels of cloud parameterizations have been tested.
- Realistic horizontally-inhomogeneous atmospheric initial conditions permit simulations during synoptically disturbed periods.

Weaknesses

- RAMS has not been used operationally for real-time air quality simulations. The code is very computationally-intensive, and simplifications to some parameterizations should be found. Communications with personnel at Westinghouse/Savannah River Laboratory, who have used RAMS extensively, indicated that simulations can be sped up by a factor of 5 on a Cray Y-MP by using sophisticated computer techniques and code restructuring.

- Before RAMS can be used operationally, a technique to parameterize cloud water effects for grid spacings of 3 to 20 km must be found. The explicit cloud microphysics scheme, while very sophisticated, is too computationally-intensive, and is not appropriate for the operational grid spacings necessary at KSC.

- Operational simulations should be performed with realistic, nonhomogeneous initial conditions and with moist convection.

- No acceptable method of data assimilation during a RAMS simulation has been described in the literature. A nudging scheme is available in RAMS that could use KSC special meteorological data, but it has not been widely tested.

- Techniques to specify the spatial variation of soil and vegetation types should be explored. Satellite-derived vegetation parameters and soil moisture patterns have been determined by Chang and Wetzel (1991) and others; perhaps some of these techniques could be used for KSC. Simulations using high resolution surface parameters should be performed to evaluate the importance of these fields on the local scale flow at KSC.

- NMC model data are on a 2.5° grid. The NOAA/ARL NMC archived model data are at higher horizontal and vertical resolutions than are available through NCAR. This data set should be tried for more realistic model initializations. NOAA/ARL is currently using these data for operational forecasts using RAMS over the mid-Atlantic coastal region.

- The RAMS group has not published model simulations with a second-order turbulence scheme for boundary layer mixing on scales of 1 km or greater. Such schemes have been used successfully by other modeling institutions and have been shown to be important for realistic dispersion modeling simulations.

6.6 Other Regional Models Used for Air Quality

Only RAMS and the hydrostatic Pielke model have been used for regional modeling simulations at KSC. However, other models for air quality simulations are available. Tables 6.1 and 6.2, from Pielke et al. (1990), list other major mesoscale models and their capabilities. The RAMS and the NCAR/PSU model are the only models which have the necessary physical (cloud effects, high resolution boundary layer physics, nonhomogeneous initial conditions) and numerical (two-way nested-grids, small grid spacings) codes. The Los Alamos (Yamada) model suffers from an inability to realistically incorporate surface synoptic data; also, working non-hydrostatic physics are not yet available. The MASS model has not yet linked cloud and regional submodels, and the Drexel and ERT models do not support the high resolution grid.
Table 6.1 Comparison of mesoscale meteorological model capabilities (from Pielke et al., 1990).

<table>
<thead>
<tr>
<th></th>
<th>San Jose Model</th>
<th>MASS Model</th>
<th>NCAR/PSU/SUNY Model¹</th>
<th>Drexel Model</th>
<th>CSU RAMS Model</th>
<th>ERT CMC/PBL Model Combination</th>
<th>Los Alamos Model</th>
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</thead>
<tbody>
<tr>
<td>Governing Equations</td>
<td>1) vorticity framework</td>
<td>1) primitive equation framework</td>
<td>1) primitive equation framework</td>
<td>1) primitive equation framework</td>
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<td></td>
<td>2) hydrostatic</td>
<td>2) hydrostatic or nonhydrostatic</td>
<td>2) hydrostatic</td>
<td>2) hydrostatic</td>
<td>2) hydrostatic</td>
<td>2) hydrostatic</td>
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<td></td>
<td>3) incompressible</td>
<td>3) anelastic</td>
<td>3) anelastic</td>
<td>3) anelastic</td>
<td>3) anelastic</td>
<td>3) anelastic</td>
<td>3) incompressible</td>
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<tr>
<td>Grid</td>
<td>staggered</td>
<td>Arakawa-A staggered</td>
<td>staggered</td>
<td>non-staggered</td>
<td>Arakawa-C staggered grid</td>
<td>staggered</td>
<td>staggered</td>
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<td>Horizontal Grid Spacing</td>
<td>1) minimum 1.6 km</td>
<td>1) minimum 7 km</td>
<td>1) 80 km</td>
<td>1) minimum ~25 km</td>
<td>1) minimum ~100 m</td>
<td>1) 127 km</td>
<td>1) minimum 380 m</td>
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<td>Vertical Grid Spacing</td>
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<tr>
<td>Model Domain</td>
<td>1) several hundred kilometers on a side</td>
<td>1) arbitrary</td>
<td>1) arbitrary</td>
<td>1) arbitrary</td>
<td>1) northern hemisphere/eastern North America</td>
<td>1) arbitrary</td>
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<tr>
<td></td>
<td>2) one-way interactive grid</td>
<td>2) two-way interactive nested version</td>
<td>2) two-way interactive</td>
<td>2) two-way interactive</td>
<td>2) one-way interactive grid</td>
<td>2) one-way interactive grid</td>
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<td>Initialization</td>
<td>1) dynamic initialization</td>
<td>1) dynamic initialization</td>
<td>1) objective analysis scheme using synoptic² analyses including satellite data removal of integrated mass divergence and 2) multivariate variational adjustment scheme planned for December 1989</td>
<td>1) objective analyses of synoptic³ data</td>
<td>1) objective analysis scheme of synoptic³ data</td>
<td>1) normal mode initial analysis of synoptic³ data/dynamic initialization with nudging towards CMC fields in PBL</td>
<td>1) objective analysis of synoptic³ data/requirement for wind field to satisfy mass conservation</td>
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<td>spectral (CMC)/finite element (PBL)</td>
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<td>sponge from synoptic data</td>
<td>from synoptic data</td>
<td>from synoptic data</td>
<td>from synoptic data</td>
<td>from synoptic data</td>
<td>from synoptic data and solution of 1-D primitive equations</td>
</tr>
<tr>
<td>Top Boundary Conditions</td>
<td>from synoptic specifications; up to present, model top confined to below mid-troposphere</td>
<td>absorbing layer</td>
<td>specified from CMC analyses; PBL model top at 2 km</td>
<td>absorbing layer</td>
<td>absorbing layer</td>
<td>specified from CMC analyses; PBL model top at 2 km</td>
<td>zero vertical gradient</td>
</tr>
<tr>
<td>Surface Boundary Conditions</td>
<td>1) heat energy and moisture surface budgets</td>
<td>1) heat energy and moisture surface budgets</td>
<td>1) heat energy budget</td>
<td>1) heat energy budget</td>
<td>1) heat energy budget</td>
<td>1) heat energy budget</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2) specified from satellite</td>
<td>2) representation of vegetation effects</td>
<td>2) representation of vegetation effects</td>
<td>2) representation of vegetation effects</td>
<td>2) representation of vegetation effects</td>
<td>2) representation of vegetation effects</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3) representation of vegetation effects</td>
<td>3) specified from satellite</td>
<td>3) specified from satellite</td>
<td>3) specified from satellite</td>
<td>3) specified from satellite</td>
<td>3) specified from satellite</td>
<td></td>
</tr>
</tbody>
</table>

¹ Note: CMC/PBL model top specified from satellite and in northern hemisphere/eastern North America for December 1989.

² Synoptic analyses from National Oceanic and Atmospheric Administration (NOAA) data.

³ Synoptic analyses from National Environmental Satellite, Data, and Information Service (NESDIS) data.
Table 6.1 Comparison of mesoscale meteorological model capabilities (from Pleike et al., 1990).

<table>
<thead>
<tr>
<th>Parameterization of Subgrid Mixing</th>
<th>San Jose Model</th>
<th>MASS Model</th>
<th>NCAR/PSU/SUNY Model</th>
<th>Drexel Model</th>
<th>CSU RAMS Model</th>
<th>ERT CMC/PBL Model Combination</th>
<th>Los Alamos Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Subgrid Mixing</td>
<td>1st and 2nd order closure</td>
<td>1st order closure</td>
<td>1st order closure</td>
<td>1st order closure</td>
<td>1st order closure</td>
<td>1st or 2nd order closure</td>
<td>2nd order closure</td>
</tr>
<tr>
<td>radiation at the surface</td>
<td>none</td>
<td>1-D cloud models</td>
<td>1-D cloud models</td>
<td>1-D cloud models</td>
<td>1-D cloud models</td>
<td>1-D cloud models</td>
<td>1-D cloud models</td>
</tr>
<tr>
<td>1) solar and longwave radiation</td>
<td>1) solar heating of surface; longwave radiation for longer than 24 hour runs (December 1989)</td>
<td>1) solar and longwave radiation at the surface</td>
<td>1) solar and longwave radiation at the surface</td>
<td>1) solar and longwave radiation at the surface</td>
<td>1) solar and longwave radiation at the surface</td>
<td>1) solar and longwave radiation at the surface</td>
<td>1) solar and longwave radiation at the surface</td>
</tr>
<tr>
<td>divergence in the atmosphere</td>
<td>2) solar and longwave radiation divergence in the atmosphere</td>
<td>2) longwave radiative flux divergence in the atmosphere</td>
<td>2) longwave radiation flux divergence in the atmosphere</td>
<td>2) longwave radiation flux divergence in the atmosphere</td>
<td>2) longwave radiation flux divergence in the atmosphere</td>
<td>2) longwave radiation flux divergence in the atmosphere</td>
<td></td>
</tr>
<tr>
<td>Stable Precipitation Algorithm</td>
<td>none</td>
<td>1) rainout for relative humidity greater than 100%</td>
<td>1) rainout for relative humidity greater than 100%</td>
<td>1) includes equations for cloud liquid water and rainwater - 1st order parameterization</td>
<td>1) includes equations for cloud ice, cloud liquid water, snow, and rain - 1st and 2nd order parameterizations</td>
<td>1) gradual rainout based on a depression threshold dependent upon large scale environment</td>
<td>none</td>
</tr>
<tr>
<td>2) ice microphysics representation in cirrus anvils clouds</td>
<td>2) includes equations for cloud liquid water and rainwater - 1st order parameterization</td>
<td>2) includes equations for cloud liquid water and rainwater - 1st order parameterization</td>
<td>2) includes equations for cloud liquid water and rainwater - 1st order parameterization</td>
<td>2) includes equations for cloud liquid water and rainwater - 1st order parameterization</td>
<td>2) includes equations for cloud liquid water and rainwater - 1st order parameterization</td>
<td>2) includes equations for cloud liquid water and rainwater - 1st order parameterization</td>
<td>2) includes equations for cloud liquid water and rainwater - 1st order parameterization</td>
</tr>
<tr>
<td>Algorithms to Link to Other Models</td>
<td>1) plume models</td>
<td>1) trajectory model</td>
<td>1) Eulerian chemical model (RADM)</td>
<td>1) trajectory model</td>
<td>1) advection diffusion (Eulerian dispersion) model</td>
<td>1) Eulerian chemistry model (ADOM)</td>
<td>1) Lagrangian particle dispersion model</td>
</tr>
<tr>
<td>2) Eulerian chemical models</td>
<td>2) 3-D nonhydrostatic cloud scale model</td>
<td>2) trajectory model</td>
<td>2) 3-D nonhydrostatic cloud scale model</td>
<td>2) trajectory model</td>
<td>2) SAI chemistry model</td>
<td>2) SAI chemistry model</td>
<td>2) SAI chemistry model</td>
</tr>
<tr>
<td>3) Eulerian dispersion models</td>
<td>3) cloud models</td>
<td>3) cloud models</td>
<td>3) cloud models</td>
<td>3) cloud models</td>
<td>3) Lagrangian dispersion model</td>
<td>3) Lagrangian dispersion model</td>
<td>3) Lagrangian dispersion model</td>
</tr>
<tr>
<td>Phenomena Studied of Relevance to Complex Terrain</td>
<td>1) extratropical cyclones</td>
<td>1) extratropical cyclones</td>
<td>1) frontal zones</td>
<td>1) orographic precipitation</td>
<td>1) acid deposition</td>
<td>1) diurnal variation of planetary boundary layer</td>
<td>1) extratropical cyclones</td>
</tr>
<tr>
<td>2) frontal system</td>
<td>2) sea-land breezes</td>
<td>2) sea-land breezes</td>
<td>2) mesoscale convective circulations</td>
<td>2) topographically-induced gravity waves</td>
<td>2) oxidant formation</td>
<td>2) sea-land breezes</td>
<td>2) frontal system</td>
</tr>
<tr>
<td>3) mesoscale convective circulations</td>
<td>3) forced airflow over rough terrain</td>
<td>3) mesoscale convective circulations</td>
<td>3) cyclogenesis</td>
<td>3) turbulence structure in the boundary layer</td>
<td>3) sea-land breezes</td>
<td>3) nocturnal drainage flow</td>
<td>3) mesoscale convective circulations</td>
</tr>
<tr>
<td>4) sea breezes</td>
<td>4) frontal circulations</td>
<td>4) extratropical squall lines</td>
<td>4) transport and diffusion of pollutants</td>
<td>4) formation of plumes over a cooling pond</td>
<td>4) mountain-valley flows</td>
<td>4) formation of plumes over a cooling pond</td>
<td>4) extratropical squall lines</td>
</tr>
<tr>
<td>5) plume transport and acid rain deposition</td>
<td>5) heavy precipitation events</td>
<td>5) transport and diffusion of pollutants</td>
<td>5) sea-land breezes</td>
<td>5) turbulence in cloud in marine boundary layer</td>
<td>5) long-range transport</td>
<td>5) turbulence in cloud in marine boundary layer</td>
<td>5) plume transport and acid rain deposition</td>
</tr>
<tr>
<td>6) squall line</td>
<td>6) mountain-valley flows</td>
<td>6) mountain-valley flows</td>
<td>6) mountain-valley flows</td>
<td>6) mountain-valley flows</td>
<td>6) mountain-valley flows</td>
<td>6) mountain-valley flows</td>
<td>6) squall line</td>
</tr>
</tbody>
</table>

*Italicized information corresponds to NCAR/PSU version of the code.

Only upper air synoptic data is used.
<table>
<thead>
<tr>
<th>Model</th>
<th>San Jose Model</th>
<th>MASS Model</th>
<th>NCAR/PSU/SUNY Model*</th>
<th>Drexel Model</th>
<th>CSU RAMS Model</th>
<th>ERT CMC/PBL Model Combination</th>
<th>Los Alamos Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>1) Able to explicitly represent clouds and fog (i.e., to prognose or diagnose cloud water or cloud ice)</td>
<td>no</td>
<td>no</td>
<td>no</td>
<td>yes (water clouds)</td>
<td>yes</td>
<td>no</td>
<td>yes, using a statistical procedure for nonprecipitating cumulus water clouds</td>
</tr>
<tr>
<td>2) Appropriate tool which could be used to estimate transport over complex terrain</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
<td>no</td>
<td>yes</td>
</tr>
<tr>
<td>3) Able to represent boundary-layer processes in complex terrain and coastal environments</td>
<td>no (no terrain in model)</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
<td>no</td>
<td>yes</td>
</tr>
<tr>
<td>4) Nested grid versions</td>
<td>no</td>
<td>yes</td>
<td>yes</td>
<td>no</td>
<td>yes</td>
<td>no</td>
<td>yes</td>
</tr>
<tr>
<td>5) Satisfactory numerical solution algorithms as based on prior performance</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
</tr>
<tr>
<td>6) Needed data for initialization</td>
<td>1) synoptic</td>
<td>1) synoptic upper air</td>
<td>1) synoptic upper air</td>
<td>1) synoptic upper air</td>
<td>1) synoptic upper air</td>
<td>1) synoptic upper air</td>
<td>1) synoptic upper air</td>
</tr>
<tr>
<td>7) Needed data for mesoscale validation</td>
<td>mesoscale resolution wind, turbulence, and air temperature data; at minimum of 20 equispaced surface stations and sounding data</td>
<td>mesoscale resolution wind, turbulence, and temperature data; at minimum of 20 equispaced surface stations and sounding data</td>
<td>mesoscale resolution wind, turbulence, and temperature data; at minimum of 20 equispaced surface stations and sounding data</td>
<td>mesoscale resolution wind, turbulence, and temperature data; at minimum of 20 equispaced surface stations and sounding data</td>
<td>mesoscale resolution wind, turbulence, and temperature data; at minimum of 20 equispaced surface stations and sounding data</td>
<td>mesoscale resolution wind, turbulence, and temperature data; at minimum of 20 equispaced surface stations and sounding data</td>
<td></td>
</tr>
<tr>
<td>8) Summary of ease of application to complex terrain (i.e., need for major model development)</td>
<td>major development work needed</td>
<td>relatively minor development work needed</td>
<td>major development work needed in SUNY version; relatively minor development work needed for NCAR/PSU research version</td>
<td>major development work needed</td>
<td>relatively minor development work needed</td>
<td>very major development work needed</td>
<td>relatively minor amount of development work needed (for nesting algorithm)</td>
</tr>
</tbody>
</table>

*Italicized information corresponds to NCAR/PSU version of the code*
spacings needed for KSC. The San Jose model does not parameterize cumulus or condensation processes.

7.0 METEOROLOGICAL DATA COLLECTION CAPABILITIES AT KSC

7.1 Introductory Comments

Previous discussions of meteorological data acquisition capabilities at KSC have emphasized flight safety issues, especially wind shear (related to aerodynamic loading of the flight vehicle) and triggered lightning episodes (see Panel on Meteorological Support for Space Operations, 1988; NASA Space Shuttle Weather Forecasting Advisory Panel, 1986; Zamora, 1992). There seems to have been relatively little discussion of data collection directly relevant to transport and dispersion of effluents released as a consequence of ground activity or flight operations at KSC, except for Myers' (1963) description of the original WIND system developed under the Ocean Breeze/Dry Gulch program.

7.2 Near-Surface Observations

An automated meteorological data collections system (WINDS, or Weather Information Network Display System) is in use at KSC. Data are updated every five minutes (although the standard deviation of wind direction, $\sigma_d$, is evaluated using 15-sec smoothing of the direction data followed by a "moving window" 30-minute average), and are stored on the Cyber computer system, where they are available for use by the MAASS system (discussed in Section 8.1, below).

