Dispersion in Non-Flat Obstructed Terrain and Advanced Modeling Techniques

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An expert panel examined the influence of complex terrain, industrial plant obstacles and thermal inhomogeneities on the dispersion of gaseous plumes or aerosols resulting from accidental releases of hazardous materials. Perturbations in transport and dispersion induced by such flow disturbances were estimated. The limitations and accuracies of current numerical and physical modeling techniques were examined. Finally, important unresolved questions concerning the estimation of transport of hazardous materials in the presence of realistic industrial building, storage and transportation environments were identified.

Introduction

This article is the chairman's report of the workshop held to discuss the implications of obstructions and terrain interacting with the dispersion of hazardous materials together with the numerical and physical model methods available to predict consequent plume perturbations. The goal of the workshop was to define the present state of knowledge of obstacle effects and to identify areas where research is needed. The specific subtopics which were discussed are listed in Table 1, and an extended list of discussion topics is summarized in Table 2. Table 3 identifies the panel members who participated in the workshop, their affiliation, and their primary presentation area.

A short presentation about each workshop subtopic was provided by a panel member. The panel member summarized what is currently known about the subtopic, noted its importance in the overall context of hazardous materials transport, and recommended areas for future research. Following each presentation, the full panel offered comments on the topic to provide alternative perspectives on the most important areas for future research. Those attending the workshop were also encouraged to ask questions and make additional comments.

This article will highlight important topics discussed and list the main research areas identified for each topic. Much of the following material was extracted by the chairman from short working papers prepared by the panel members to help encourage panel discussion. A short list of references is provided for those who would like further information.

Atmospheric Processes Over Complex Terrain

Engineers and meteorologists are often faced with the problem of predicting transport and dispersion of hazardous materials in the presence of hills, valleys, escarpments and mountains. These objects distort streamlines producing regions where plumes stagnate in separation regions, loft upwards or descend downwards, meander due to channeling, and disperse more rapidly due to shear enhanced mixing. The American Meteorological Society Meteorological Monograph on "Atmospheric Processes Over Complex Terrain" edited by W. Blumen [*1*] provides an exhaustive review of thermally forced flows over mountains and valleys, the effect of rugged terrain on diffusion, and the role of physical and numerical methods in predicting such flows.

There has been notable progress in the analysis and modeling of terrain related thermal circulations, drainage flows, moun-

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TABLE 1 WORKSHOP SUBTOPICS

a. Complex terrain effects on vapor cloud transport.
b. Industrial plant and obstacle effects on dispersion.
c. Surface temperature effects on dispersion-sea or land breezes and heat islands.
d. Characteristics and limitations of 3d grid models.
e. Characteristics and limitations of spectral and alternative models.
f. Characteristics and limitations of physical modeling of flow over complex terrain.
g. Physical modeling of dispersion over complex terrain including dense gas effects.

tain waves, and downslope wind storms. Qualitatively, we understand more about the fundamental mechanisms which drive such flow fields. However, paucity of field data, the unsteady nature of the flow fields, and the non-linear response of some flows to apparently small perturbations in terrain features and atmospheric stratification pose formidable barriers to quantitative prediction of turbulent processes and the transport of pollutants. The primary recommendations to clarify complex terrain physics are to initiate research to:

- Determine what are the lee-side effects in complex terrain including stratification and separation influence on the wake region,
- Determine the effect of calms and light winds on cloud pooling and drainage behavior, and
- Examine how cloud generated heavy plume motions interact with obstacle and terrain perturbed flows.

Industrial Plant and Building Complex Effects on Dispersion

Flow and dispersion around even simple building shapes can be more complex than many terrain flows. Building geometry and spacing, local surface characteristics, local meteorology, the dynamics of the effluent release, and the presence of surrounding terrain can all modify particle path lines and dilution rates. Building architecture can induce downwash, deflect plumes along alleys and street canyons, induce channeling between adjacent structures, and produce local vortices which can induce mixing or secondary motions. Hosker [2] and Meroney [3] summarize some of the attributes of flow and diffusion near obstacles.