The original network contained 28 towers instrumented at 6 ft and 54 ft (about 1.8 m and 16.4 m) above ground level, two 204 ft (62 m) towers, and one 492 ft (150 m) tower. These towers are deployed mainly between the northern and southern KSC site boundaries on Merritt Island. An additional 19 "Mesonet" towers have been added, mostly on the mainland. The original instruments and data loggers are presently being replaced with state-of-the-art equipment. Variables monitored include wind speed and direction, air temperature, and dewpoint. Figure 7.1 illustrates the tower network. Wind observations off the coast are not available.

The MAASS system (discussed below) performs a number of automatic quality control checks on the incoming data stream. The simplest are "out-of-range" checks, which ensure that the 5-minute averages of wind speed and direction, air temperature, and dew point are all within specified plausible ranges of possible values for the particular variable. Statistical tests are performed as well, to determine if any values fall outside the 99% confidence interval calculated for the particular sample. Suspicious data are flagged and removed from the data normally used for meteorological calculations.

The MAASS system uses the Barnes objective analysis method (Barnes, 1964, 1973; Caracena et al., 1984; Caracena, 1987) to create a regularly spaced gridded wind field from the irregularly spaced tower data by horizontal interpolation. The method includes a smoothing technique that allows retention of significant irregularities in the observed winds. An empirically adjusted weighting coefficient has been determined for KSC. Probably the principal shortcoming of the method is that, as presently implemented, it deals only with near-surface data, so the wind field is two-dimensional. In the meteorologically complex region of KSC, this is a severe limitation. It should be noted that alternatives to the Barnes method now exist; for example, kriging
Figure 7.1  Map of meteorological tower network in the KSC/CCAFS area. The symbol ▲ indicates the original wind towers; ▼ indicates the newer "Mesonet" towers; and ◊ indicates electric field mill sites.
techniques look promising (see Goodin et al., 1979, 1980; and the review by Eckman and Dobosy, 1989).

A 30-station network of electric field mills (the Launch Pad Lightning Warning System, or LPLWS) has been installed at KSC to detect electrified clouds. A Lightning Location and Protection (LLP) system detects and locates cloud-to-ground strikes within roughly 200 km of KSC.

Real-time data on water surface temperatures (very important for sea or river breeze prediction) are sparse, especially off the Atlantic coast. Satellite sea surface temperature observations have rather coarse resolution, and have only recently become available in real-time. The NOAA/NOS Coast Watch program has initiated dial-up service for 1 km and 4.4 km resolution sea surface temperatures acquired from the NOAA Polar Orbiter AVHRR satellite, for the Florida coast.

The National Weather Service operates basic and synoptic observing stations along the main Florida peninsula at Jacksonville, Daytona Beach, Orlando, and West Palm Beach. FAA surface stations (FSS) at Jacksonville, Gainesville, St. Petersburg, Melbourne, Vero Beach, Fort Meyers, and Miami supplement this network.

7.3 Data Aloft

A standard rawinsonde is launched daily at Cape Canaveral Air Force Station (CCAFS) at 0615 hrs EST, providing wind speed and direction, temperature, and humidity data at height intervals of about 1000 ft (roughly 300 m). For special events (e.g., launches), high-resolution (200 ft, about 60 m, or smaller height intervals) rawinsonde data can be obtained by special arrangement. Similarly, windsonde and "Jimsphere" wind data can be acquired at 100 ft (30 m) or larger height intervals at CCAFS by special arrangement only. A Tethersonde (tethered balloon) system is available, but is not used routinely. In Florida, the NWS launches rawinsondes on the worldwide standard morning and evening schedule from Apalachicola, Tampa Bay, West Palm Beach, and Key West.

The NOAA team was advised during a November 15, 1991 meeting that three Doppler sodar systems have been procured for near-continuous wind measurements at KSC up to about 1 km AGL (depending on local atmospheric conditions); however, these units had not been installed at the time of the briefing. A Doppler radar wind profiler is also planned for installation; the system will provide wind speed and direction data and vertical velocities at heights between roughly 1.5 km and 18 km. Zamora (1992) has recently recommended a network of six such systems to resolve weather moving through the Cape Canaveral area. It is not known whether RASS temperature data will also be provided with this equipment; the cost for this additional capability is generally modest, and should be seriously considered.

Weather radar is in use at Patrick AFB and at Daytona Beach; it is used primarily to monitor the development of thunderstorms and precipitation. A NEXRAD Doppler radar system is presently operational at the NWS station at Melbourne, FL, just south of the Cape area; this system has greatly improved ability to resolve vertical and horizontal variability in the wind. Additional systems will be installed by the NWS over the next few years.
8.0 DISPERSION MODELS IN PRESENT USE AT KSC

8.1 The MARSS System

The Meteorological and Range Safety Support (MARSS) system used at KSC is documented in several places (Bobowicz, 1985; ENSCO, 1988; Lane and Evans, 1988; Taylor and Schumann, 1986; Wiley et al., 1988). Only a brief summary, based largely on those references, will be provided here. The system is intended to provide the user or users with color graphics displays of meteorological and safety-related data, model predictions of concentrations and toxic corridors resulting from releases of various effluents, and results from the Rocket Exhaust Effluent Diffusion Model (REEDM). The information is provided as overlays on a high-resolution digitized background map of the KSC/CCAFS and surrounding area.

MARSS version 3.1 (Sonnier et al., 1990) is a stand-alone system implemented on three identical DEC MicroVAX II microcomputers, each driving multiple (up to eight) Tektronix model 4111 or 4211 color graphics terminals through a terminal server. This provides redundancy in the system in case of hardware problems. All calculations, display generation, and user interactions take place on the MicroVAXes. Meteorological data from the Weather Information Network Display System (WINDS), effluent dispersion information from REEDM, and BLAST damage assessment model outputs are obtained as ASCII files from the Cyber 860 mainframe by the MicroVAXes using a communication link. MARSS is otherwise independent of the mainframe computer. A mouse-driven user interface allows the selection of menu items or icons from the screen. Fast graphics are provided by the Tektronix PLOT 10 software package. Four main processes are available: meteorology, diffusion, safety map, and auxiliary displays. The meteorology process provides access to the tower network data, and the diffusion process provides the paths and toxic corridors predicted by the dispersion models OB/DG and/or LOMPUFF. The safety map process allows the user to construct customized map overlays of safety-related information. The auxiliary displays process provides access to other data such as the REEDM-generated isopleths of effluent concentrations. Help displays are associated with each of the processes. A zoom function allows the user to magnify a particular portion of the map, or to look at a larger area than is being displayed. Overlays such as concentric range rings around dispersion source locations and crash grids or USGS grids are available.

The major functions available on MARSS version 3.1 are graphic weather data displays (wind vectors in "wind barb" form, wind field, towers display, flow divergence contours, and area divergence time series); tabular weather data displays; weather data update and display every five minutes; historical weather data archiving, retrieval, and redisplay; concurrent runs of up to 12 OB/DG and one LOMPUFF scenarios; graphic overlay preparation; REEDM concentration isopleth display; and help (both tutorial and context-sensitive).

8.2 The Source Terms

Dispersion models are often described and discussed in general terms, using a so-called "normalized" or relative concentration, wherein the concentration in the plume or puff is divided by the emission rate (for a continuous source) or by the amount of material emitted (for an instantaneous source). For any application however, the actual concentration is needed as a function of space and time, so information about the emission rate or emitted quantity must be supplied in some way. In the discussion below, we will use the term "source strength" to mean either emission rate or emitted quantity, depending on the nature of the release.
It should be noted that accurate estimation of the source strength is often one of the most difficult parts of an assessment, especially under emergency conditions when the release characteristics are still poorly defined. Yet the predicted concentrations depend directly on the source strength; a factor of two error in source strength translates directly to a factor of two error in predicted concentration. Kunkel (1983) indicates that a 100% increase in source strength results in roughly a 50% increase in the length of a toxic corridor. It is clear that the method used to predict the source strength deserves considerable attention.

Accurate specification of the source strength is straightforward only for the cases of routine operational releases where a stack or vent operates at a known flow rate, discharging a known amount of material over a given time span, or when a known quantity of gaseous material is discharged completely into the atmosphere. Many releases are not very well-defined, however, especially under accident conditions. Often the release is in the form of a rupture of a container or conduit of some kind, and it is uncertain how much material is spilled, and what discharge rate applies; sometimes only the conservative assumption can be made that all the material was released. More uncertainties arise if the spilled material is liquid or solid, and undergoes a phase change, eventually moving off in gaseous form. As a result of these complications, an entire subclass of models has arisen, to help quantify the emission process. These models incorporate a wide range of complexity and assumptions about the physics and chemistry of the processes acting, and there is still disagreement in the literature as to which models do the best job of predicting the source strength for any particular type of release. Analogies to heat transfer and evaporation of water are often drawn. The situation is even worse if the effluent is very cold or dense when released, or reacts chemically with atmospheric constituents or other environmental materials during the release process, altering both the composition and the energy associated with the release.

8.2.1 OB/DG source term

The NOAA team believes that the OB/DG source term is rather poorly documented. The source term model apparently assumes that all liquid spills will form a puddle or pool, from which the effluent material will evaporate. The model assumes a fixed value for the evaporation rate (units of mass time\(^{-1}\) area\(^{-1}\) ) that depends only on the chemical species; the model does allow for a user-specified evaporation rate, but the NOAA team believes that most users are not capable of guessing a value for this, and will simply rely on the specified values. Then the model calculates the source strength using this evaporation rate and a user-specified or computed pool surface area (ENSCO, 1988; Sonnier et al., 1990). If the spill site is diked, the maximum pool size is limited to the diked area. If there is no dike, and no on-site estimate of the pool size, an estimate is made from the estimated total spill volume, assuming a 0.1 inch pool depth.

Table 8.1 shows the evaporation rates presently used in the MARSS system. The rates seem to be average values based on evaporation pan tests conducted during the 1960s (Henderson and Brown, 1970; McNerney et al., 1966; Matsak, 1963) and consolidated by Stewart (1972). Stewart (1972) plotted the average evaporation rate data for UDMH, N\(_2\)H\(_4\), N\(_2\)O\(_4\), and liquid O\(_2\) versus their respective boiling points, and found that a straight line fit the data fairly well. He apparently then used this same line and the known boiling points of other materials to estimate the evaporation rates of those materials. He observed that (for the limited number of compounds considered) the materials seemed to fall into five clusters along the line. For conservatism, he then assigned the highest evaporation rate within the group to all members of that group. It is unclear where the MARSS values for FREON-21 and NO\(_2\) were obtained; however, if the boiling point method of Stewart is applied, both compounds fall into Stewart's
Group II, as does \( \text{N}_2\text{O}_4 \). The evaporation rate values assigned in MARSS to FREON-21 and \( \text{NO}_2 \) are indeed the same as that for \( \text{N}_2\text{O}_4 \), suggesting that the Stewart approach has been followed.

**TABLE 8.1.** Evaporation rates assumed for various spilled materials in the MARSS system.

<table>
<thead>
<tr>
<th>MATERIAL</th>
<th>EVAPORATION RATE (LBS/MIN)/FT(^2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MMH (monomethylhydrazine)</td>
<td>0.02</td>
</tr>
<tr>
<td>( \text{N}_2\text{H}_4 ) (hydrazine)</td>
<td>0.02</td>
</tr>
<tr>
<td>( \text{N}_2\text{O}_4 ) (nitrogen tetroxide)</td>
<td>0.10</td>
</tr>
<tr>
<td>( \text{NH}_3 ) (ammonia)</td>
<td>0.13</td>
</tr>
<tr>
<td>FREON-21</td>
<td>0.10</td>
</tr>
<tr>
<td>HCl</td>
<td>---</td>
</tr>
<tr>
<td>( \text{UDMH} ) (unsymmetrical dimethylhydrazine)</td>
<td>0.02</td>
</tr>
<tr>
<td>A-50 (Aerozine-50, a 50-50 mix of UDMH and ( \text{N}_2\text{H}_4 ))</td>
<td>0.02</td>
</tr>
<tr>
<td>( \text{NO}_2 )</td>
<td>0.10</td>
</tr>
</tbody>
</table>

The above approach neglects several important features of the evaporation process that are clear in the detailed data from the original tests. The most important is that evaporation is not constant in time; for some materials (e.g., \( \text{N}_2\text{O}_4 \)) the evaporation rate peaks quickly, and then drops off; for others (e.g., liquid \( \text{O}_2 \)), the dropoff may or may not occur. A-50 is a peculiar material for which a kind of fractional distillation takes place (see Henderson and Brown, 1970); UDMH has a vapor pressure roughly an order of magnitude larger than that for hydrazine, and so the initial evaporation is mostly UDMH. As the percentage of hydrazine in the pool increases, its hygroscopic nature causes atmospheric water vapor to be absorbed increasingly rapidly, to the point that the overall evaporation rate becomes roughly constant.

The approach also neglects the sensitivity of evaporation to factors known to affect mass transfer, such as wind speed, turbulence level, ambient temperature, fluid temperature, and heat transfer from the surroundings. The use of evaporation pans (rather than evaporation directly from a spill on the ground) for the test series may also introduce uncertainties. The meteorological community regards the use of pans even for water evaporation studies with considerable caution; Brutsaert (1982) remarks that "although of uncertain and often dubious applicability as a measure of evaporation in nature, evaporation pans continue to be used..."
widely*. Future evaporation rate studies should attempt to evaluate spills more realistically, so as not to influence heat and mass transfer processes by the presence of the pan. Spills directly on to surfaces typical of KSC work regions are advised.

8.2.2 LOMPUFF source term

The LOMPUFF model uses a much more complex approach to formulating the source term, relying on the so-called SPILLS model (Fleischer, 1980), which was originated by the Shell Oil Development Company, and is rather well known in the air quality community. Among other capabilities, SPILLS uses the thermodynamic and physical properties of a chemical of concern to estimate the evaporation rate of a spilled liquid for both continuous and instantaneous releases. For LOMPUFF, only this capability was of interest. SPILLS considers three possible physical processes leading to a vapor source from a liquid release. Adiabatic flashing can occur when the released material is initially at high pressure and its boiling point is below the ambient temperature. Evaporation can occur due to heat transfer from the ground and air, causing the material’s vapor pressure to rise. And evaporative mass transfer occurs when the wind blows over a pool of liquid.

A continuous release of liquid generally is due to a modest break in a storage tank or a pipeline. The model assumes the liquid is discharged at a known release rate into a quiescent, ambient temperature pool on the ground, and that there is no heat transfer between the pool and its surroundings. Mass transfer is assumed to occur only because of the wind passing over the pool surface. The pool surface area and the evaporation rate must both be specified by the user or calculated. The pool area can sometimes be specified if the release occurs within a diked or otherwise confined area.

An instantaneously formed pool is generally due to a large break in a tank or pipe, so that the total available amount of liquid is dumped on the surface. The particular evaporation mode then depends on the nature of the spilled chemical. If the chemical’s boiling point is below the ambient temperature, we expect the material to flash off adiabatically at first, because of the abrupt decrease in pressure from the storage vessel to local atmospheric pressure. After this initial loss of material, the remaining pool is assumed to be at its boiling point; the resulting heat transfer from the surroundings to the fluid occurs by conduction (from ground surface) and convection (from air). Mass is transferred to the air passing over the pool. However, if the boiling point of the release is higher than the ambient temperature, then only convective mass transfer removes material from the pool.

The user must specify a good deal of information to use SPILLS (and hence LOMPUFF). Table 8.2 shows the properties of the material that must be given; as is typical for models of this type, these values are stored in the MARSS/LOMPUFF data base, so the user only needs to specify the material’s name. The user must also specify one of three possible sets of information: emission rate (taken to be the release rate) and the spill duration for a continuous spill; the spill amount for an instantaneous spill into an unconfined area; or the pool size and spill quantity for an instantaneous spill into an area with restricted runoff. The code then estimates a source strength for the release.
Table 8.2. Chemical data required for LOMPUFF.

<table>
<thead>
<tr>
<th>NAME</th>
<th>UNITS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular weight</td>
<td>g/mole</td>
</tr>
<tr>
<td>Specific heat at constant volume for gas phase at ambient temperature</td>
<td>J/g/°K</td>
</tr>
<tr>
<td>Specific heat at constant pressure for gas phase at ambient temperature</td>
<td>J/g/°K</td>
</tr>
<tr>
<td>Heat of vaporization at normal boiling point</td>
<td>cal/g-mole</td>
</tr>
<tr>
<td>Energy of molecular interaction</td>
<td>J</td>
</tr>
<tr>
<td>Effective diameter of molecule</td>
<td>Å</td>
</tr>
<tr>
<td>Critical temperature</td>
<td>°K</td>
</tr>
<tr>
<td>Critical pressure</td>
<td>atmospheres</td>
</tr>
<tr>
<td>Critical volume</td>
<td>cm³/g-mole</td>
</tr>
<tr>
<td>Normal boiling point</td>
<td>°K</td>
</tr>
<tr>
<td>Surface tension of liquid phase at normal boiling point</td>
<td>N/m</td>
</tr>
<tr>
<td>Viscosity of liquid phase at normal boiling point</td>
<td>kg/m/s</td>
</tr>
<tr>
<td>Liquid phase enthalpy with temperature dependence a, b, and c</td>
<td>cal/mole</td>
</tr>
<tr>
<td>Saturated liquid molar volume with temperature dependence a, and b</td>
<td>cm³</td>
</tr>
<tr>
<td>Vapor pressure with temperature dependence a, and b</td>
<td>atmospheres</td>
</tr>
</tbody>
</table>
8.3 OB/DG

8.3.1 OB/DG model description

The Ocean Breeze/Dry Gulch model (OB/DG) depends on the OB/DG diffusion prediction equation, a purely empirical statistical best fit (least-squares multiple linear regression) to tracer data collected in the Ocean Breeze (Cape Canaveral, FL), Dry Gulch (Vandenberg AFB, CA), and Prairie Grass (O’Neill, NB) experiments. The variables considered (see Nou, 1963) when developing the equation were the concentration on the plume centerline $C_p$, the source strength $Q$, the mean wind speed $U$, the standard deviation of wind direction $\sigma_\theta$, the vertical temperature difference $\Delta T$ between two specified heights, and the distance $x$ downwind from the source. A variety of formulations were tested using Prairie Grass data; the form $C_p/Q = K x^a U^b \sigma_\theta^c (\Delta T + K)^d$ gave the best results, and was the simplest to use. The terms $K$, $a$, $b$, $c$, and $d$ are the parameters of fit; $K$ is just a temperature offset added to $\Delta T$ to avoid raising a negative number to a power. Following some preliminary work, the combined data sets from Ocean Breeze, Dry Gulch, and Prairie Grass were divided in half using a random selection technique; one half ("Ocean Gulch Grass") was used to derive the best fit equation, and the other half ("Dry Prairie Breeze") was used to test the equation. The two data sets each include 31 runs from Prairie Grass, 35 runs from Ocean Breeze, and 44 runs from Dry Gulch. The diffusion equation finally selected was:

$$C_p/Q = 0.00211 x^{-1.96} \sigma_\theta^{-0.506} (\Delta T + 10)^{-1.33}$$  \hspace{1cm} (8.1)$$

where $C_p/Q$ is the relative pollutant centerline concentration in sec/m$^3$, $x$ is the downwind distance from the source in metres, $\sigma_\theta$ is the standard deviation of wind direction in degrees, and $\Delta T$ is the difference in air temperature in °F between 54 ft (16.4 m) above ground and 6 ft (1.8 m) above ground ($\Delta T = T_{54} - T_6$).

Tests against the second half of the combined data set showed that this expression predicted 72% of the cases within a factor of two, and 97% within a factor of four. The mean predicted value was 145% of the mean observed value of $C_p/Q$. The equation did slightly better with the Ocean Breeze portion of the data; 79% of the cases were predicted within a factor of two, and 98% were predicted within a factor of four. Figure 8.1a shows the observed vs. predicted values of $C_p/Q$ for the complete independent data set, while Fig. 8.1b shows the same thing but for the independent Ocean Breeze data only.

The OB/DG equation is "inverted" to solve for the distances downwind to the short- and long-term exposure limits for the particular chemical released; these limits are part of the chemical data base. Isopleths of estimated ground level concentrations corresponding to these two limits are then calculated by assuming a Gaussian distribution in the cross-wind direction. A wedge-shaped toxic corridor is also calculated; the length of the corridor is equal to the long-term exposure limit, and its angular width is $4 \sigma_\theta$ (e.g., Taylor and Schumann, 1986).

8.3.2 OB/DG model strengths and weaknesses

8.3.2.1 Source treatment

The OB/DG source model is restricted to "cold spills" (no fire or explosion); the atmospheric release must behave as a passive (non-dense) gas. As discussed above, OB/DG computes the evaporation rate (source strength) for a liquid spill by multiplying a constant evaporation rate
for each chemical by the pool size of the spill (ENSCO, 1988). The evaporation rate is fixed and specific for a particular class of chemicals. Only an estimate of the spill area is then needed to calculate the source strength. This approach is very fast and easy to use, but it neglects the influence of phenomena (wind, temperature, local heat transfer, individual chemical characteristics) that are known to affect evaporation rate. By selecting fairly high values for the fixed evaporation rate, a moderately conservative approach is maintained. However, higher values can probably occur in extreme circumstances (strong winds and/or high local turbulence intensity; strong solar insolation, etc.), leading to a stronger source than predicted. There is also a risk of being too conservative; under light winds and weak insolation, for example, the source term may be significantly smaller than this simple scheme would predict, leading to overly pessimistic predictions about the extent of danger zones. In short, the scheme is inflexible and simplified to the point of being unable to recognize or deal with cases outside the usual range of conditions.

8.3.2.2 Transport treatment

OB/DG must consider only wind direction in its treatment of effluent transport. There is no dependence on wind speed at all; this is apparently absorbed within its dependence on the vertical temperature gradient, which is correlated with wind speed. In its original form OB/DG is a straight-line model — it cannot take advantage of the voluminous wind field data available at KSC, and so can't deal with the horizontally and vertically complex local wind fields observed in the KSC area. In practice, the plume path is "bent" by the computer program to accommodate the wind direction changes in the gridded winds produced by the MARSS system from the meteorological tower network data. This seems to be a purely ad hoc attempt to force the model to behave in what is believed to be a more realistic fashion, and seems to violate the assumption under which the model equation was originally derived. The OB/DG algorithm is based specifically on data from the KSC area (but see the discussion below). It is a very simple algorithm derived from a statistical best-fit to the data, and so executes very rapidly on even a simple computer. The user interface as implemented in the MARSS system is very friendly, making the code easy to operate. The graphical displays of the "plume" are easy to interpret and apply (but see Section 8.3.2.3, below).

8.3.2.3 Diffusion treatment

The OB/DG algorithm provides estimates of the centerline effluent concentration only. As implemented on the MARSS system, the crosswind extent of the plume is estimated very simply by assuming a Gaussian distribution, and the toxic corridor's width is assumed to be $\pm 2 \sigma_x$ measured from the local centerline. This is extremely easy to calculate and provides an easy-to-interpret display for the user.

The primary argument in favor of the OB/DG model is that some of the tracer data used in the model derivation (regression analysis) were collected in the KSC area. Hence, the model is "tuned" to the specific conditions at KSC. This strength is also its main weakness. The real problem with OB/DG is that it must be limited to cases for which its data-based statistics are valid. The method most emphatically should not be extended to different source heights or configurations, or meteorological conditions other than those of the original Ocean Breeze tracer test sequence. The argument that the model is site-specific may instill a false sense of security for three reasons:
(a) The Ocean Breeze tracer experiments mostly took place during daytime periods of unstable onshore flow, when strong turbulence tends to homogenize the local flow. Since horizontal and vertical variability of the wind field is at a minimum during these periods, a simple model like OB/DG may be adequate. But during other times, such as at night, OB/DG may be inadequate.

(b) The tracer measurements during the Ocean Breeze (and Dry Gulch) experiments extended only to downwind distances of about 5 km (note: it is roughly 20 km from the eastern edge of the KSC/CCAFS site to Titusville). Extrapolating the OB/DG model beyond 5 km is risky. This is especially true in the presence of an elevated inversion, limiting the depth of the mixing layer; no attempt was made to include this effect in the OB/DG model, and its concentration estimates may therefore become too small (non-conservative) at large distances downwind. Ohmstede et al. (1983) observed this effect in comparisons to other models that do allow for a mixed layer of finite depth.

(c) OB/DG arises from a multiple regression analysis using one-half of the Prairie Grass, Ocean Breeze, and Dry Gulch tracer data sets. The model was then validated with the other half of these data sets. Since there may be significant statistical dependencies (i.e., temporal and spatial correlations) between the two halves of these data sets, this validation method may have overestimated the skill of the OB/DG model. A truly independent set of tracer data would be required to provide a fair evaluation of the OB/DG model's skill.

A number of investigators have tested the OB/DG model against other models, and (occasionally) against data. Kunkel (1984) compared OB/DG to the Shell SPILLS dispersion model, and to his modification of the latter, for a hypothetical ground level release of benzene, evaporating at 1 kg/s. Kunkel estimated the "hazard distance," the distance from the source where the centerline concentration drops to a prescribed threshold value of 10 ppm, for a range of meteorological conditions. He found that for a high sun angle and clear skies, OB/DG predicted shorter hazard distances than the original Shell model, but agreed quite well with the modified Shell model. For low sun and clear skies, OB/DG again predicted shorter hazard distances than the original Shell model for most wind speeds; the modified Shell model was found to agree well with OD/DG for winds > 4 m/s, but OB/DG predicted much shorter hazard distances for lighter winds. Overcast skies affected both Shell variant predictions. At night, the hazard distance predictions of the Shell variants depended on wind speed and cloud cover, as well as stability. The greatest discrepancy between OB/DG and the two Shell variants occurred for light winds and clear or partly cloudy skies, when OB/DG predicted much smaller hazard distances than either Shell model. It should be recalled that OB/DG was derived from daytime data, and so should not be applied to nocturnal stable conditions anyway. Kunkel's recommendation was that the modified Shell dispersion model should be considered as a replacement for OB/DG because it agreed with OB/DG for situations where OB/DG was believed to be accurate, and it was suitable for a much wider range of applications than OB/DG.

Ohmstede et al. (1983) performed a very comprehensive comparison of OB/DG to the EPA's Industrial Source Complex Short-Term (ISCST) model, the Army's Volume Source Dispersion Model (VSDM), and the Army's Toxic Corridor Prediction Program (TOXCO). They found that OB/DG agreed reasonably well with the other models for unstable and neutral conditions for sites with relatively smooth ground cover, and that OB/DG was much more conservative than the other models for rough ground cover. However, at long travel distances, especially in stable conditions, OB/DG began to underpredict concentrations relative to the other models, because OB/DG has no provision for including the confining effects of an elevated inversion layer. The
The worst case was OB/DG's underprediction of hazard distances during very stable conditions over smooth ground; Ohmstedt et al. warn that this could be serious in case of accidental releases of large quantities of effluent at night, when not even the probability multiplier (safety factor) generally used with OB/DG predictions could prevent an underestimate.

McRae (1985a) compared OB/DG and several other models to field data obtained from a planned spill of about 6000 kg of N₂O₄ in the Eagle 3 test in Nevada. OB/DG underpredicted the concentration by a factor of four or more at about 800 m downwind. In fairness to OB/DG, the other models did not do very much better. It should be recalled that OB/DG was developed for passive gas releases only; application to a dense gas spill is outside its range of proper use.

Hanna et al. (1988) reviewed a number of commonly used hazard assessment models including OB/DG, and discussed quantitative statistical evaluation procedures. For the Ocean Breeze, Dry Gulch, Prairie Grass, and Green Glow data sets, AFTOX and OB/DG were found to be not significantly different in performance; OB/DG was, of course, "tuned" during its development to the first three of these data sets, and was therefore expected to perform well.

8.4 LOMPUFF

8.4.1 LOMPUFF model description

The Local Meteorological Puff (LOMPUFF) model is presently not widely known in the air quality research community. For this reason, a detailed discussion is given here. The model has been described by ENSCO (1988), Evans and Taylor (1988), and Lane and Evans (1989); the ENSCO discussion is largely followed here, with some additions. LOMPUFF was added to the MARSS system by ENSCO, Inc. as an alternative to the OB/DG model. It was developed by combining the Shell SPILLS model (discussed above; see also Flescher, 1980) as a source term with the EPA's INPUFF dispersion model (Petersen et al., 1984). The component models were modified to run within the MARSS system, using available meteorological and chemical data.

The dispersion model used in LOMPUFF is the well known INPUFF model (Petersen et al., 1984; an improved version, INPUFF-2, is now in use – see Petersen and Lavdas, 1986), developed for the EPA to deal with time-varying releases into a spatially and temporally varying wind field. LOMPUFF uses the meteorological data (wind speed and direction, standard deviation of wind direction, and temperature gradient) from the CCAFS/KSC tower network, updated every five minutes. The model works by periodically releasing a puff of effluent from the source location, allowing it to advect with the (spatially varying) wind observed at that time, and diffusing as a Gaussian puff at rates derived from empirically driven similarity theory, described in more detail below. Mixing height estimates are also obtained from similarity theory.

LOMPUFF calculates the dispersion parameters for the puffs as follows (see Draxler, 1976; Irwin, 1983):

\[
\begin{align*}
\sigma_y &= \sigma_x t f_x \\
\sigma_z &= \sigma_w t f_z
\end{align*}
\]

where \(\sigma_y\) and \(\sigma_z\) are the horizontal and vertical dispersion parameters, respectively; \(\sigma_x\) and \(\sigma_w\) are the standard deviations of the crosswind and vertical wind direction components, respectively; \(t\) is the elapsed time of travel of the puff since leaving the source; and \(f_x\) and \(f_z\) are semi-empirical functions of \(t\):
\[ f_y = [1 + 0.9(t/1000)^{0.5}]^{-1} \]  
\[ f_z = 1, \text{ for unstable conditions} \]  
\[ f_z = [1 + 0.9(t/50)^{0.5}]^{-1}, \text{ for stable conditions} \]

Because the evaporation generally occurs from a pool of non-zero size (i.e., an area source), the initial value for the horizontal dispersion parameter is assumed to be \( \sigma_{\infty} = \text{pool width}/4.3 \) (see Turner, 1969).

Atmospheric stability is assessed from the temperature gradients observed on the meteorological towers, converted to potential temperature \( \theta \); data are collected at 54 ft (16.5 m) and 6 ft (1.8 m). Let \( \Delta\theta = \theta_{54} - \theta_6 \), where the subscripts refer to measurement height in ft, to be consistent with other notation. Then \( \Delta\theta > 0 \) is stable, \( \Delta\theta = 0 \) is neutral, and \( \Delta\theta < 0 \) is unstable. In terms of measured temperatures, with \( \Delta T = T_{54} - T_6 \), \( \Delta T > -0.257^\circ F \) is stable, \( \Delta T = -0.257^\circ F \) is neutral, and \( \Delta T < -0.257^\circ F \) is unstable. Note: it is unclear in the description of the LOMPUFF model how \( \Delta\theta \) and \( \Delta T \) are defined there; the original work on the OB/DG model specifies \( \Delta T \) as it is defined here. The NOAA review team is not familiar with the details of the temperature measurement system used at KSC; we note that determining atmospheric stability via temperature gradients requires high accuracy sensors, as well as high flow rate fan-aspirated radiation shields to assure measurement of the actual air temperature. A direct difference measurement scheme (e.g., an electrical bridge approach) is normally recommended. If these precautions are not taken, the results may be misleading. Schemes based on net radiation or surface energy balances may be more accurate.

The term \( \sigma_v \) is related to the standard deviation of wind direction and the wind speed, both determined from the meteorological tower data:

\[ \sigma_v = \sigma_e u \]  

The ENSCO (1988) document does not specify the elevation where these data should be taken; it is believed to be 54 ft (16.5 m) AGL. It should be noted that there is no accepted method for extrapolating Eq. 8.4 above the surface layer, especially when \( \sigma_v \) values are relatively large.

The standard deviation of the vertical velocity component, \( \sigma_w \), must be estimated in some way because a suitable measurement technique is not available in the KSC network. It should be noted that it is now possible to use remote sensing systems such as sodars to provide direct evaluations of \( \sigma_w \); if this capability is added to the KSC meteorological system, LOMPUFF's indirect evaluation can be eliminated (but see Neff and Coulter, 1986, for some cautionary advice). In the absence of such data, surface layer similarity theory was chosen as a means to estimate this term.

The approach of Venkatram and Paine (1985) is used in LOMPUFF to estimate \( \sigma_w \) for neutral and stable conditions:

\[ \sigma_w = 1.3 u_* (1 - z/z_i)^{0.55}, \]  

where \( u_* \) is the friction velocity, \( z \) is the height above ground and is (arbitrarily) set to 1 m, and \( z_i \) is the mixing layer height in m, estimated as \( z_i = 1300 u_*^{1.5} \). It is unclear to the NOAA team why \( z \) was set to 1 m; it would seem more appropriate to evaluate it at the source height, or perhaps at the height of the wind measurements. Also, Eq. 8.5 applies only to small-scale
turbulence, rather than to gravity wave scales, which may produce different dispersion characteristics.

For unstable conditions, it is assumed that

$$\sigma_w = 1.3 \, u_\ast \, (1 + 3 \, z/L)^{1/3}, \quad (8.6)$$

where $z$ again is set to 1 m (see comment above), and $L$ is the Monin-Obukhov length in m. For unstable conditions, $z_0$ is set to 1000 m, but does not seem to be used. The Monin-Obukhov length (in m) is defined as $L = u_\ast^2/(k \, g \, T_\ast/T)$, where the von Karman constant $k$ is taken as 0.35, $g$ is the gravitational acceleration (m/sec$^2$), $T$ is the average temperature ($^\circ$K) in the boundary layer, and $T_\ast$ is the similarity temperature. The NOAA review team points out that Eq. 8.6 should have a minus sign (rather than a plus sign) within the parentheses; see Panofsky et al. (1977). Also, this equation is valid only in the surface layer. In the outer layer (i.e., for $z > 0.1 \, z_0$) in strong convection, for horizontally homogeneous conditions, $\sigma_w = 0.6 \, w_\ast$, where $w_\ast$ is the convective velocity scale (see, e.g., Weil, 1985).

The above approach requires the evaluation of $u_\ast$, $T_\ast$, and $L$, to evaluate $\sigma_w$. LOMPUFF uses measured profile data and similarity assumptions to do this. The method is as follows: the wind speed $u$ at a height $z$ is given by

$$u(z) = u_\ast \, k^{-1} \, [\ln(z/z_0) - \Psi_m(z/L)] \quad (8.7)$$

where $z_0$ is the aerodynamic roughness length of the area, which is assumed to be 0.2 m for KSC. Note that $\Psi_m$ is zero for neutral stability conditions, so in this case $u_\ast = 0.07936 \, u_s$; this is sufficient to evaluate $\sigma_w$ for neutral conditions. The situation is far more complex for non-neutral atmospheric conditions.

For unstable (e.g., typical daytime convective conditions),

$$\Psi_m = 2 \ln[(1 + x)/2] + \ln[(1 + x^2)/2] - 2 \tan^{-1}(x) + n/2 \quad (8.8)$$

where $x = \phi_{m^{-1}} = [(1-1.5z)/L]^{1/4}$.

The temperature profile is given by

$$T_\ast = 1.35 \, k \, \Delta \theta \, [\ln(z_2/z_1) + \Psi_{h1} - \Psi_{h2}]^{-1/2} \quad (8.9)$$

where $T_\ast = 0$ for neutrally stable conditions. For unstable conditions,

$$\Psi_{h1} = 2 \ln[(1 + \phi_{h1^{-1}})/2] \quad (8.10a)$$

$$\phi_{h1} = [1 - (9 \, z_2/L)]^{-1/2} \quad (8.10b)$$

$$\Psi_{h2} = 2 \ln[(1 + \phi_{h2^{-1}})/2] \quad (8.10c)$$

$$\phi_{h2} = [1 - (9 \, z_2/L)]^{-1/2} \quad (8.10d)$$

An iterative solution is used. Estimate $u_\ast$ using Eq. 8.7 for the neutral stability case, with $z = 16.5$ m, and $z_0 = 0.20$ m. Use this first estimate in Eq. 8.9 for $T_\ast$, taking $z_2 = 16.5$ m, $z_1 =$
1.8 m, and \( \Psi_{h2} = 0 = \Psi_{h1} \). Then calculate \( u_2^2/(k g T_2/T_1) \) as a first approximation to \( L \). Use it to estimate \( \phi_m \), so that \( \Psi_m \) can be evaluated. Use this result to calculate an improved solution for \( u_2 \) using Eq. 8.7. Calculate an improved value for \( T_2 \) using Eq. 8.9, and then re-estimate \( L = u_2^2/(k g T_2/T_1) \). Repeat the procedure until the new value of \( L \) differs from the previous one by less than 5%.