A vapor cloud source may itself interact with the charac-

TABLE 2 DISCUSSION TOPICS

a) Limitations and accuracies of current prediction methods,
b) Significant physical phenomenon not being considered in current prediction methods,
c) Dominant time and space scales required to predict hazardous gas dispersion in complex terrain,
d) Implications of terrain channeling or pooling of hazardous gas releases,
e) Incorporation of chemical kinetics, phase change, and aerosol formation in advanced models,
f) Use of complex models in the regulatory environment,
g) Incorporation of non-stationary atmospheric effects into complex terrain models (e.g. diurnal effects, sea or lake breeze effects, weather),
h) Incorporation of obstacles (buildings, fences, water spray curtains) into numerical prediction models, and
i) The role of proprietary versus open-domain programs in meeting the needs of the industrial and regulatory communities.
j) New turbulence or numerical model schemes which should be incorporated into future models.
k) Inclusion of variability (concentration statistics and meandering) into modeling methods to permit prediction of probability distributions.
l) Approaches to improve verification of proposed models.

TABLE 3 WORK SHOP PANEL

Name	Affiliation	Topic Presented
Julian C. R. Hunt	Cambridge University	Complex terrain effects
Ray Hosker	ATDL, NOAA, Oak Ridge	Industrial plant effects
Ted Yamada	Yamada Science & Art	Sea and land breeze effects
John Leone, Jr.	Lawrence Livermore National Laboratory	Three-dimensional grid models
Steven Ramsay	University of Western Ontario, London	Spectral and alternate models
William H. Snyder	Fluid Modeling Laboratory, EPA	Fluid modeling of complex terrain effects
Nick Isyumov*	University of Western Ontario, London	Fluid modeling of dispersion

*Dr. N. Isyumov was unable to attend; therefore, Dr. S. Ramsay, kindly presented Dr. Isyumov's material.

TABLE 4 SCREENING CRITERIA FOR NEGLECTING OROGRAPHIC EFFECTS

In neutral and unstable conditions

- the gradient of the surrounding terrain should be less than about 1 in 10
- for a ridge upwind of the source
  - either $h > 1.5\ H$ [2 or 2.5 H]
  - or $x > 20\ H$ in neutral conditions [15 H]
  - $x > 10\ H$ in very unstable conditions
- for an isolated hill upwind of the source
  - either $h > 1.5\ H$ [2 H]
  - or $x > 7\ H$ [10 H]
- for a hill or ridge downwind of the source
  - either $h > H + \sigma_z(x)$ [2D: $x > 8$ H or $h > 2$ H]
  - $\sigma_z(x) > H$ [3D: $x > 7$ H or $h > 1.5$ H]

In stable conditions

- the gradient of the surrounding terrain should be less than about 1 in 100
- for an obstacle upwind of the source
  - either $h > H$
  - or $x > 40\ H$ in slightly stable conditions
  - $x > 100\ H$ in very stable conditions
  - or $x > 10\ H$ if local meteorological data is available
- for an obstacle downwind of the source
  - either $h > H + \sigma_z(x)$
  - or $\sigma_z(x) > H$

Notes:

The criteria are based on a change of 30% in the wind speed between flat and complex terrain.

The 10 m wind speed must be at least 1 m s^{-1}.
h = the release height.
H = the obstacle height.
x = the distance between the obstacle and the source.
$\sigma_z(x)$ = the vertical plume standard deviation.

[modified values suggested by W. H. Snyder during workshop] teristics of the building flow to produce a new flow field. The release rate (puff vs plume) and total quantity of gas can effect plume trajectories. Initial plume momentum and buoyancy determine whether the gases ascend and escape near-field building circulations, or descend and follow wake movements. The conclusions reached by the companion review in this journal of the Vapor Cloud Source Modeling Workshop (Lantzy, 1992) are relevant to a better understanding of transport from sources released near building complexes.

Numerical Modeling of Dispersion in Complex Flow Fields

With the wide spread availability of computers and the increasing understanding of air flow over complex terrain, it is becoming quite usual in many countries to base environmental decisions concerning the location or control of sources of pollution in complex terrain on models. Yet an important initial question must be *Is it necessary to consider complex terrain effects for the dispersion problems of interest?*

Hunt argued for some screening procedures such as those proposed by Jones (1986), shown in Table 4. During subsequent workshop discussions Snyder proposed the modifications shown in brackets [--] on the same table based on experience gained during EPA research. Another approach is to ask whether a source lies within a sensitive region or space near a hill (within an influence 'window'), because, if it does, the surface concentrations may increase. Physical model studies and parametric studies of computational models are particularly valuable for this purpose.