For the stable case, the LOMPUFF code uses the expressions

\[
\Psi_m = -6.85 \ln(z/L) - 4.25 (z/L)^{1/2} + 0.5 (z/L)^2 - 0.598
\]

\[
\Psi_{h1} = -6.35 (z_1/L)
\]

\[
\Psi_{h2} = -9.257 \ln(z_2/L) - 5.743 (z_2/L)^{1/2} + 0.676 (z_2/L)^2 - 0.808
\]

A rather complex sequence of steps is then used to solve for \( u_m \), \( T_m \), and \( L \). The exact method depends on the value of \( L \); an exact solution is feasible for some range of values, while an iterative method works for others. Refer to ENSCO (1988) for details. The NOAA reviewers feel that the simple log-linear profile relations of Businger et al. (1971) would be better suited for stable case calculations than the complicated forms in Eqs. 8.11 and 8.12, which are unreferenced in the ENSCO document. Also, previous experience suggests that the method given above requires a good first guess and sophisticated iterative techniques to minimize the possibility of non-convergence of the solutions, especially for stable cases with low wind speeds.

8.4.2 LOMPUFF model strengths and weaknesses

8.4.2.1 Source treatment

The LOMPUFF source model, like that of OB/DG, is restricted to "cold spills" (no fire or explosion); the atmospheric release must behave as a passive (non-dense) gas. As discussed above, LOMPUFF computes the source strength for a liquid spill using the Shell SPILLS model. This approach is believed to be superior to that used for OB/DG, in that it allows variations in ambient conditions to affect the evaporation rate.

There are many other source strength models available. Kunkel (1983) compared six models, including the SPILLS model, for evaporation rate predictions for hydrazine, MMH, UDMH, and \( \text{N}_2\text{O}_4 \). Unfortunately, some of the necessary data for the SPILLS code were unavailable for these chemicals. Kunkel therefore performed a comparison of the SPILLS model and the "Army" (Whitacre and Myirski, 1982) evaporation rate model for 17 other chemicals, and found that the results agreed within about \( \pm 10\% \); his conclusion was that the Army and SPILLS models would produce similar results in other cases. Hence the behavior of the Army model could be used as a surrogate for that of the SPILLS model (note: a study by McRae, 1985a, indicated that this is not always true). The other models he considered were the Ille and Springer (1978) model, based on work by Mackay and Matsugo (1973); a modified version of this (Kunkel, 1983); the USAF Engineering and Services Laboratory model (Clewell, 1983); and the USAF Air Weather Service (1978) model. Kunkel tested the models as functions of wind speed and air temperature, with and without solar radiation (important for the Ille and Springer code only). He observed that the Army model (and therefore also the SPILLS model) consistently produced the lowest source strength. The Ille and Springer model and the Air Weather Service model
generally produced the largest estimates for evaporation rate (and therefore would produce the most conservative toxic corridor assessments). Kunkel suggested that the Army and the SPILLS models would give reasonable estimates of source strength for nocturnal releases; but would underestimate the source strength of daytime spills because they do not account for the substantial effect of solar radiation. Kunkel stated that the Ille and Springer model has a more realistic treatment of the problem, because it allows for changes in pool temperature that are induced by evaporative cooling and solar warming.

Vossler (1989) compared results from the Kunkel (1983; modified Ille and Springer) model, the Air Force Dispersion Assessment Model (ADAM; Raj and Morris, 1987), the Kawamura and Mackay (1987) model, and a new composite model, developed by considering the sensitivities of the evaporation rates predicted by earlier models to various processes. The Vossler model generally behaves like the Kunkel model, except in sparse woods where Vossler predicts a smaller evaporation rate, and in desert terrain, where the Vossler prediction is higher. Both the Kunkel and Vossler models predict significantly smaller evaporation rates than ADAM and the Kawamura and Mackay model. It is worth noting that the evaporation models are becoming increasingly complex, and require a great deal of site-specific information from the user. For example, the Vossler model needs the month, day, and time of the spill; the elapsed time since the spill occurred; the site latitude and longitude; the cloud cover fraction and thickness; the terrain and ground types; the volume of material spilled and the depth of the pool; the temperatures of the air, ground, and chemical storage container; wind speed; and barometric pressure. An equally large amount of information on the chemical and thermodynamic properties of the spilled material, the air, and the ground is needed for the heat and mass transfer calculations.

The real question to be answered is which source strength models - if any - are able to predict observed evaporation rates accurately. ENSCO (1988) attempted to answer this by comparing OB/DG and LOMPUFF source strength estimates to evaporation rates from spill experiments with N₂O₅, hydrazine, and Aerozine-50. For N₂O₅, ENSCO found that the OB/DG and Lompuff predictions were in reasonable agreement (about 30%) with each other, but were only about one-half of the evaporation rates determined during the Eagle 3 field test (McRae, 1985b). ENSCO found that the hydrazine evaporation rate predicted by LOMPUFF was less than half of the observed value (Ille and Springer, 1978), while that predicted by OB/DG was roughly an order of magnitude larger than the observed. The evaporation pan studies of Henderson and Brown (1970) provided the data for Aerozine-50; ENSCO's scatter plots show that LOMPUFF predictions are generally within a factor of two of the observed values, although there does not appear to be a great deal of skill in the predictions, and there is a tendency to under-predict. OB/DG predicts the same (high) evaporation rate for all cases, and overestimates the observed values in all but one case.

These results seem inconclusive. Given the importance of the source term, a series of coordinated and definitive source term/model comparison studies are needed to determine the best available source term model. If such an experiment is conducted, it is imperative that (a) the spills be performed in as realistic a manner as possible, and (b) high quality data be collected on all processes and variables that may affect the heat and mass transfer process, so that all models may be fairly tested.
8.4.2.2 Transport treatment

The LOMPUFF model relies on the MARSS wind field derived using Barnes' smoothing technique (Barnes, 1964, 1973; Caracena et al. 1984; Caracena, 1987) to horizontally interpolate the spatially and temporally varying wind field from the tower network data. This is a considerable improvement over the horizontally homogeneous wind field assumed for typical Gaussian plume models and for the original version of OB/DG. However, LOMPUFF uses a purely two-dimensional wind field to move the puffs, so it cannot account for vertical variations in the wind. This lack of vertical variability may be an important disadvantage at KSC, because of the frequent presence of sea and river breezes having significant vertical wind speed and direction shears.

LOMPUFF is a very typical puff-trajectory model. Its success relies on a realistic depiction of the local wind field as it changes in time and space, responding to changes in terrain, surface characteristics, and meteorological conditions. At present, the best hope for such a wind field rests on a good interpolation scheme, using data from a dense wind observation network. The KSC area is perhaps unique in the availability of near-surface observations for generating a wind field. As noted above, a two-dimensional wind field and advection scheme may be inadequate for the KSC. Significant improvements in predicting effluent transport will probably be possible only when a three-dimensional wind field and a three-dimensional puff advection technique are developed. Use of a power-law wind speed profile may allow some adjustment of puff transport speed to the height of the effluent release, but the direction uniformity imposed by the present method makes the technique appropriate mainly for a well-mixed atmosphere with little direction shear -- perhaps it is most useful for strongly convective conditions with a weak sea breeze.

8.4.2.3 Diffusion treatment

If on-site measurements of $\sigma_u$ or $\sigma_w$ are available, Irwin's (1983) dispersion parameterizations are superior to other common dispersion schemes such as the Pasquill-Gifford curves. At KSC, the tower network provides fairly detailed measurements of $\sigma_u$, but the estimation of $\sigma_w$ using similarity theory is somewhat suspect. Similarity theory is based on assumptions of stationarity and long expanses of horizontal homogeneity; it essentially applies to equilibrium situations (Pasquill and Smith, 1983; Stull, 1988). The KSC area in no way approximates a meteorologically suitable site for the application of similarity theory. However, the use of similarity theory for the vertical dispersion is probably better than using the Pasquill-Gifford $\sigma$-curves, because it can help account for the influence of moisture on local turbulence. The best solution would be measurements of $\sigma_w$, so that the on-site methods could be used.

Another potential weakness of LOMPUFF is that the modeled puffs apparently can grow indefinitely. A basic assumption in a puff model is that large-scale atmospheric motions appear explicitly in the wind field, whereas small-scale turbulent eddies appear statistically in the diffusion parameters. This distinction between large-scale and small-scale eddies becomes blurred when the puffs become significantly larger than the grid cells used in the wind field. Some puff models avoid this problem by breaking individual puffs into smaller ones when the horizontal or vertical dimensions become too large. LOMPUFF does not have this capability.

8.4.2.4 Testing and user issues

From a short introduction to LOMPUFF as presently implemented on the MARSS system, the NOAA team believes that the potential users of the model are not really aware of its utility, and
are inadequately trained in its operation. We believe this is simply because the model is not mandated by KSC for regular use.

From the available LOMPUFF documentation and from discussion with ENSCO scientists, it is clear that there has not been enough testing of the LOMPUFF model to formulate well-founded estimates of the model's accuracy and precision, especially in the complex environment of KSC. If LOMPUFF (or any other dispersion model) is to be employed for decision-making involving hazardous chemicals, then it should be subjected to in situ testing. Such tests should cover as wide a range of likely operational conditions as possible (diurnal and seasonal variability, various synoptic conditions, a range of plausible release heights, etc.). LOMPUFF (or any other dispersion model -- including OB/DG) should not be applied outside ranges where it has been tested and found to behave satisfactorily.

The limited demonstration provided also indicates that the user interface may need some work. However, LOMPUFF's principal shortcoming for emergency use on the MARSS system is the excessive run time (roughly five min) required on the existing MicroVAX computers. It is believed that long run times on this system will be characteristic of any puff-trajectory model, and that this will become much worse if a three-dimensional code is established. The situation can be remedied only by an improvement to the computer system. In the short term, it may be sufficient to replace the MicroVAX machines with state-of-the-art RISC workstations, which would provide roughly a two order-of-magnitude improvement in execution speed; in the long run, relatively inexpensive parallel processing machines may be the optimum choice. The Tektronix display terminals appear to be generally satisfactory; because much of the graphics apparently relies on these terminals and their associated software, it may be that the user interface can remain relatively undisturbed. If so, a computer upgrade would be greatly facilitated.

9.0 ALTERNATE SOURCE MODELS

A number of alternatives exist to the source strength models that are used in OB/DG and LOMPUFF (see Section 8.4.2.1, above, for examples). However, there currently seems to be little objective information that can be used to recommend one model over another. For example, many of the model evaluations (e.g., Kunkel, 1983) intercompare different source strength models, but do not compare the models with field data. The few field-data comparisons that are available do not provide highly encouraging results. McNaughton et al. (1986) compared six source strength models -- including the Shell SPILLS model -- with two experimental releases of N₂O₄ and found that all the models greatly overestimated the observed evaporation rates. They also compared the models with two experimental releases of liquified propane. These comparisons indicated that the models were highly sensitive to some of the input parameters. For one model, the estimated evaporation rate decreased by almost a factor of three when the pool temperature was changed from -43°C to -51°C. The evaporation-rate estimates of the Shell SPILLS model changed by a factor of three to seven when wet soil was assumed instead of dry soil.

Given the uneven performance of the source strength models, the NOAA team currently does not see any clear alternatives to the source strength models that are used in OB/DG and LOMPUFF. The OB/DG source strength model is overly simplistic from a physical standpoint, but this simplicity can also be a strength, in the sense that the model is not sensitive to indeterminate data such as pool temperature or soil type. The SPILLS model used in LOMPUFF is physically more complete, but this increased complexity is also a weakness, in that the
estimated evaporation rates can be highly sensitive to indeterminate information. As mentioned previously, it is probably necessary to perform a series of field experiments to determine which source strength model is most appropriate for KSC.

It has been the experience of the NOAA team that critical information regarding the source term is difficult or impossible to obtain while an accident is in progress. For this reason, the NOAA team believes that release scenarios should be developed for each location where significant quantities of toxic material are located. If a large quantity of N₂O₄ is located at a certain location, for example, a "small", "medium", and "large" release scenario could be developed. The "large" scenario could be a instantaneous release of the entire inventory. The "medium" and "small" scenarios might represent tank leaks below and above the liquid level, respectively. Such scenarios are likely to produce more rapid and robust estimates of the source term than attempts to obtain all the necessary input data while an accident is in progress. Perhaps the information could be stored in a multi-dimensional matrix, allowing for variations in solar radiation, wind speed, turbulence intensity, local surface characteristics, chemical characteristics, and the like, for easy use during emergency conditions.

10.0 ALTERNATE DISPERSION MODELS

Several alternate dispersion models that are suitable for emergency response and management at KSC are briefly discussed here. Some of these models are already being used for similar applications elsewhere, while others are currently undergoing development and/or evaluation. The models described below cover a wide range of formulations and capabilities, though the list does not claim to be complete. For example, atmospheric dispersion of reactive or dense gases are special topics covered by a large number of models and published work. Recent reviews of dense gas dispersion models can be found in Witlox (1991), Hanna and Drivas (1987), and Eckman (1990).

10.1 Plume Models

The AFTOX model, described by Kunkel (1988), is a Gaussian plume/puff dispersion model for uniform terrain and wind conditions. The program, written in BASIC, will run on IBM PC-compatible and Zenith-100 microcomputers. The model can handle continuous or instantaneous, liquid or gas, elevated or surface releases from a point or area source. An option is available for treating continuous heated plumes from stacks. The model can plot concentration contours, and compute concentration at a given point and time, and maximum concentration at a specified elevation and time. The model has many unique features such as the computation of a continuous stability parameter, inclusion of the concentration-averaging time and surface roughness, capabilities to save/print later and to correct input data without restarting, easy access to the chemical data file for changing data, and a plot of the plume and 90% hazard area with automatic scaling. Nitrogen tetroxide, hydrazine, Aerozine-50, and other chemicals of interest at KSC are available within the AFTOX chemical data base.

Kunkel (1988) presented results of an evaluation of AFTOX using diffusion data from the well-known USAF Projects Ocean Breeze, Dry Gulch, Prairie Grass, and Green Glow. A total of 243 tests covering a wide range of wind, stability, and terrain conditions were used in the evaluation. Kunkel also compared AFTOX predictions to those of the OB/DG model.
10.2 Puff-Trajectory Models

Puff-trajectory models are widely used to simulate the atmospheric transport of pollutants because of their ability to address short-term releases, spatially and temporally variable winds, and variable emission rates. For example, the TRIAD model (Hicks et al., 1989), developed by the Atmospheric Turbulence and Diffusion Division of NOAA, can model an accidental release of a chemically reactive gas into the atmosphere over several minutes, or the typical buoyant continuous plume from a stack, in a moderately complex terrain. The puff trajectories are determined from temporally and spatially varying wind fields, which are obtained by objective interpolation among wind data supplied to the model from suitably located meteorological towers. The model adjusts wind speeds for different tower heights and ground elevations, and can use on-site turbulence measurements to estimate puff diffusion parameters.

TRIAD's Gaussian puff dispersion routine, which is based on EPA's INPUFF-2 (Petersen and Lavdas, 1986), can simulate both moving and stationary point sources. Concentrations can be estimated for one or more sources at up to 100 receptors, on scales ranging from tens of m to tens of km. TRIAD can account for gross differences in ground elevations of sources and receptors in complex terrain. Given suitable parameterizations, TRIAD can optionally account for the effects of fast exothermic chemical reactions in the atmosphere to estimate the concentrations of toxic contaminants and the reaction products. Other options include plume downwash, dry deposition and gravitational settling, user-specified dispersion schemes and plume rise routines, and several other useful features.

The TRIAD model has been evaluated by Rao et al. (1989) and Tangirala et al. (1992) by simulating ASCOT (Atmospheric Studies in C0mplex Terrain) concentration data from passive tracer releases at different heights in the nocturnal drainage flows in a deep mountain valley in western Colorado. Evaluations with data sets from other locations are currently in progress. TRIAD does not account for density effects on gas dispersion, and it uses a two-dimensional wind field to transport the puffs, so it cannot account for vertical variations in the wind. These limitations are similar to those discussed earlier for LOMPUFF. Among the future improvements planned for TRIAD are the development of a suitable three-dimensional wind field and puff transport technique in complex terrain, and break-up of an individual puff into several smaller puffs when it grows too large either horizontally or vertically. Such desirable features are available now in a few puff models such as RIMPUFF (Thykier-Nielsen and Mikkelsen, 1991).

Another puff-trajectory model suitable for heavy gas dispersion problems and emergency response applications is the HARM-II model developed by NOAA's Atmospheric Turbulence and Diffusion Division. This model incorporates a large chemical data base, and has been designed to address chemical spills as well as radiological releases. Model capabilities include source strength estimation, wind-field interpolation, multi-tasking and communications, and a wide range of graphics outputs. HARM-II is currently being used for emergency management application at the Department of Energy's facilities in Oak Ridge, TN, and other locations in neighboring states. A tracer experiment intended to collect suitable data for model evaluation is under consideration.

10.3 Particle-in-Cell (PIC) Models

A three-dimensional Particle-in-Cell Model for Atmospheric Dispersion (ADPIC) model described by Lange (1978) computes turbulent diffusion velocities based on empirically-determined eddy viscosity coefficients and pollution concentration gradients. The pollutant is represented by a
large number of Lagrangian "marker" particles which are transported in a three-dimensional Eulerian grid by the combined mean and turbulent velocities. The pollutant concentrations are obtained by counting particles within each grid cell. MATHEW, a three-dimensional diagnostic mass-consistent wind field model developed by Sherman (1978), provides ADPIC with hourly averaged wind fields which are used to simulate pollutant transport by the mean winds.

The MATHEW/ADPIC models form part of the ARAC (Atmospheric Release Advisory Capability) system (Dickerson et al., 1985) which has been widely used for emergency management applications, especially those associated with radiological releases. The ability of models such as ADPIC to be coupled to different wind field models for emergency response or emergency preparedness applications, and for simulating irregular concentration distributions in a complex terrain is a distinct advantage. For example, in a recent ASCOT study, ADPIC was coupled with both MATHEW and SABLE, a prognostic conservation-equation model, in separate simulations of passive tracer dispersion in a nocturnal drainage flow.

Two disadvantages of the original ADPIC code are that it (1) used the gradient diffusion method, which requires high grid resolution in order to resolve the concentration gradient, and (2) was restricted to first-order K-theory turbulence models, which have been found to be inadequate for convective conditions and elevated releases. Lange (1990) modified ADPIC to include a second-order stochastic turbulence model based on the Langevin approach of Legg and Raupach (1982). Other recent modifications to ADPIC include dense gas dispersion (Ermak and Lange, 1991). It is not clear that the effects of skewed velocity distributions and unequal updraft/downdraft volumes observed in strongly convective conditions can be adequately simulated, and extended for buoyant or dense gas dispersion modeling with MATTHEW/ADPIC. The stair-stepped approximation of the terrain in the models may also lead to unrealistic flow stagnation in steep terrain.

10.4 Stochastic Dispersion Models

Stochastic dispersion models, also referred to as Lagrangian particle models or random walk models, describe the atmospheric dispersion of a contaminant in terms of the random motion of fluid elements or particles. Given the statistical properties of a flow, many particle trajectories are calculated, each corresponding to a different flow realization, by assuming the motion of a particle to be a random process. Thousands of such trajectories can be considered to build up a picture of the ensemble-average concentration distribution. The simplicity and flexibility of the approach, and the ability to incorporate spatial variations in turbulence properties are among the advantages of these models. A comprehensive review of the Lagrangian particle models is given by Hurley and Physick (1991).

Williams and Yamada (1990) described a microcomputer-based forecasting model, HOTMAC/RAPTAD, for potential applications to emergency response plans and air quality studies. RAPTAD (RAndom Particle Transport and Diffusion) is a random particle statistical model, which is driven by HOTMAC (Higher Order Turbulence Model for Atmospheric Circulations), a prognostic three-dimensional mesoscale flow model. The latter, based on a turbulence kinetic energy closure, was developed by Yamada (1985). These two models were initially run on a supercomputer such as a CRAY X-MP, but also on a SUN 4/260 workstation and an IBM/PC-AT with a 32-bit OPUS PM-350 board. Similar models have been reported by a few research groups in the U. S. and other countries. While the prognostic mesoscale flow model conveniently provides the winds and turbulence quantities needed in the Lagrangian particle diffusion model, this approach may not be suitable for emergency management.
applications because of: (i) the relatively long computation times required, (ii) difficulties in model initialization and managing the large volume of I/O data, (iii) grid resolution and numerical problems, and (iv) the lack of suitably-trained personnel to run the complex meteorological codes and interpret the results.

The NOAA review team feels that, for emergency response applications, a better approach to realize the benefits of the Lagrangian particle models is to combine them with interpolative or mass-consistent wind field models based on the observed meteorological data. NOAA's Atmospheric Turbulence and Diffusion Division is currently following this approach in developing the Lagrangian Stochastic Dispersion Model (LSDM), a three-dimensional random walk model suitable for pollutant dispersion in nocturnal flows over complex terrain. In addition to accounting for the variations in wind speed and direction, LSDM is capable of describing dispersion in highly inhomogeneous and skewed turbulent flows. A description of this nonlinear random walk model with Gaussian random forcing can be found in Luhar and Britter (1989), where it was applied to diffusion in a convective boundary layer.

11.0 CONCLUSIONS AND RECOMMENDATIONS

The review team's conclusions and recommendations follow. These have been divided into three sections dealing with data requirements for operational model use, modeling needs to assure defensible and practical transport and dispersion models for use in the MARSS system, and obtaining the data needed to develop and test those models. *Bullets* have been used as headings to call attention to specific items.

11.1 Meteorological Data Requirements

- Test the existing tower network for optimum density and distribution.

The existing KSC surface data network appears to have good spatial density. However, it is not clear if any statistical tests have been done to determine whether an optimum tower configuration has been achieved for accurate wind field modeling. If no such tests have been performed, it is recommended that they be carried out using several months of existing tower data spread over a calendar year, to assure adequate sampling of meteorological conditions. Individual towers can be "dropped" from the data set to determine their effect on the overall wind field. Correlations among the various towers can also be examined. Eckman et al. (1992) have developed a procedure to determine optimum tower spacing using data from a dense network of temporary stations located in moderately complex terrain. The object is to verify that the towers are placed close enough together to resolve important wind field features, and (conversely) to determine whether any stations are superfluous, and might be better used elsewhere in the network. Comparisons with fine-resolution A•RAMS results might be helpful; for example, recent modeling results using a 3 km grid spacing seem to adequately resolve the main flow features. However, a 3 km spacing for towers may not be adequate for emergency response work, especially in the near field. This recommendation is believed to have a low cost and a high benefit to the program.

- Wind direction alignment is a critical item; the averaging time for $u_6$ should be shorter.

The verbal description provided to the NOAA review team at the November, 1991 briefing concerning the tower network operation, including its calibration checks and external audits,
suggests that the network is well run, and provides credible data. The provision of data updates every five minutes seems adequate for all practical purposes. It would be useful to make 10 or 15 minute moving-window average values for $a_{\theta}$ available in MARSS for use in LOMPUFF or similar models; however, the 30-minute averaging technique should be retained for OB/DG, which was derived on that basis. One last point should be made: in view of the critical nature of wind direction data for effluent dispersion calculations, particular attention should be paid during network maintenance to the alignment of the direction vanes to true north; alignment to $\pm 1^\circ$ should be sought. This recommendation is believed to have a low cost and a moderate benefit.

- Continuous data are needed on winds and temperature aloft.

The principal weakness in the existing KSC measurement system is the lack of continuous data on winds and temperatures aloft. There is a real need to be able to determine vertical profiles of wind speed and direction shear to predict the trajectories of elevated plumes, especially during stable atmospheric conditions when strong shears can occur. A useful tool in this regard would be a high-frequency Doppler profiler for wind vector and $a_{\theta}$ data, with RASS for virtual temperature profiles. The preferred approach for KSC would be a multi-station network, such as the six station system recommended by Zamora (1992). It seems likely that the MARSS system must eventually use a combination of regional scale high resolution modeling and four-dimensional data assimilation techniques to provide an adequate representation of the wind fields in the KSC area; the data assimilation is required to keep the model honest and linked to current observations, thus improving predictions. The availability of both surface and elevated data in the KSC computer system would help considerably in implementing this approach. This recommendation carries a high cost, but should be of great benefit to the program.

11.2 Modeling Needs

- OB/DG is limited in capabilities and should be replaced.

Given recent advances in dispersion modeling and computer technology, the NOAA review team considers the empirical/statistical OB/DG model to be obsolete. The model has only a rudimentary ability to take advantage of the extensive meteorological data available at KSC, and no ability to account for vertical variations in the wind. Moreover, its applicability is limited to daytime periods of unstable onshore flow. Also, OB/DG is unable to deal with elevated releases of effluents, for operational uses such as launch vehicle fueling. The source strength submodel is another major weakness of OB/DG, although its lack of complexity may have some advantages.

- LOMPUFF has broader applicability, but also has important limitations.

The LOMPUFF model is a significant improvement over OB/DG, but it too cannot account for vertical variations in the wind, and it does not represent the latest generation of puff models. Its main advantage is its ability to use the extensive wind and turbulence data provided by the KSC WINDS system; it also has reasonably good theoretical underpinnings that contribute to user confidence. However, it has not yet been put into routine use on the MARSS system. The LOMPUFF source strength model is much more sophisticated than that of OB/DG, but all of the data needed to run it must be collected into the MARSS data base for at least the 44 identified likely source locations. The LOMPUFF source model should be compared to the latest USAF source model (Vossler, 1989), as well as to data. Improvements to the LOMPUFF source
strength model might be patterned after that used in AFTOX. Dispersion improvements to LOMPUFF might begin by using the latest INPUFF version, INPUFF-2 (Petersen and Lavdas, 1986). Neither OB/DG nor LOMPUFF can deal with the dense gas effects that may be important for large, fast releases of N₂O₄.

- In the short term, an existing dispersion model should replace OB/DG.

As a defensible interim improvement, the NOAA team recommends that OB/DG be replaced by either LOMPUFF or another easy-to-implement model such as AFTOX (latest version). AFTOX has the advantage of being accepted and utilized routinely at many USAF sites, and can deal with a wide range of atmospheric conditions without violating the assumptions of its derivation. However, AFTOX uses data from only a single meteorological tower, and cannot recognize the complexity of the flows often encountered at KSC – a serious shortcoming. This recommendation is believed to have a low cost, with a substantial benefit to the program.

- In the long term, a new transport and dispersion model should be developed for KSC.

For the longer term, it is therefore recommended that a more sophisticated dispersion model that can deal with both horizontal and vertical variations in wind speed and direction be selected for use at KSC. The dispersion portion of the model could be a recent-generation puff model or a Lagrangian particle (random walk) model; either of these could be coupled with a suitable three-dimensional wind interpolation/assimilation model. This recommendation is believed to have a moderate cost, with a high benefit to the program.

- The RAMS model should be made operational, and used to help understand KSC conditions.

On the local to regional scale, the non-hydrostatic RAMS model using a 3 km grid should be made operational by simplifying the moist convection treatment, and using nested grids. Code optimization work could help execution speed, but it may be necessary to run RAMS on a Cray Y- MP class machine for operational purposes. At this time, it may be best to consider this code to be a research tool, or as a model for leisurely simulations prior to an accident, or for post-accident assessments – at least until supercomputer capabilities are available on affordable workstations. Simulations performed with RAMS should include non-homogeneous initial atmospheric and ground surface conditions. Enhancements to the initial conditions using special KSC data sets should be added whenever possible. The ability to ingest these special data sets during a model run should be included in RAMS by using four-dimensional data assimilation procedures. The RAMS planetary boundary layer scheme should be improved by incorporating a second-order closure parameterization for boundary layer turbulence valid for grid spacings greater than 1 km. Realistic techniques should be explored to derive land use and ground and water surface characteristics in an operational mode. An improved data assimilation technique should be devised for RAMS to interface with all MARSS meteorological data sets. This recommendation is expected to have a high cost, but a substantial benefit.

- MARSS computer hardware should be upgraded.

For application of the transport and dispersion models discussed above, the present MARSS computer system should be upgraded to state-of-the-art UNIX-based computer workstations; for example, IBM model 560 or Hewlett-Packard model 750 RISC machines could be configured to run existing and improved codes efficiently. Almost a two order-of-magnitude improvement in execution speed is expected over the existing MicroVAX machines. The new DEC "Alpha"
workstation could conceivably provide somewhat better compatibility with existing codes, but this is uncertain. In the long run, continuing improvements in computational capability will allow operation of sophisticated model codes in real time or faster. A program to phase enhanced computer systems into the MARSS system on a regular basis should be inaugurated. In the short run, more complex but realistic models should be used to build a scenario data base, for easy reference during an accident, when access to detailed source data, local ground surface data, and the like will be impossible. In any case, machine-specific coding should be avoided to permit easy improvements to the computer system without requiring major revisions of existing code. This recommendation is believed to have a moderate to high cost, with a high benefit to the program.

11.3 Modeling Tests

- The source strength submodel should be verified with realistic tests.

The NOAA review team recommends that the source strength submodel(s) be verified by realistic field tests, under conditions similar to those likely at KSC. It is not clear that the evaporation pan tests previously used are accurate simulations of chemical spills on concrete or other surfaces; it is significant that the meteorological research community does not use evaporation pans any more, even to evaluate water transfer over vegetation. Perhaps it would be possible to attempt direct (eddy correlation) flux measurements over a chemical spill if a fast (10 Hz or better) sensor for hydrazine or \( \text{N}_2\text{O}_4 \) can be identified. New remote sensing techniques (e.g., laser absorption) being developed at NOAA's Aeronomy and Wave Propagation Laboratories and elsewhere may be capable of determining path-averaged fluxes across an evaporating pool. Some of the source strength models should be able to deal with the evaporation of surrogate materials, rather than hazardous chemicals such as hydrazine. It may therefore be feasible to design an experimental program to thoroughly explore the source model's range and sensitivities using a relatively innocuous substance. A few carefully selected cases should then be studied using the chemicals of interest, to verify the overall conclusions.

Regardless of the experimental design, it must be emphasized that the concentration calculations depend directly on the accuracy of the source term estimates; any transport and dispersion model can do no better than these estimates allow. Verification of the source strength submodel is therefore a key issue. This recommendation is believed to have a high cost, but should be of major benefit to the program.

- Transport and dispersion models require tracer studies over a wide range of conditions.

The transport and dispersion model(s) require a careful tracer study. It is worthwhile to distinguish between transport (trajectories) and diffusion. For the former, "tagged air parcels" are extremely useful for verifying the predicted path of a plume or puff. Radar-tracked or self-tracking (LORAN or GPS) constant-volume balloons (tetroons) could be released at various times of the day and year, to sample a wide variety of conditions. For example, one might release a cluster of three tetroons every six hours every other day for about two weeks, during each of the four seasons. Costs of such a study are presently high (roughly comparable to a tracer study alone), but are expected to drop with continued development of low-cost GPS. Tetroon flights are especially useful for determining over-water trajectories, where predictions based on extrapolation of land-based data are risky. On the other hand, tetroons cannot follow the changes of altitude experienced by an air parcel caught within a recirculating cell; gaseous tracers and measurements aloft are necessary to test such predictions.
The diffusion studies would be best conducted using multiple tracer sources, with simultaneous elevated and surface releases, and fixed and mobile sampling out to distances of perhaps 30 km. Both day and night releases are needed. These could be coupled with studies of photos, videotapes, and possibly aerosol backscatter lidar scans of non-buoyant exhaust plumes or other targets of opportunity, to evaluate model predictions of effluent path and spreading. These data would be very useful to (a) test the basic model selected for general use, and (b) verify the predictions for a few key (highly probable or highly dangerous) scenarios developed using sophisticated modeling tools. In any case, a very comprehensive data set, covering mean and fluctuating meteorological variables and surface conditions and characteristics, should be collected along with the tracer data, so that future tests will be unnecessary. A high quality data set will be very useful for evaluating meteorological and dispersion models for KSC, and elsewhere. This recommendation carries a very high cost, but will provide major benefits to the program in terms of credibility and scientific understanding.

A tentative design for a transport and dispersion study has been developed.

While the initial draft of this report was in review, NASA requested that a tentative design for a comprehensive transport and dispersion study for the KSC region be added. Accordingly, a "strawman" experimental plan is given in Appendix A. This Appendix suggests the collection of trajectory data over both land and sea using special balloons, and dispersion data using simultaneous releases and sampling of multiple tracer materials from both surface-based and elevated sources. The emphasis is on concentration measurements near ground level, and on detailed wind and turbulence measurements at the surface and aloft. A full suite of supporting meteorological data should be collected, so that both present-day and future modeling techniques will have adequate information for development and testing. The review team recommends that this experiment should be viewed as the logical successor to the original Ocean Breeze study at KSC. That study was conducted using the best available technology of its day; its replacement should be as comprehensive as presently feasible.

The NOAA review team has heard some discussion of the need for a similar transport and dispersion study at Vandenberg Air Force Base. We believe that this is warranted for the same reasons described above with regard to KSC. We also believe that it would make good sense for NASA and the Air Force to pool their resources, and design a joint bi-coastal study program to replace the old, limited OB/DG data sets. For shorthand purposes, this might be described as "OB/DG-II." A logical first step in this process would be to identify a small (less than ten people) design team, charged with developing detailed design specifications for the study, and identifying potential sources of expertise and experimental capability. The team should include at least two modelers with rather broad-based experience, as well as specific expertise in current flow and dispersion modeling, to ensure that all data likely to be needed in present and future model development and assessment are included in the experimental plan. The remainder of the team should have experience in designing and executing large scale transport and dispersion studies, including the use of visible tracers (balloons and smoke), simultaneous multiple gaseous tracers, and meteorological measurements including direct and remote sensing systems.
ACKNOWLEDGEMENTS

This work was accomplished under an Interagency Agreement between the National Aeronautics and Space Administration and the National Oceanic and Atmospheric Administration. The authors thank Jose A. Caraballo, the NASA/KSC project officer, for his help in providing vast quantities of documentation and his patience during the preparation of this report, Gregory E. Taylor and Randolph J. Evans (ENSCO, Inc.) for their help in providing documents and technical papers on the MARSS system, Walter A. Lyons and Roger A. Pielke (ASTER, Inc.) for providing the latest RAMS documentation, and LaLa Chambers (Oak Ridge Associated Universities/ATDD) for her ability to obtain obscure reports from unusual sources in practically no time at all. Review comments by Bruce B. Hicks (NOAA/ARL), Ray F. Kamada (Naval Postgraduate School), Donald L. Ermak (Lawrence Livermore National Laboratory), and Kevin R. Birdwell (Oak Ridge Associated Universities/ATDD), and supplementary materials furnished by Torben Mikklesen (Riso National Laboratory) are greatly appreciated.
12.0 REFERENCES


A comprehensive experiment to provide adequate transport and dispersion data to develop and test numerical models of effluent releases at KSC is needed. The earlier Ocean Breeze study at KSC has limitations because data were collected primarily during daytime episodes of onshore winds and unstable atmospheric conditions. Furthermore, all releases were near the ground, close to the beach, and are not relevant to scenarios at KSC that involve releases at heights well above ground level, and from different locations. Releases at any time of the day or night, and in any season of the year, are likely. An experiment of greater generality is therefore needed to test predictive dispersion capabilities, especially for poor dispersion conditions (e.g., stable nighttime conditions with a low inversion) that present a high pollution or hazard potential. Furthermore, the Ocean Breeze/Dry Gulch experiments at Cape Canaveral and Vandenberg AFB may have experienced significant deposition of the particulate tracer between the source and receptor locations, so that the measured concentrations were lower than would be found using a non-depositing passive tracer material; a model (e.g., OB/DG) based on these data will therefore underpredict airborne concentrations. Data from conservative, passive tracer releases are needed. A comprehensive set of supporting meteorological data and local surface characteristics will be necessary to allow development and testing of present-day and future models; these data should include a full suite of mean and fluctuating meteorological variables and surface conditions and characteristics, so that future tests will be unnecessary.

At NASA request, a tentative design for a comprehensive transport and dispersion study for the KSC region was developed after the review of the main report, and is presented here. This design suggests the collection of trajectory data over both land and sea using special balloons, and dispersion data using simultaneous releases and sampling of multiple tracer materials from both surface-based and elevated sources. A full suite of supporting meteorological data is strongly recommended, so that both current and future modeling techniques will have adequate information for development and testing. The review team recommends that this experiment be viewed as the logical successor to the original Ocean Breeze study at KSC. That study was conducted more than 30 years ago using the best available technology of its day; its replacement should be as comprehensive as is presently feasible.