Once the need to account for terrain effects on dispersion is determined the model user must also focus on

a. the surface area required (if it is larger than 30×30 km^2 then unsteadiness has to be considered);
b. the accuracy and completeness of meteorological and topographic data in the area of interest;
c. the credibility of the predictive method and the expertise of the users;
d. the capacity and speed of the computer system, or the size and nature of the fluid modeling facility; and
e. the number of cases to be considered.

Alternative Numerical Codes for Complex Terrain Flows

Today there are a wide variety of numerical models available for predicting dispersion in complex terrain situations. Hunt et al. [*6*] review recent research developments in models suitable for regulatory purposes. Such models must be scientifically justifiable and they must be fast. Hunt suggested that currently there are three main types of computational schemes being developed for regulatory purposes: a) *Microscale formulae models* which are appropriate for steady limited area (100 m-30 km) dispersion. They involve simplification of the physics and crude approximations to flow processes (CTDMPLUS, FLOWSTAR, MS3DJH, and MERCURE). b) *Mesoscale models* which are used for areas less than synoptic scales (< 300 km) and unsteady conditions. Computations are based on discretized equations suitable for large super-workstations (RAMS, HERMES, HOTMAC, RAPTAD), and c) *Interpolation codes* which are developed for areas less than synoptic scales (< 300 km) and unsteady conditions, but are based on interpolation between velocity fields given at data points within the flow field (MATHEW, ADPIC).

Meroney (1990a) has also reviewed classes of models applied to dispersion over complex terrain. He identified some seven model types used for plume dispersion in complex terrain:

i) Gaussian plume models,
ii) Hill intercept models,
iii) Phenomenalogical models,
iv) Mass consistent or objective analysis models,
v) Depth integrated models,
vi) Linear perturbation models, and
vii) Full primitive equation models.

Table 5 summarizes important characteristics of such models. Avissar et al. [*15*], Paegle et al. [*8*], and Pielke [*9*] discuss the numerical limitations of meso-scale numerical computational processes as applied to complex coastal mountain flow fields. The calculations of Yamada, Kao and Bunker [*10*] demonstrate the flexibility of new prognostic models like HOTMAC which solves a set of time-dependent conservation equations. RAPTAD is a three-dimensional diffusion code based on the Monte Carlo statistical method. Yamada et al. showed that calculations of dispersion in the presence of surface inversions, shifts in wind direction, sea and land breezes, and coastal mountains are quite credible. Predictions were at least as good as those obtained by diagnostic models when real-time meteorological data were available, and they were far better than diagnostic models when wind data were not available.

There are several difficulties in applying complex numerical models to regulatory purposes: heavy computational requirements, the necessity of a knowledgeable user, and the absence of verification data. Nonetheless, Leone and Yamada both agree that hazard analysis should move toward the "best science" techniques. Regulatory models have tended to emphasize

TABLE 5 SUMMARY OF ADVANTAGES AND DISADVANTAGES OF VARIOUS MODEL CLASSIFICATIONS

Gaussian Plume Models:

Advantages

1. Programmable on small micro computer systems for very fast execution,
2. A number of scenarios can be quickly run to assist planning,
3. Minimal meteorological data required, and
4. Predicts maximum hourly concentrations well when time and space variations are not critical.

Disadvantages

1. Validations show models do not predict hourly observations at a specific time and location beyond the immediate vicinity of the release,
2. Models cannot track changing meteorological conditions such as lead to fumigation in valley flows,
3. Cannot treat spatial inhomogeneities like wind shear or terrain specific features,
4. Requires an empirical specification of sigmas versus stability and distance, and
5. Does not provide any estimate of variance from predicted values.

Gaussian Puff Models:

Advantages

1. Can be implemented on local minicomputers,
2. Can track changing wind and stability, and
3. Accuracy is limited only by resolution of meteorological data and the scale of the tracked puffs.

(Continued on following page)

Table 5 (Continued)

Disadvantages
1. Requires significant local wind data,
2. Models do not generally treat dispersion augmentation due to wind shear,
3. Requires an empirical specification of sigmas versus stability and distance, and
4. Does not provide any estimate of variance from predicted values.