The NOAA review team has recently heard discussion of the need for a similar transport and dispersion study at Vandenberg AFB. We believe that this is warranted for the same reasons given above for KSC. We also believe that it would make good sense to design a joint NASA/USAF bi-coastal study program to replace the OB/DG data sets. A logical first step in this process is to identify a small (six to eight people) design team (called the "Steering Committee" hereafter), charged with developing detailed design specifications for the study, and identifying potential sources of expertise and experimental capability. Considerable expertise in these matters already exists within a number of government laboratories, especially in NOAA, DOE (through the ASCOT complex terrain dispersion program), and some DOD facilities. It is hoped that this draft experimental design for KSC can serve as a starting point for the study.
The Conclusions and Recommendations of the main report itemize some key technical improvements and features which should be considered for modernization and improvement of the MARSS dispersion modeling capability. Table A-1 shows a draft outline for a systematic KSC modeling upgrade program that draws on these recommendations. It attempts to list the stages required to assure a reasonably thorough modernization and upgrade of the MARSS system. It is recognized by the NOAA team that the intensity of focus on any particular stage within the system upgrade plan may vary substantially according to NASA management policy decisions. However, each step of the outline in Table A-1 has some relevance to the design and implementation decisions which must be made during the formulation of the modernization plan. This conceptual MARSS system upgrade plan is similar in content to the program plan recently implemented for the successful San Joaquin Valley Air Quality Study in California over the last two years. It is believed that an analogous approach, tuned to NASA goals and funding levels, would be useful and aid the development of a sound program. The experimental design that follows, of course, addresses only a single issue in this outline; the remaining issues are necessary for success.

A-2. KEY ASSUMPTIONS

A number of assumptions have been made in developing the material below, some for technical reasons, and some for budgetary ones. These are:

1. The team has not directly addressed testing of the source strength submodel, although this is an important safety issue, directly affecting the accuracy of concentration predictions. The chemical and thermodynamic aspects of the problem are complex enough that a separate test program should be designed. This could be conducted simultaneously with the transport and dispersion studies, but need not be. It is believed that the design of the source strength test program should consider the questions of (a) possible surrogate materials, to allow less hazardous and more comprehensive tests, and (b) direct mass transfer measurements by eddy correlation or other state-of-the-art methods.

2. It is assumed that the existing meteorological tower network at KSC will be statistically evaluated for optimum quantity and placement, and that at least some supplementary towers will be recommended for eventual inclusion in the permanent network. For the transport and dispersion study, it is assumed that about 15 supplementary towers will be added temporarily, using portable units operating from solar power and radio telemetry, because it seems unlikely that the permanent towers could be added quickly. If the statistical study indicates that the existing network is adequate, or if any needed permanent supplementary towers can be added to the existing system before the transport and dispersion study, then this portable network will be unnecessary, and the expenses associated with it can be ignored. If the portable network is needed, it should be put in place for a full calendar year, to cover the intensive experiments discussed below.

3. Winds and turbulence aloft are critical to the success of the study. After discussions with NOAA/Wave Propagation Laboratory specialists, three Doppler radar profilers paired with three Doppler sodars have been suggested, to provide data from heights just above the "tower layer" to 10 km or more AGL. Because these data are needed for all experimental components associated with the study, it is recommended that the Doppler units be installed for a full year, complementing the tower network data. These data, besides
TABLE A-1. OUTLINE OF KSC MARSS UPGRADE PROGRAM PLAN

- Initial assessment of MARSS system
  - Identify system strengths and weaknesses
  - Conclusions and recommendations
    - Model and system changes
    - Necessary measurements and evaluations
- Establish core working group (Steering Committee) to design program and oversee implementation
- Develop draft overall system upgrade plan
- Develop draft dispersion study work plan
- Perform technical support studies and initial preparations
- Obtain external plan review; revise work plan accordingly
- Execute field measurement program(s)
- Perform QA processing and data archival
- Analyze existing and new data sets
- Identify candidate improvements (hardware and software) for MARSS system
- Test and evaluate candidate improvements
- Select and recommend development, procurement, or installation (as appropriate) of improvement components
- Assemble system components, perform initial testing, refine as needed.
- Test upgraded system for scientific performance and for ease of use
- Prepare new MARSS system user manuals and other documentation
- Train MARSS' operators
being crucial to the transport and dispersion studies, will be extremely useful in testing the predictions of the new A•RAMS model.

(4) Transport and dispersion experiments over a wide range of times and meteorological conditions are necessary, to simulate the range of possible conditions during potential atmospheric releases at KSC. On the basis of previous experience, the following schedule is suggested: (a) Each intensive experimental period should allow for three weeks in the field, including setup and removal time. (b) Within this three-week window, about seven experimental days should be completed, working on an every-other-day basis, with a day or two available in case of weather slippage or equipment problems. (c) Each experimental day should be 24 hours in duration, to cover the diurnal cycle. (d) There should be four experimental periods (e.g., January, April, July, October) to cover the seasons, sampling a variety of synoptic weather conditions. During each experimental period, both trajectory studies (e.g., with tetroons) and dispersion studies (with multiple gaseous tracers) should be conducted simultaneously.

(5) Modern meteorological models require detailed information on surface heat fluxes, surface layer turbulence characteristics, local vegetation patterns and species, soil moisture content, and the like. An intensive effort to obtain this information at KSC will be needed. Much of the information can be obtained using present-generation turbulent flux measurement systems mounted on towers. It is assumed here that at least two flux measurement stations will be operated over two different surface types during the four intensive studies.

(6) Recent advances in flux measurement methods permit the study of turbulent fluxes from moving platforms such as boats and light aircraft at relatively modest cost, allowing the possibilities of (a) assessing flux variability over the KSC area (believed to be substantial because of the proximity of many different surface types), and (b) off-shore flux measurements, to test model predictions and provide parameterizations for future modeling use. It is assumed here that off-shore and airborne flux studies will be conducted in coordination with two of the land-based flux studies. Note: there is a good deal of present interest in near-coastal zone studies; NOAA, DOE, and the Office of Naval Research are all funding new research programs aimed at flow dynamics and air-surface exchange. The Steering Committee should explore the possibility of collaborating with one or more of these programs, so as to 'leverage' the funding available to NASA and the other agencies.

(7) Because remote sensing of aerosols is rather costly and is expected to be useful primarily in the near field, only a single three week study using lidar has been included; if funds permit, an additional study would be very useful.

A-3. TRAJECTORY DATA

The most important test of any dispersion model examines its ability to transport effluent in the proper direction at the correct speed, so that the modeled pollutant cloud or plume passes over the correct receptor points at the correct time. The model should be able to do this regardless of the time of day or the season of the year. At KSC, on-shore winds (often but not always associated with daytime conditions) will carry released material across Merritt Island toward the Florida mainland, where significant population centers may be impacted. Off-shore winds (often
but not always a nighttime phenomenon) may carry material out to sea, where it may be transferred to the ocean, or may be caught up in a recirculating flow and carried back toward land the next day.

Neutrally buoyant balloons offer a convenient means to observe the trajectories of atmospheric releases from various locations. The tetroon (tetrahedral balloon; see Angell and Pack, 1960) has been used for decades for this purpose. Until fairly recently, tetroons were tracked either optically, with theodolites, or by radar, generally using active transponders. This required a skilled team of several observers, limiting the number of balloons in flight at any given time, and restricting the number of hours of possible observations. Newer technologies have emerged. A method using a miniature on-board LORAN-C navigation system and radio telemetry was introduced and used effectively. More recently, a miniature Global Positioning System (GPS) has been developed for balloon-borne use. Both of these tracking systems place the active equipment on board the balloon, allowing a simple, easy-to-use system on the ground — in essence, the balloons become a self-tracking system. No extensive sampling network or other dispersed tracking equipment is needed.

There are many uncertainties in the cost estimates for this portion of the study because the technology is still evolving. In particular, it is presently possible to track tetroons using active radar, LORAN, or GPS transponders. Using radar for tetroon tracking could save about $200,000 compared to the GPS method at present prices, because GPS transponders are still expensive, but radar requires transportation, setup, and use of bulky complex equipment by a skilled crew, which is also costly. GPS transponder costs are falling, and it is anticipated that the cost premium of GPS over radar will be small by the time of the experiment. Right now the LORAN approach may be the most cost-effective; the transponder cost would also be about $200,000 less than GPS, and the system should perform well in the Florida coastal navigation environment. However, the GPS approach is given in the budget below because of its probable superior accuracy, the simultaneous availability of horizontal position and altitude, and the likelihood that transponder prices will fall considerably over the next year or two. The costs shown are present-day, and should therefore represent an upper bound on the trajectory study.

Regardless of the technology selected, it is recommended that a moderately large number of self-tracking neutrally buoyant balloons be launched at various times of the day and year, to determine trajectories under a range of observed atmospheric conditions. For example, a cluster of three tetroons could be released at 0600 hrs Eastern time. Four hours later, three more balloons would be released; this would be repeated at four hour intervals throughout the day (launch times of 0600, 1000, 1400, 1800, 2200, and 0200), thus sampling early morning, mid-morning, mid-afternoon, early evening, mid-evening, and late-night conditions. Data should be collected for each balloon for at least 24 hours, or until the balloon is more than, say, 100 km from KSC. These flights would be repeated every other day for about two weeks, to sample several synoptic conditions. This sequence would be repeated every three months, for one calendar year, to sample conditions across the full seasonal cycle. The experiment would require about 504 balloons, plus a number of spares in case of equipment failures.

For developing and testing transport models, numerous supporting meteorological data are needed, along with direct observations of trajectories. These meteorological data are discussed separately, below.
A-4. DIFFUSION DATA

Direct observations of effluent diffusion are needed to develop and test numerical models of this phenomenon. A variety of realistic source locations should be used; source height and horizontal location should both be considered. Non-reactive, non-depositing gaseous tracers are required for this effort. Over the last fifteen years or so, mainly under U. S. DOE funding, a very sensitive multi-tracer capability has been developed using perfluorocarbon tracers (PFTs). With existing technology, four different tracers can be released simultaneously, and captured by a single sampler at each desired receptor location. Gas chromatography is used to separate the individual tracers, and provide concentration values for each. This greatly reduces the number of tracer releases needed to determine the concentration patterns resulting from different source locations.

The review team has extensive experience with the PFT technology. We have found it to be a costly method, though very sensitive, which is probably best reserved for long range (hundreds to thousands of kilometres) dispersion studies, where there is no real substitute for PFTs. For the KSC study, it is assumed here that NASA's primary interest is in distances less than a few tens of kilometres. For such distances there are several fluorocarbon materials that are more cost-effective, are easy to deal with, and easy to sample. These include bromotrifluoromethane (13B1), bromochlorodifluoromethane (1211), and dibromodifluoromethane (12B2). The effective cost per sample for these materials is expected to be only about 50% of the PFT tracers. An additional tracer can be added to the system by using sulfur hexafluoride, if there are no significant sources (e.g., electrical switchyards) of this material in the KSC area.

It should be emphasized that concentration data alone will be inadequate; detailed observations of the winds, turbulence, atmospheric temperature structure, local surface characteristics, and other variables are essential to drive numerical prediction schemes for effluent concentration. These data must be collected simultaneously with the tracer releases. Furthermore, it is recommended that all tracer releases be conducted simultaneously with balloon trajectory studies, to provide additional data on the likely paths of the emitted material.

An extensive network of samplers is needed for adequate resolution of an effluent puff or plume. If the spacing is too open, the material may pass between samplers without being captured. Even with fairly close spacing, it is possible under some circumstances that only the edges of the cloud will be sampled, and the central concentration will be undetermined. On the other hand, if the samplers are very close together, the sampling and analysis costs become prohibitively large. Separate (but simultaneous) trajectory data from the balloon studies will help determine the path of the material, and whether it has been only partially sampled. An angular spacing of about 2° is probably optimal, based on previous experience, and should allow calculation of horizontal dispersion parameters.

Four sampling arcs, logarithmically spaced at distances about 1 km, 3 km, 10 km, and 30 km from the sources are recommended. An additional arc at 50 to 80 km was considered but rejected because the costs for servicing the outermost arc would have amounted to nearly half of the total cost. Because of the geography of the KSC area, it will be impossible to place more than a few samplers in the two quadrants east of the site, unless numerous boats are deployed. This is not believed to be feasible on cost grounds. Hence the samplers are assumed to be distributed mainly in the two westerly quadrants, so that about 91 samplers per arc will be needed. Allowing for a few co-located samplers for QA/QC purposes, about 400 samplers will be needed for the study.
Fixed site sampling is done using battery-powered "bag" samplers, which can be programmed to draw in air and tracer gases at a controlled flow rate for a given length of time. It is assumed here that the tracer releases will be about 12 hours in duration, with sampling performed in hourly increments. Hence there would be 12 sample bags collected per sampler per release, or about 4800 bags total per release.

Four tracer release sites can be operated simultaneously, simulating four possible effluent sources. These might include two surface and two elevated sources, for example. The geometry of the sampler arcs will depend on the location of these sources. Tracer releases every other day seem feasible, based on previous experience. Within a three-week field campaign, it should be possible to complete seven tracer studies. Some of these should cover nocturnal periods, and some should cover the daytime. The 12 hour duration of each run was selected to allow coverage of the important transition periods in the morning and evening.

Under the above assumptions, about 33,600 samples would be collected during one experiment. The experiments should be carried out in several seasons, to sample a wide variety of meteorological conditions. With experiments in all four seasons, as recommended, about 134,400 samples will be collected. To hold down costs, the sample bags can be cleaned and reused from one seasonal experiment to the next, and this is assumed in the following cost estimates.

Real-time ground-based mobile sampling of SF₆ is feasible using a commercially available sampler in a van equipped with a GPS and data logger. A switched dual cold-trap sampling system feeding a single GC could probably be deployed in the same vehicle, to provide sampling of the fluorocarbon tracers with a sample averaging time of less than five minutes. Use of such a system would allow determination of the various plume paths in near-real time, greatly facilitating understanding of plume motions and impacts on the fixed sampler network. Preparation and deployment costs for such a system have not been calculated, but would probably amount to $300,000 to $400,000 for four three-week studies.

A-5. VISIBLE TRACERS

It may be very cost-effective to use oil fog releases to document both the trajectories and the dispersion of materials released at selected locations using a combination of airborne and ground-based photography. Over the years, a number of techniques have been developed to provide quantitative dispersion estimates from geometric analyses of smoke photographs, including aerial photos (Gifford, 1957, 1959, 1980; Nappo, 1980, 1984; Eckman and Mikkelsen, 1991). Furthermore, smoke releases can be used to determine dispersion close to the sources, and to evaluate the significance of the very large buildings at KSC for locally affecting dispersion. This may be useful in determining the proper placement of monitoring equipment near potential release sites. In addition, repeated photos allow the averaging of results, providing both time-averaged data and instantaneous realizations. These can be very helpful in testing models, especially for emergency response use, where plume fluctuations and peak-to-mean concentration ratios may be very important.

Aerosol backscatter lidars offer a powerful means to determine through-plume average concentrations at multiple locations along the length of a visible or sub-visible aerosol plume. Ground-based lidars provide side views of the plume; airborne lidars can be used for plan views. At night, some lidars can scan simultaneous releases of different colored fluorescent particles to evaluate dispersion from multiple sources. The quantitative data obtained can be
used to test model calculations directly. The necessary equipment is available through a few government laboratories, universities, and commercial firms that have specialized in this technique. The experimental plan suggested here would use a ground-based lidar during one experimental period to evaluate dispersion patterns from two or more different source locations, providing more quantitative detail on the near field characteristics than can be inferred from the gaseous tracer samplers. A new lidar system being developed by NOAA's Wave Propagation Laboratory will combine concentration measurement capabilities with Doppler wind measurements (not simultaneously); this system will be operational this winter, and would provide a greatly improved capability for the KSC study.

A-6. METEOROLOGICAL DATA

An excellent surface meteorological tower network is already operating across the KSC region, with well-instrumented meteorological towers reporting data at five-minute intervals. However, as indicated in the main report, a statistical analysis should be carried out on the existing data to verify that the towers are sufficient in number and optimally located so as to resolve the surface wind field peculiarities at KSC. During the short-term intensive trajectory and diffusion studies, it may be advisable to supplement the existing tower network with temporary towers, to help resolve flow field features. Portable towers using radio telemetry and solar power would be ideal for this task, and are readily available from both government and commercial sources. It is assumed here that about 15 such towers will be utilized during the study.

The tower network provides essential data on near-surface wind speed and direction. These are important for testing the RAMS predictions, as well as the dispersion models. However, turbulence data are also needed. The towers presently provide a somewhat indirect measure of turbulence, \( \sigma_x \), the standard deviation of the horizontal wind direction. It would be possible to add bivanes to these towers, to provide a similar measure of the vertical turbulence, \( \sigma_z \). However, modern flow and dispersion models generally require more direct information about the local turbulence; in particular, commonly used scaling parameters depend on the local heat flux, the turbulent kinetic energy, the standard deviations of the fluctuating velocity components, the eddy dissipation rate, and other terms.

Direct turbulence measurements using sonic anemometry (or less effectively, u-v-w propeller anemometers), remote sensors, instrumented airplanes, etc., can provide these data. Current technology has reached the point where full eddy correlation turbulent fluxes of momentum, heat, and water vapor can be conducted on a nearly continuous basis; two-week continuous runs in conjunction with the transport and diffusion measurements would certainly be feasible. As a quality control measure, the accuracy of the turbulence measurements should be checked by performing a full suite of energy balance measurements; if closure of the energy budget is achieved within a few per cent, then the measured fluxes can be assumed accurate. The data required for this check will include net radiation, soil heat flux, and the turbulent fluxes of heat and moisture. Standard technologies and procedures are available for all of these. Some of these data will be required themselves, for surface parameterizations in large scale numerical models.

It should be rather inexpensive to add some measures of steadiness of the prevailing conditions to the data set using higher than normal sampling speeds on the mean instruments. If this is difficult to implement on the permanent tower network (because of data acquisition system limitations), it can be handled on the supplementary network. For example, an electronic microbarograph array can be added and used with one-minute average measurements of
temperature, wind speed and direction standard deviations, and (perhaps) ozone concentrations to determine the passage of coherent atmospheric "events" or "structures" across the measurement array. These events are apt to be especially important at night, when they may significantly increase local turbulent dispersion for short periods, or when convective storms are moving through the Cape area. Documentation of their presence may be very important in understanding the characteristics of the tracer concentration distributions, and the coupling of the near-surface layer flow to the winds aloft.