Phenomenological Models:

Advantages
1. Models are designed to reproduce specifically the dominant features of the identified flow system,
2. Models like VALMET can inherently handle complicated temporal variations of valley flows, and
3. Recent versions of the model can operate on mini size computers.

Disadvantages
1. Models are limited to terrain geometries for which they were created (e.g. VALMET is limited to narrow valleys of simple planform),
2. Models usually cannot handle flow systems beyond their design range (e.g. cross-valley flows, tributary flows, sudden change in terrain shape or direction), and
3. Models will require extensive development to make them more flexible.

Mass Consistent Objective Analysis Models:

Advantages
1. Models can be terrain specific and provide for terrain steering of winds,
2. Models can handle wind shear,
3. Versions of these models can handle stratification, surface roughness and lee wave behavior, and
4. Recent versions of the model can operate on mini or micro computers.

Disadvantages
1. Requires substantial input data to yield accurate results (results are possible with minimal input, but accuracy degrades),
2. Turbulent diffusion parameters such as sigmas must be determined separately,
3. Models cannot handle flow separation or strong drainage flows, and
4. Does not provide any estimate of variance from predicted values.

Depth Integrated Models:

Advantages
1. Grid reduction by depth integration increases substantially the computer space available for horizontal domain size or horizontal resolution; hence, large domains can be examined on mini or micro size computers, and
2. Models have been extensively validated against oceanographic and atmospheric flows as well as heavy gas spills.

Disadvantages
1. Models cannot handle flow separation, strong vertical shear, or recirculation situations, and
2. Models are effectively limited to situations where inversions or other boundaries cap the layer being examined.

Linear or Perturbation Models:

Advantages
1. Models can be terrain specific and provide for terrain steering of winds,
2. Models can provide almost infinite resolution over the domain chosen,
3. Models can adjust for atmospheric stratification, wind shear, and inhomogeneities in surface roughness, and
4. Models can operate on mini or micro computers.

Disadvantages
1. Requires substantial input data to yield accurate results (results are possible with minimal input, but accuracy degrades),
2. Turbulent diffusion parameters such as sigmas must be determined separately,
3. Models cannot handle flow separation or strong drainage flows, and
4. Models do not provide any estimate of variance from predicted values.

Primitive Equation Models:

Advantages
1. Models can provide simulations of almost all meteorological variables,
2. Models contain all the necessary physics to predict wind shear, flow separation, secondary flows, etc., and
3. Models can be structured to take advantage of almost all of available data in providing a best-guess simulation.

Disadvantages
1. Models require very large computing resources,
2. Further development work will be required to reduce response time and make input and output modules user friendly,
3. Boundary condition data may often be difficult to obtain,
4. Some tests suggest many models contain large numerical pseudo-viscosity which distorts the predictions, and
5. Many of these models are still not very well validated.

"user friendliness" and simplicity, but super-computer capacity workstations, the use of precalculated wind fields, the availability of new computer graphic enhancements, and expert system methodologies may provide similar flexibility for the more calculationally intense methods.

Hosker noted that the continued use of simple regulatory models can be defended only if the models can be shown to be "conservative" for the site and phenomena of interest. This kind of conservatism may be so severe as to put an unwarranted economic burden on local facilities under many other conditions. Simple models generally have the advantage of requiring only very limited amounts of local meteorological data; but on the other hand, limited data probably gives a limited picture of the local flow and turbulence characteristics, especially in complex flow situations. Even the costs of data collection have dropped dramatically. So most of the traditional obstacles to the use of complex models seem to be disappearing.

Numerical Codes for Building Complex Flows

Numerical prediction of the transport of hazardous gases in about buildings or in the midst of an industrial complex is in its infancy. Research by Murakami et al. [*12*] recently evaluated the limitations of various turbulence models when predicting flow around simple cubical buildings. Calculations have compared predictions by κ-e, algebraic stress (ASM) and large-eddy simulation (LES) models with wind tunnel measurements. ASM and LES models appear to reproduce laboratory measurements of streamline location, separation, reattachment, and turbulence magnitudes.

Currently there is no operational numerical model to predict diffusion around buildings suitable for regulatory purposes. The primary constraint seems to be the fine computational grid and resultant large memory required to resolve the smaller scales of motion found near building surfaces. Leone observed that the continued development of massively-parallel computers will allow a significant increase in model resolution, improved representation of flow physics, and real-time modeling of some emergency response situations.

The panel felt that it would be timely now for research to focus on the:

- Development of the ability to incorporate the variability of individual plume realizations into prediction techniques,
- Extension of spectral models for complex terrain flows to include plume behavior over steeper terrain and broader stratification conditions,
- Incorporation of cloud induced motions into 3-D numerical models,
- Development of realistic "clock-time" models to apply to hazard response situations in complex environments, and
- Incorporation of the capabilities of the new massively-parallel computers into future prediction schemes.

Physical Modeling of Dispersion in Complex Flow Fields

There is a tendency for mathematical modelers to look askance at fluid models. They tend to think that wind-tunnel modeling is some kind of toy that does not match reality. It is true that not all processes that occur in the atmosphere can be simulated in the laboratory, but, on the other hand, there are a number of phenomena that are handled *much better* in the wind tunnel than in mathematical models—a fine example is the separated, recirculating wake on the downwind side of a building. To paraphrase Corrsin, a wind tunnel is, in effect, an analog computer and, compared with digital computers (numerical models), it has the advantage of "near-infinitesimal" resolution and "near-infinite" memory. If a mathematical model cannot simulate the results of an idealized and well-controlled laboratory experiment, how can it possibly be applicable to the atmosphere. A *well-designed* and *carefully executed* fluid modeling study will yield valid and useful information—information that can be applied to real environmental problems—with just as much and generally more credibility than any current mathematical models.

The similarity constraints and limitations of laboratory modeling for wind engineering problems is described by Snyder [*20*], Meroney [*3*] and Plate [*19*]. Special information related to the simulation of dense gas clouds is provided by Meroney [*17*], and a review of physical model experience for complex terrain flows is summarized by Meroney (1990b).

The panel recommends research which will:

- Develop a hybrid methodology to routinely combine fluid and numerical model information to extend hazard predictions in complex environments, and
- Develop a routine fluid modeling ability to simulate stratified flows for hazard analysis.

Modeling Tools and Operational Strategies Needed to Predict Accident Consequences

Pragmatically better hazard predictability is useful only if it can result in better strategies to avoid or mitigate hazardous material release situations. Similarly new computational models are acceptable in a regulatory environment only if they are harmonious with existing field-data collection systems, are verifiable over the range of purported applicability, and consistently result in regulatory decisions which conservatively protect the public. Hence, a specialized model that better represents dispersion physics in complex flows will generally not be approved by permitting agencies without extensive and expensive testing. What is then the best way to protect the public, while not unduly burdening economic development?

The panel and audience were not able to conclusively resolve the above dilemma; however, it was proposed that research should begin to:

- Develop a feedback between predicted dispersion behavior and plant operation strategies to control source releases and mitigate impacts,
- Develop methods to combine short-term weather prediction with hazard prediction schemes, and
- Develop a methodology to extrapolate field and laboratory data measured in non-typical flat Nevada type environments to chemical processing plant sites.

Finally, a variety of proposals was made to improve numerical and fluid modeling tools which would enhance the ability to predict consequences of accidents. It was proposed that research begin on methods to:

- Incorporate real time remote sensing data (satellites, lidar, profilers) into predictive models,
- Develop methods to incorporate weather forecast model information into predictive models,
- Recast dispersion problems in complex terrain as variational problems which permit routine updating as information flows during a hazard event,
- Use topology methods to identify important or dominant input to hazard events during modeling,
- Develop image capture, graphic imaging and "speckle" velocimetry methods in fluid modeling to improve understanding of 3-D fields of motion and resultant concentrations in complex environments,
- Incorporate data visualization and display methods into the presentation of numerical and fluid modeling results to enhance the value and understanding of predictions,
- Develop an expert system framework for the interaction of complex environments with hazard incidents, and
- Use sensitivity analysis, chaos techniques or bifurcation arguments to determine sensitivity of release scenarios to uncertainties in initial conditions and bounding conditions.

Conclusions

In summary the workshop discussions ranged over a wide range of topics related to the release of hazardous materials in "complex" environments associated with the built-up region which may surround a release site. The panel members concluded that significant progress has been made in understanding such flows. The potentials for improved hazard prediction through the use of numerical and fluid modeling are bright. The integration of prediction techniques into plant safety operational strategies should significantly decrease the impact of routine or inadvertent releases of hazardous materials.

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Panel of Experts

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