Near-surface data are not sufficient to define the complex flows characteristic of KSC. It is recommended that a small network (6 or more stations) of remote sensing systems (e.g., acoustic sounders or sodars) be installed to provide wind speed and direction aloft, at heights up to 500 m AGL, with a vertical resolution better than 50 m, to permit resolution of thin zones of wind speed and direction shear, especially under stable conditions. Actually, the current generation of mini-sodars can provide even better vertical resolution (15 m or so) up to heights of perhaps 250 m; a combination of mini-sodars and standard commercial phased-array-antenna sodars should be able to provide high-resolution data near the surface, with reasonable resolution above 250 m AGL. Determination of the variability of wind speed and direction aloft will also be useful in understanding the transport and dispersion of elevated clouds or plumes of effluent. Some indications of this variability are available from sodars, but there is still uncertainty and debate as to the accuracy of these statistics.

Wind speed and direction data are needed at heights up to at least 10 km AGL, for evaluating the synoptic flows, for testing the RAMS predictions, and for resolving the return flow components of the land and sea breezes. Up to three 915 Mhz Doppler radar profilers should be installed, at least for the duration of the study, to provide frequent updates on the synoptic wind conditions. These would be used together with the NWS and USAF rawinsonde data, to determine the prevailing synoptic flows, and to evaluate their steadiness. The three Doppler profilers should be co-located with three Doppler sodars, to provide data within the first few hundred metres AGL.

The new NWS NEXRAD Doppler radar system operating at Melbourne, FL can provide additional wind information aloft with frequent updates. If NEXRAD stations are installed throughout Florida prior to the experiment (a possibility), it is important that their output should be acquired as well.

Mixing layer depth will be needed as a function of space and time. The required information can be obtained from the remotely sensed data aloft. During the night and early morning, the range of the sodar systems will probably be adequate to determine the mixing layer depth, but in a convective daytime boundary layer, the longer range of the radar profiler(s) will be needed. The scheduled twice-daily NWS and USAF rawinsonde balloon launches will supplement these more frequent data. Slow-rising special rawinsondes released from Patrick AFB or from Cape Canaveral AFS should be considered, to provide higher than normal resolution of the vertical profiles of wind and temperature in the lower planetary boundary layer. Without remote sensor-equipped ships offshore, over-water mixing layer data will have to be collected by an instrumented airplane, or by over-water radiosonde launches.

Vertical temperature structure will be important for understanding the tracer dispersion and for testing models of it. Data from the few tall towers near KSC should be exploited. However, remote sensing systems probably offer the best hope of obtaining frequently updated temperature data throughout the mixing layer. So-called radio acoustic sensing systems (RASS)
should be deployed near the Doppler radar profilers, to determine the virtual temperature profile. Data on the moisture profile are needed to recover the actual air temperature.

During the intensive experimental programs, it is recommended that satellite data on sea surface temperature off the east coast of Florida be obtained, for testing models of sea breeze onset. Also, satellite photos of the cloud patterns over the Cape region would be useful, to determine zones of flow convergence and uplift; these data will also serve to test RAMS predictions.

A-7. DATA HANDLING METHODS

The Steering Committee will need to establish comprehensive data collection, handling, and storage techniques. Given present desktop computer and workstation capabilities, the NOAA review team suggests that "raw" data be collected on readily available removable media (e.g., high-density diskettes, "Bernoulli" cartridges, etc.) for initial editing and QA/QC testing. Acceptable data should then be recorded on write-once optical media, to assure the data set's integrity. "Meta-data" describing the data and its format should be attached to each data file for future reference. Backup copies should be made and stored in a safe location for archival purposes. Data files can then be copied on to suitable media for analysis on fast PCs or workstations. A data systems manager should establish and follow well-documented protocols for this work.

Most data will be in digital format. Some raw lidar or profiler records may be obtained as false color screen images that can be used to interpret flow or diffusion patterns at least semi-quantitatively; however, the processed data from these systems will be in digital format. Data from smoke releases will also include time-lapse photographic sequences and videotape records. These data should be duplicated for archival purposes. The photos and tapes can then be analyzed. This somewhat tedious process can be partially automated using video digitization methods and special software to analyze the resulting digital records. The results will include estimated plume dispersion parameters, peak-to-mean relative concentration estimates, and the like. These results depend on the assumptions made during the analysis, so it is imperative that the underlying assumptions be thoroughly documented.

A-8. QA/QC PROCEDURES

QA/QC procedures should be carefully defined and well documented. There is ample guidance in the meteorological literature; see, for example, Finkelstein et al. (1983) and Kaimal et al. (1984). The procedures should include equipment calibration methods for all sensors or samplers used (whenever possible), as well as defining the statistical tests to be imposed on the data to assure that they are well-behaved. It is recommended that an external auditor be engaged to perform in-situ tests of the direct sensing meteorological equipment. Data acquired from the tower network should continue to be checked as presently done, with in-range and time-series consistency checks. Supplementary tower data should be tested in the same way. Surface flux measurements acquired for model parameterizations and scaling parameters should be verified by requiring local energy budget closure; if the measured fluxes satisfy the energy budget within 10% or better, then the measurements can be considered accurate. Remote sensing equipment such as lidars and sodars present special calibration problems, and can

\[^1\text{Virtual temperature } T^* = (1 + 0.61q)T, \text{ where } q \text{ is the specific humidity, or mass of water vapor per unit mass of humid air, and } T \text{ is the dry bulb temperature. The difference between } T^* \text{ and } T \text{ may be very important in determining local atmospheric stability.}\]
generally be tested only for conformance to the published design and operating specifications. The science of concentration sampler and analysis quality control has become well defined over the last decade or so, and includes careful sensor calibrations and cross-calibrations against reference gases, blanks, reference samples, etc. These should all be used to assure high quality concentration data.

A-9. TENTATIVE BUDGET ESTIMATES

The following pages of budget estimates are an attempt to associate somewhat better than order-of-magnitude costs with the components of the above-outlined study. The costs should not be assumed to be exact, but are based on practical experience with recent similar studies. Some savings are possible by reducing the duration of the study from four intensive experimental periods to three; these have been indicated in the text below. This of course affects the study's seasonal coverage. Note: this document is not a proposal by NOAA to perform this study at these prices; it is intended only as a planning and discussion guide.

The transport and dispersion study component cost estimates may be summarized as follows:

<table>
<thead>
<tr>
<th>Component</th>
<th>Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steering Committee</td>
<td>$242,000</td>
</tr>
<tr>
<td>Trajectory Experiments</td>
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<tr>
<td>Supplementary Tower Data</td>
<td>121,603</td>
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<td>Profiler Data</td>
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<td>Mini-sodar Data</td>
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<td>Land-based Flux Data</td>
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<td>Off-shore Flux Data</td>
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<tr>
<td>Tracer Concentration Data</td>
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</tr>
<tr>
<td>Smoke Study Data</td>
<td>445,490</td>
</tr>
<tr>
<td>Field Director and Administration</td>
<td>175,088</td>
</tr>
<tr>
<td>TOTAL:</td>
<td>$5,407,643</td>
</tr>
</tbody>
</table>

It should be noted that these figures do not include funds for numerical model development or testing, nor for hardware improvements to the MARSS computer system. Those costs would have to be estimated separately.
A-9.1 Steering Committee Budget

Assumes eight people on design and oversight team. Assumes four planning meetings at KSC, and site inspections of two intensive studies.

Equipment costs:
none

Supplies:
plan and report materials and printing $2,000

Labor (includes benefits and overheads):
8 scientists, miscellaneous assistants; total of about 15 FTE months 180,000

Lodging and per diem:
8 people @ $88 x 4 days x 4 meetings 11,264
8 people @ $88 x 7 days x 2 trips 9,856

Travel:
airfare: 8 people @ $600 RT (ave.) x 6 trips 28,800
car rental: 8 @ $45/day x 28 days 10,080

STEERING COMMITTEE TOTAL: $242,000

Note: If the steering committee membership is reduced to six people (reducing the expertise available) and the number of intensive experimental periods is reduced to three, then the estimated cost for the steering committee decreases to about $182,000.
A-9.2 Trajectory Experiments Budget

Assumes 18 tetroons per 24 hours, every other day for two weeks, in each of four seasons. Assumes NASA provides space and electrical power for rented field office.

**Equipment costs:**
- 504 tetroons @ $105 = $52,920
- 504 transponders @ $800 = $403,200
- 7 antennas @ $250 = $1,750
- GPS ground station = $1,700

**Supplies:**
- Nitrogen (about 27 cylinders) = $1,350
- Helium (about 126 cylinders @ 4 balloons/cylinder) = $9,450
- Batteries = $1,008
- Computer media = $500

**Labor (includes benefits and overheads):**
Preparations and setup, operations, data editing and reporting
- 3 scientists, about 272 FTE days effort = $145,248

**Lodging and per diem:**
- 3 people @ $88 x 21 days x 4 trips = $22,176

**Travel:**
- air fare, 3 people @ $920 RT x 4 trips = $11,040
- car rental, 2 @ $275/week x 3 weeks x 4 trips = $6,600

**Rental:**
- Computers, 3 @ $35 month x 4 months = $420
- Balloon inflation van, $50 x 18 days x 4 trips = $3,600
- Field office, $1.5K x 4 trips = $6,000

**Shipping:** Air freight = $4,000

**QA/QC expenses:**
- Calibrate/check transponders $534 x 16 FTE days = $8,544
- Documentation = $5,340

**Meetings:** 2 planning, 1 reporting = $4,500

**Miscellaneous:**
- $1,000

**TETROON TOTAL:**
- $690,346

Note: if the number of intensive experimental periods is decreased to three, the cost of the trajectory studies decreases to about $521,000.
A-9.3 Meteorological Data Budget

A-9.3.1 Supplementary tower network budget

Assumes 15 portable towers set up and operating in the KSC area for one calendar year, with radio telemetry recovery of data to a local computer, with telephone retrieval of data from that computer. Assumes refurbishment of instruments will be necessary at the end of the year, due to harsh environment. Assumes eight days to set up and five days to remove system, plus travel. Assumes NASA provides space for receiving antenna and computer, and a telephone line. Assumes all towers located on Government property so that no land rental is required.

Equipment costs:

- Replacement/refurbishment of instruments after study: $12,825

Supplies:

- Computer media: 1,500
- Repair parts: 4,500

Labor (includes benefits and overheads):

- Includes preparation, travel, setup and removal, data retrieval and editing.
- 1 scientist, 2 engineers, 1 technician; total of about 143 FTE days: 71,500

Lodging and per diem:

- 3 people @ $88 x 21 days x 2 trips: 11,088

Travel:

- car rental, 1 @ $250/week x 2 trips: 500

Rental:

- truck rental, 2 @ $175/week x 3 weeks + $0.22/mile: 2,370

Shipping:

- air freight for repair parts: 500

QA/QC expenses:

- calibrations, documentation: 12,500

Meetings:

- 2 planning, 1 reporting: 3,600

Miscellaneous:

- fuel for trucks: 720

TOWER NETWORK TOTAL: $121,603

Note: meteorological data should be collected for a full year, regardless of how many intensive experimental periods are conducted. No changes in tower costs are envisioned.
A-9.3.2 Profiler network budget

Assumes three Doppler radar profilers and three co-located Doppler sodars set up and operating in the KSC area for one year. Assumes all are located on Government property, so that no property rental is required. Assumes that NASA will provide electricity and telephone lines for each system. Labor includes data editing, QA/QC costs. Assumes one person on site during each of four intensive studies, plus four short trips during year for maintenance and testing.

Equipment costs:
- 3 profiler systems (915 MHz) @ $45K $ 135,000
- 3 sodar systems @ $15K $ 45,000

Supplies:
- Computer media. $ 3,000

Labor (includes benefits and overheads):
- 2 scientists, 1 engineer, 1 programmer, total of about 8 FTE months 105,000

Lodging and per diem:
- 1 person @ $88 x 21 days x 4 trips 7,392
- 1 person @ $88 x 6 days x 4 trips 2,112

Travel:
- airfare, 1 person @ $500 RT x 8 trips 4,000
- car rental, 1 @ $250/week x 3 weeks x 4 trips 3,000
- 1 @ $250/week x 1 week x 4 trips 1,000

Rental: none

Shipping:
- ship systems by truck 10,000

QA/QC expenses:
- lumped with Labor category, above

Meetings:
- 2 planning, 1 reporting 4,500

Miscellaneous: 2,000

PROFILER NETWORK TOTAL: $ 322,004

Note: meteorological data should be collected for a full year, regardless of how many intensive experimental periods are conducted. No changes in profiler costs are envisioned.
A-9.3.3  Mini-sodar network budget

Assumes six mini-sodars set up and operating in KSC area for one year. Assumes all sites are located on Government property, so that no land rental is required. Assumes NASA will provide electricity and a telephone line for each system.

Equipment costs:
   2 additional systems $ 50,000

Supplies:
   Computer media, hardcopy. 2,000

Labor (includes benefits and overheads):
   2 scientists, 2 engineers, total of about 12 FTE months 175,000

Lodging and per diem:
   2 people @ $88 x 21 days x 4 trips 14,784

Travel:
   airfare, 2 people @ $500 RT x 4 trips 4,000
   car rental, 1 @ $250/week x 3 weeks x 4 trips 3,000

Rental:
   field office, $1.5K x 4 trips 6,000

Shipping:
   air freight 6,000

QA/QC expenses:
   testing, calibrations, documentation 4,000

Meetings:
   2 planning, 1 reporting 4,500

Miscellaneous: 2,000

MINI-SODAR NETWORK TOTAL: $ 271,284

Note: meteorological data should be collected for a full year, regardless of how many intensive experimental periods are conducted. No changes in mini-sodar costs are envisioned.
A-9.3.4 Land-based flux measurements budget

Assumes two tower-mounted flux systems are operated during four three-week periods. Assumes both sites are located on Government property, so that no land rental is required. Assumes NASA will provide electricity and a telephone line for two equipment huts/offices.

Equipment costs:
None.

Supplies:
Computer media. $1,800

Labor (includes benefits and overheads):
2 scientists, 1 engineer, total of about 8 FTE months 100,000

Lodging and per diem:
2 people @ $88 x 21 days x 4 trips 14,784

Travel:
airfare, 2 people @ $400 RT x 4 trips 3,200
car rental, 1 @ $250/week x 3 weeks x 4 trips 3,000

Rental:
field office, 2 @ $1.5K x 4 trips 12,000

Shipping:
air freight and truck 3,500

QA/QC expenses:
calibration gases, testing, documentation 3,500

Meetings:
2 planning, 1 reporting 3,600

Miscellaneous: 1,000

SURFACE FLUX TOTAL: $146,384

Note: meteorological data should be collected for a full year, regardless of how many intensive experimental periods are conducted. Flux measurements during all four seasons are highly desirable, so no changes in land-based flux costs are envisioned.
A-9.3.5 Off-shore flux measurements budget

Assumes simultaneous use of one flux measurement system mounted on a rented boat operating off the Florida coast, and a flux measurement system on a light airplane, during two experimental periods, with collection of about 50 hours of eddy correlation data by each system during each experimental period. Assumes a field office can be placed on Government property so that no land rental is required. Assumes NASA will provide electricity and a telephone line for the field office.

Equipment costs:
- Refurbish sonic anemometer after study

Supplies:
- Computer media

Labor (includes benefits and overheads):
- 4 scientists, 2 engineers, total of about 18 FTE months

Lodging and per diem:
- 4 people @ $88 x 21 days x 2 trips

Travel:
- airfare, 3 people @ $400 RT x 2 trips
- car rental, 3 @ $250/week x 3 weeks x 2 trips
- airplane ferry flights, 2 RT @ $50/hr x 9 hrs

Rental:
- field office, $1.5K x 2 trips
- hanger space, $100/week x 3 weeks x 2 trips
- airplane operation, $50/hr x 50 hrs x 2 trips
- boat operation, $400/day x 20 days x 2 trips

Shipping:
- air freight and truck

QA/QC expenses:
- calibration gases, testing, documentation

Meetings:
- 2 planning, 1 reporting

Miscellaneous:

OFF-SHORE FLUX TOTAL: $ 291,284

Note: meteorological data should be collected for a full year, regardless of how many intensive experimental periods are conducted. Flux measurements during all four seasons are highly desirable, so no changes in off-shore flux costs are envisioned.
A-9.4 Tracer Concentration Experiment Budget

Assumes 7 tracer releases in each of 4 seasons, with 4 simultaneous surface and elevated sources of 12 hours duration, and hourly sampling along 4 arcs with 400 samplers in operation. Assumes NASA provides access to release locations and about 160 sampler sites, so that land rental for only 200 sites is needed. Assumes NASA provides electricity and telephone line for a rented field office. Assumes sampler bags are reused across the 4 seasonal studies.

**Equipment costs:**
- GC systems: 10 + 2 spares @ $13K
- Tracer release equipment $156,000
- Supplies:
  - Sample bags: 33,600 @ $4 134,400
  - Pumps, parts, controllers: 100 @ $800 80,000
  - Tracer materials: 13,440 lbs @ $5/lb x 4 tests 268,800
  - Sampler batteries: 4 x 400 x 4 changes @ $1 x 4 tests 25,600
  - Computer media 2,000

**Labor (includes benefits and overheads):**
- GC technology development: 90 FTE days 45,000
- sampler and source prep: (400 units @ 2 hrs, + 15 days) x 4 tests 110,000
- field study: 20 people x 21 days x 4 tests 587,600
- GC analysis & maint.: (4 people/shift x 2 shifts x 40 days + 10 days) x 4 tests 372,000
- report preparation: 45 FTE days x 4 tests 108,000

**Lodging and per diem:**
- 20 people @ $88 x 21 days x 4 tests 147,840

**Travel:**
- airfare, 20 people @ $900 RT x 4 trips 72,000
- sampler van rental, 15 @ $300/week x 3 weeks x 4 tests 54,000
- car rental, 3 @ $250/week x 3 weeks x 4 tests 9,000

**Rental:**
- samplers: 300 @ $50/mo x 1 mo x 4 tests 60,000
- sampler land rental: 200 sites @ $50/mo x 4 tests 40,000
- bag storage building: $2K/mo x 4 tests 8,000
- field office, $1.5K/mo x 4 tests 6,000
- computer and scales: $2K/mo x 4 tests 8,000

**Shipping:**
- sampler and source equipment: $15K x 4 tests 60,000
- sample shipping: $9K x 4 tests 36,000

**QA/QC expenses:**
- calibration gases: 8 @ $700 x 4 tests 22,400
- bag cleaning and QC checks: $6K x 4 tests 24,000
- data QC and reintegration: 40 days/test x 4 tests 80,000
Meetings:
  2 planning, 1 reporting

Miscellaneous:
  site selection and permissions: 364 sites @ 1hr, + 30 days followup 45,000
  site survey and documentation: 364 sites @ $80 29,120
  contingency: 100,000

TRACER TOTAL: $2,702,160

Note: if the number of intensive experimental periods is decreased to three, the cost of the tracer concentration studies decreases to about $2,122,000.
A-9.5 Smoke Studies Budget

Assumes one three-week aerosol backscatter lidar campaign with seven 12-hour measurement sessions. Assumes some nocturnal releases using fluorescent particles, to evaluate multiple source dispersion in the near field. Assumes quite complete analysis of the output data; some cost savings would be feasible with reduced analysis effort. Assumes all equipment set up on Government property, so no land use rentals are needed. Assumes NASA provides electricity (lidars are heavy power consumers) and telephone line for lidar unit, as well as access and assistance in releasing tracer from suitable locations. Comprehensive photographic and video coverage of visible tracer releases is assumed, but costs for those are believed to be negligible compared to lidar costs. Aerial reconnaissance photos of visible tracer releases would be very useful; these could be obtained by USAF aircraft, and a cost estimate is not included here.

<table>
<thead>
<tr>
<th>Equipment costs:</th>
<th>$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lidar and tracer dispenser modifications, parts</td>
<td>35,000</td>
</tr>
<tr>
<td>Supplies:</td>
<td></td>
</tr>
<tr>
<td>Tracer oil and fluorescent particle tracer, computer media, etc.</td>
<td>50,000</td>
</tr>
<tr>
<td>Computer costs:</td>
<td>10,000</td>
</tr>
<tr>
<td>Labor (includes benefits and overheads):</td>
<td></td>
</tr>
<tr>
<td>3 scientists, 2 engineers, 1 programmer, 2 computer aides; total of about 64 FTE months</td>
<td>308,000</td>
</tr>
<tr>
<td>Lodging and per diem: 5 people @ $88 x 21 days</td>
<td>9,240</td>
</tr>
<tr>
<td>Travel:</td>
<td>3,500</td>
</tr>
<tr>
<td>airfare, 7 people @ $500 RT</td>
<td></td>
</tr>
<tr>
<td>car rental, 3 @ $250/week x 3 weeks</td>
<td>2,250</td>
</tr>
<tr>
<td>Rental:</td>
<td>none</td>
</tr>
<tr>
<td>Shipping:</td>
<td>16,000</td>
</tr>
<tr>
<td>air freight and truck</td>
<td></td>
</tr>
<tr>
<td>QA/QC expenses: calibration, testing, documentation</td>
<td>5,000</td>
</tr>
<tr>
<td>Meetings:</td>
<td>4,500</td>
</tr>
<tr>
<td>2 planning, 1 reporting</td>
<td></td>
</tr>
<tr>
<td>Miscellaneous:</td>
<td>2,000</td>
</tr>
<tr>
<td>SMOKE STUDIES TOTAL:</td>
<td>$ 445,490</td>
</tr>
</tbody>
</table>

Note: if the measurements of the smoke studies are reduced to just photographic coverage of the oil fog releases (no lidar), the cost reduces to about $75,000, including analysis.
### A-9.6 Field Director Budget

Assumes the Field Director will attend all planning meetings, and will spend about one month on site during each test sequence. Assumes he/she will spend about four months planning and coordinating activities, and about two months documenting and reporting the general results.

**Equipment costs:**
- notebook computer and portable printer $3,500
- portable 5-channel GPS $4,500

**Supplies:**
- paper, computer media, maps, digital terrain data $3,000

**Labor (including benefits and overheads):**
- Covers 4 tests @ 1 mo, 4 planning mtgs, 4 mo preparation/coordination, 2 mo reporting $137,500

**Lodging and per diem:**
- 1 person @ $88/day x 30 days x 4 tests $10,560
- 1 person @ $88/day x 4 days x 4 meetings $1,408

**Travel:**
- airfare: 1 person @ $600 RT x 8 trips $4,800
- car rental: 1 @ $250/week x 4 weeks x 4 tests $4,000
- 1 @ $45/day x 4 days x 4 meetings $720

**Rental:**
- cellular telephone, $400/mo x 4 tests $1,600

**Miscellaneous:**
- reproduction and mailing costs $2,500
- telephone costs $1,000

**FIELD DIRECTOR TOTAL:** $175,088

Note: if the number of intensive experimental periods is decreased to three, the cost for the Field Director decrease to about $135,000.
REFERENCES FOR APPENDIX A


APPENDIX B

CURRICULA VITAE OF REPORT AUTHORS
CURRICULUM VITAE

Rayford P. Hosker, Jr.

TITLE AND AFFILIATION

Director and Physical Scientist
Atmospheric Turbulence and Diffusion Division
NOAA/ERL/Air Resources Laboratory
456 South Illinois Avenue, Post Office Box 2456
Oak Ridge, TN 37831-2456

(615) 576-1233; FAX (615) 576-1327

EDUCATION

M.S. Aeronautics/Fluid Mechanics, University of Minnesota, 1967.
B.S. Physics, Boston College, 1965.

PROFESSIONAL EXPERIENCE: 26 years total

Director, NOAA, Atmospheric Turbulence and Diffusion Division, Oak Ridge, Tennessee, December 1990 - present.

Acting Director, NOAA, Atmospheric Turbulence and Diffusion Division, Oak Ridge, Tennessee, November 1989 - December 1990.

Assistant Director (since 1982) and Physical Scientist, NOAA, Atmospheric Turbulence and Diffusion Division, Oak Ridge, TN, August 1971 - October 1989.


PROFESSIONAL MEMBERSHIPS

Air and Waste Management Association
American Association for Advancement of Science
American Meteorological Society
American Society for Testing and Materials (Subcommittee D-22.11, Standards for Meteorological Instruments).
PROFESSIONAL INTERESTS

Research interests include fluid mechanics, atmospheric turbulence, air pollution meteorology, and related fields, including instrumentation. Dr. Hosker has participated in numerous national and international symposia, workshops, and short courses devoted to these topics, and has authored or co-authored numerous journal articles, reports, book chapters, and a book. He is involved with theoretical and experimental studies of flow and dispersion near buildings, transport and diffusion in complex terrain, and dry deposition of acidifying materials. Dr. Hosker served for five years as the Field Director for the U.S. Department of Energy's multi-laboratory program for Atmospheric Studies in Complex Terrain (ASCOT), and participated in the design, direction, and performance of large-scale field studies of flows in complex terrain. He collaborated in the design of a prototype meteorological and filterpack sampling network, and oversees its continuing operation at 13 sites across the U.S. as part of the National Acid Precipitation Assessment Program. He recently collaborated in the design and testing of a new recirculating-flow environmental chamber to assess the uptake of radioactively-tagged pollutants by stone and other building materials. He established the ATDD's Applied Fluid Dynamics Laboratory. Previous research work has included dry deposition modeling, over-water dispersion estimation, atmospheric effects of energy generation, and forest meteorology.

Before joining ATDD in 1971, Dr. Hosker was a post-doctoral fellow at NATO's von Karman Institute for Fluid Dynamics, where he studied laboratory modeling of flows near buildings. His dissertation research at Northwestern University was on the behavior of shock waves traveling in chemically reactive gases, and he was a research assistant at the University of Minnesota during a study of supersonic parachutes.
CURRICULUM VITAE

K. Shankar Rao

TITLE AND AFFILIATION

Senior Physical Scientist

Atmospheric Turbulence and Diffusion Division
NOAA/ERL/Air Resources Laboratory
456 South Illinois Avenue, P. O. Box 2456
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EDUCATION

Ph.D. Geophysical Fluid Dynamics, Dept. of Mechanical Engineering,
University of Notre Dame, USA, 1972.
M.A.Sc. Fluid Mechanics, University of Windsor, Canada, 1968.
B.S. Mechanical Engineering, Andhra University, India, 1962.

PROFESSIONAL EXPERIENCE: 26 years total

Senior Physical Scientist, Atmospheric Turbulence and Diffusion Division, NOAA, Oak Ridge, TN, 1988-present.


Research/Teaching Assistant, Department of Aerospace and Mechanical Engineering, University of Notre Dame, IN, 1968-1972.

Research Assistant, Department of Mechanical Engineering, University of Windsor, Ontario, Canada, 1966-1968.
PROFESSIONAL MEMBERSHIPS

American Geophysical Union
American Meteorological Society
American Society of Mechanical Engineers

PROFESSIONAL INTERESTS

Dr. Shankar Rao is a Senior Physical Scientist in the Atmospheric Turbulence and Diffusion Division (ATDD) of the National Oceanic and Atmospheric Administration (NOAA), Oak Ridge, TN, where he has been working since 1976. He has over 23 years experience in atmospheric boundary layer and turbulence modeling, and air quality model development and evaluation. He developed several regulatory air quality models such as PEM-2, PAL-DS, PEM, and MPTDS for the U.S. EPA. Dr. Rao formulated the mathematical theory and derived the concentration algorithms for these models, and evaluated them using data from field studies in St. Louis and Philadelphia. Among the models Dr. Rao developed for the U.S. DOE are second-order closure PBL models for understanding the turbulence structure and studying the meteorological effects of large-scale power generation; TRIAD, a puff-trajectory model for atmospheric dispersion of highly reactive gases such as uranium hexafluoride; nocturnal drainage flow models for parameterization studies, and pollution dispersion models such as VALPUFF and LSDM for application in complex terrain. The latter models were evaluated by analyzing and simulating the meteorological and tracer data from DOE's Atmospheric Studies in Complex Terrain (ASCOT) program in which he participated since its inception in 1979.

Dr. Rao has extensive research and consulting experience in micrometeorology, atmospheric turbulence and diffusion, numerical modeling, and statistics. He is active in international collaborative research and scientific exchange programs of the U.S. National Science Foundation. He is keenly interested in promoting atmospheric sciences and air pollution studies in developing countries, which are facing urbanization and rapid industrialization. In the past 10 years, Dr. Rao gave many lectures and offered short courses on air pollution modeling at leading academic institutions in India. He serves on ASME's Technical Committee on Atmospheric Transport and Diffusion, and on the NOAA/ATDD Committee reviewing the emergency preparedness models used at DOE's Oak Ridge facilities. He has considerable experience in tracer data analysis and model evaluation techniques. Among his recent interests are air toxics sampling and data analysis, model uncertainty, Lagrangian stochastic dispersion modeling, concentration fluctuations, and climate change.

Dr. Shankar Rao is a member of the American Meteorological Society, American Geophysical Union, and American Society of Mechanical Engineers. He is the author or co-author of approximately 100 research papers and reports, many of which are published in scientific journals, and peer-reviewed government agency reports available from NTIS. He serves as a reviewer for scientific and professional journals, and government agencies.
CURRICULUM VITAE

Richard M. Eckman

TITLE AND AFFILIATION

Physical Scientist

Atmospheric Turbulence and Diffusion Division
NOAA/ERL/Air Resources Laboratory
456 South Illinois Avenue, P. O. Box 2456
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EDUCATION

M.S. Meteorology, Pennsylvania State University, 1984.
B.S. Meteorology, Pennsylvania State University, 1982.

PROFESSIONAL EXPERIENCE: 10 years total

Physical Scientist, Atmospheric Turbulence and Diffusion Division, Oak Ridge, TN, 1986-present.

Research Associate, Risø National Laboratory, Denmark, and Pennsylvania State University, State College, PA, 1982-1985.

Research Assistant, Pennsylvania State University, 1982.

PROFESSIONAL MEMBERSHIP

Member, American Meteorological Society

PROFESSIONAL INTERESTS

Dr. Eckman's primary area of research has been atmospheric diffusion in the planetary boundary layer. From 1982 to 1985, he worked at Risø National Laboratory in Denmark, where he conducted both theoretical and experimental investigations on relative diffusion and the effects of sampling time on measurements of atmospheric diffusion. He continued the work on sampling-time effects after moving in 1986 to the Atmospheric Turbulence and Diffusion Division in Oak Ridge, Tennessee.
More recently, Dr. Eckman's research activities in atmospheric diffusion have centered on developing an improved understanding of transport and diffusion in complex terrain. Part of this work has been funded by the U.S. Department of Energy under the ASCOT (Atmospheric Studies in COMplex Terrain) program. The ASCOT program conducted large field experiments in the Brush Creek Valley of western Colorado, and in the Tennessee River Valley near Oak Ridge. Dr. Eckman was involved in diffusion-model simulations of tracer releases within Brush Creek Valley, and has used the Oak Ridge data set to develop improved techniques for measuring and simulating pollutant transport in complex terrain.

Dr. Eckman has also been involved in studies of atmospheric gravity waves. In the stable boundary layer, instabilities produced by gravity waves are thought to be a source of turbulence. Dr. Eckman has been using microbarograph data collected near Oak Ridge and in southeastern Wyoming to study wave-turbulence interactions and their importance in the stable boundary layer.

In addition to research projects, Dr. Eckman has experience in the operational aspects of emergency management. For several years he has served as a meteorological advisor to the Department of Energy's Oak Ridge Operations (ORO). In this capacity, he provides meteorological support to ORO during accidents that involve the potential or actual release of hazardous contaminants. Dr. Eckman also spent three weeks in Saudi Arabia and Kuwait shortly after Operation Desert Storm as part of a U.S. government effort to assess the effects of the Kuwait oil fires. He helped to install a meteorological tower network that was used to estimate the movement of the oil smoke.
CURRICULUM VITAE

Jeffery T. McQueen

TITLE AND AFFILIATION

Meteorologist
NOAA/ERL, Air Resources Laboratory
1325 East West Highway
Silver Spring, MD 20910

(301) 713-0295; FAX (301) 713-0119

EDUCATION

B.A. Environmental Sciences, University of Virginia, 1982.
M.S.  Atmospheric Sciences, Colorado State University, 1985.

PROFESSIONAL EXPERIENCE:  7 years total

Meteorologist, NOAA, Air Resources Laboratory, Silver Spring, MD, 1991 to present.


PROFESSIONAL MEMBERSHIPS

American Meteorological Society

PROFESSIONAL INTERESTS

Research interests involve improving numerical simulation of atmospheric transport and dispersion through the use of mesoscale meteorological models. Recent work has involved experimentation with the RAMS model code for the Persian Gulf, to simulate meteorological conditions during the Kuwait oil fires. This output was used to drive Lagrangian dispersion models to predict the oil fires' smoke plume. Evaluation of model performance was conducted by comparing the dispersion model output to NOAA/AVHRR satellite images of the smoke plume. Mr. McQueen is presently involved in techniques for ingesting high resolution land use, sea surface temperature, and soil data into the RAMS code, and studying their effects on transport and dispersion.

Previous research work at NASA involved designing, implementing, and evaluating the MASS numerical meteorological model to study the effects of soil and vegetation parameters and cloud-derived mesoscale moisture fields on intense frontogenesis simulations.
CURRICULUM VITAE

George E. (Gene) Start

TITLE AND AFFILIATION

Deputy Director and Research Meteorologist

Field Research Division
NOAA/ERL/Air Resources Laboratory
1750 Foote Drive
Idaho Falls, ID 83402

(208) 526-2329; FAX (208) 526-2549

EDUCATION

B. S. Physics, Washington State University, Pullman, WA, 1959.

PROFESSIONAL EXPERIENCE: 32 years total

Deputy Director and Research Meteorologist, NOAA, ARL, Field Research Division, Idaho Falls, ID, May 1966 - present.


PROFESSIONAL MEMBERSHIPS

American Meteorological Society
Air & Waste Management Association

PROFESSIONAL INTERESTS

General areas of experience include meteorological measurements, gaseous tracer technologies, data analysis and reporting, design and performance of field measurement programs, and management of large field programs. Major interests include building wake effects, aircraft wake turbulence and vortices, coastal and shoreline settings, complex terrain settings, extended and regional scale settings, puff-trajectory modeling, and local-scale measurement networks. During the past 26 years, extensive experience has been gained in
experimental design, test plan development, program supervision, and the logistics and contingency planning required during field measurement programs.

The work has encompassed many types of conventional meteorological measurements and tracer monitorings, including extensive use of tower-mounted sensors, local and regional scale Lagrangian balloon trajectory markers (e.g., tetroons), high-resolution data on winds aloft using pibals, rabals, and rawinsondes, laser anemometry, high-frequency turbulence using hot-wire and hot-film anemometry, visible tracers, remote sounding systems, and particulate and inert gaseous tracers.

Programs for tracer technology implementation and field measurements have been planned, prepared and implemented. Extensive technology applications have been developed to optimize and automate the laboratory analysis of perfluorocarbons, sulfur hexafluoride, and numerous fluorocarbons by gas chromatography. Prototype systems for sampling and tracer analysis were exercised and evaluated during the 1970s. A highly-refined tracer analysis laboratory system was designed, constructed and utilized for many tracer programs for 1982 to the present. An advanced gas chromatograph system was designed, tested and implemented during 1988 and 1989. A more automated, modular and adaptable gas chromatograph system design is nearing completion. System testing is scheduled for mid 1992.

Applied model development has been performed for local and regional transport and diffusion calculations. Early model development included MESODIF, a pioneering puff diffusion approximation for plumes. Follow-on work included incorporation of time- and spatial-varying fields of winds, deposition and plume depletion, and time related transformation processes. The MESODIF puff-trajectory modeling system was adapted and used to perform diagnostic assessments for design and checking of the WASH 1400 Reactor Safety Study.

The S.E. Idaho mesoscale meteorological network was designed and established in 1968 and 1969. The acquisition, use, and diagnostic researching of those data have been performed, supervised, and reviewed. Follow-on applications of those models and data collections have resulted in the design and computerized implementation of operational support and emergency preparedness capabilities for the Idaho National Engineering Laboratory. Consultation has been provided to federal agencies, private industry, universities, local governments, and foreign scientists.