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Monterey, California

An Evaluation of Diagnostic Atmosphereic Dispersion Models for "Cold Spill" Applications at Vandenberg Air Force Base, California

by
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Six diagnostic atmosphereic dispersion modeling groups: NUATMOS/CITPUFF, CALMET/CALPUFF PGEMS, WOCSS/MACHWIND/Adaptive plume, and LINCOM/RIMPUFF/HEAVYPUFF are evaluated for use in specifying toxic hazard corridors for rocket propellent and oxidizer "cold spills" at Vandenberg AFB. Other models are also considered briefly. Physical assumptions, speed, cost, availability, ease of use, compatibility with existing risk assessment systems, validation, data requirements, and Vandenberg suitability are discussed. Underlying physical basis and modeling technique are emphasized. Dispersion models consist of separable windflow and dispersion sub-models. A MACHWIND/LINCOM windflow tandem with ADPIC, RIMPUFF, or CALPUFF diffusion may provide the most robust diagnostic modeling suite. A cost/benefit analysis of computer hardware and modeling accuracy is given.

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INTRODUCTION

Because it is the west coast satellite launch center for DOD, Vandenberg AFB supports on-going improvement of atmospheric dispersion models used in risk assessment for potential "hot" and "cold spills" of stored rocket propellents and oxidizers or those in transport or transfer around the active launch sites.

Potential "hot spill" assessments are now treated with the REED-M model. "Cold spills" use the Ocean Breeze/Dry Gulch model (to be replaced by the AFTOX Gaussian plume model). More defensible "hot" and "cold spill" models have been mandated for emergency response, normal launch, and routine venting purposes. Thus, together with the other ranges, Edwards AFB and Cape Canaveral, Vandenberg is actively considering a number of diagnostic (time invariant) and prognostic (time varying) models for on-base operational use.

The creation of timely, accurate predictions using prognostic models strains the limits of existing computers. So the Vandenberg risk assessment community has deemed diagnostic model upgrading the initial priority. As available computer power increases, the focus will shift to selecting and tailoring improved prognostic models.

Within this two-tiered approach, step one is to evaluate end user needs at the Vandenberg launch pads and storage facilities. This was done by survey, with input from other test ranges. Next was preliminary survey of all available existing dispersion models. Twelve candidate models were discussed at the USAF Toxic Release Advisory Group semi-annual meeting. Further assessment narrowed the group to the following serious contenders: NUATMOS/CITPUFF, CALMET/CALPUFF, PGEMS, WOCSS/MACHWIND/Adaptive plume, LINCOM/RIMPUFF/HEAVYPUFF, MATHEW/ADPIC. The following evaluates these six diagnostic atmospheric dispersion modeling groups on the basis of technical merit and suitability for the Vandenberg environment. This is being pursued as part of Phase I of the diagnostic model evaluation, testing, validation, and installation effort.

We attempt here to recommend an optimal modeling grouping, preliminary to detailed code testing, operational simulation, and the validation and installation phases.

We begin with lists of important modeling issues and models, specific model features, Vandenberg requirements, and figures assessing the current cost and availability of dispersion modeling resolution and computer hardware. We then assess the degree of fulfillment of Vandenberg requirements and modeling issues on the basis of available documentation. The format consists of a narrative description and evaluation of six modeling groups and summary. The appended reference list is lengthy, but includes much of the standard literature considered useful in assessing the current state of atmospheric dispersion modeling.

MODEL ISSUES

1. Cost and Ease of Procurement and Use, Life-Cycle Utility

   a. Site license availability
   b. Right to modify
   c. Technical support
   d. Right to upgrades
   e. Total hardware/software cost including transition costs from current system
   f. Estimated time and effort for validation
   g. Time to operational status
      i. Current model readiness
      ii. Effort/benefit analysis
   h. Estimated training time and user salary
   i. Estimated time to obsolescence

2. Military, Regulatory, and Legal Requirements

   a. Military mandates
   b. Beyond Base regional/state/federal regulatory requirements
   c. Legal defensibility

4. Input Data Requirements, adequacy of current measurements

   a. Towers
   b. Sodar
   c. Rawinsonde
   d. Radar
   e. Buoy
   f. Radiation/Cloud cover
   g. Soil parameters
   h. Variable/homogeneous initialization

5. Domain issues

   a. Domain size
   b. Grid spacing
   c. Domain type constraints: hills, land/water, buildings
   d. Surface, Lateral, and Top Boundary conditions

6. Windflow Model

   a. Initialization procedures and objective analysis
   b. Stable/Neutral/Unstable Physics
      i. Turbulence closure order
      ii. Moisture treatment
      iii. Boundary layer parametrizations
   c. Grid solver, e.g. finite difference/element/spectral

7. Diffusion Model

   a. Source parameters
   b. Chemistry
   c. Type of physics, e.g., Gaussian plume, puff, particle
   d. Stable/Neutral/Unstable Physics
   e. Dense/Neutral/Buoyant gas treatment
   f. Numerical solution procedures

8. Fire and Explosion Model

9. Risk Assessment Model

10. Total system issues
    a. Comprehensiveness
    b. Internal consistency, module sophistication balance
    c. Modularity/Upgradability
    d. Portability

MAJOR MODELS EVALUATED

1. **CALMET/CALPUFF**

   Sigma Research (J.S. Scire, D.G. Strimaitis, R.J. Yamartino)
   for California Air Resources Board regional air quality

2. **PGEMS**

   Battelle Northwest Laboratory (K.J. Allwine, C.D. Whiteman, V. Ramsdell)
   for Pacific Gas and Electric Co. at Diablo Canyon Nuclear Power Plant

3. **NUATMOS/CITPUFF**

   USDA (D.G. Ross, D.G. Fox)
   for U.S. Environmental Protection Agency

4. **WOCSS/Adaptive Plume**

   SRI Int. (F.L. Ludwig, Roy Endlich)
   for SRI Int.

5. **MACHWIND**
   U.S. Army Atmospheric Sciences Laboratory (R. Meyers)

6. **LINCOM/RIMPUFF/HEAVYPUFF**

   RISO National Laboratory/Naval Postgraduate School
   (I. Troen, G. Lai, T. Mikkelsen, M. Nielsen)
   for USAF Space and Missile Systems Center Vandenberg AFB
   THC dispersion model

7. **MATHEW/ADPIC**

   Lawrence Livermore Laboratory (M. Dickerson, R. Lange, D. Ermak)

MODEL SYSTEM CHECKLIST:

MODELS:	CALMET/ CALPUFF	PGEMS/	WOCSS/ MACHWIND/ Adaptive	LINCOM/ RIMPUFF/ HEAVYPUFF	NUATMOS/ CITPUFF	MATHEW/ ADPIC
1. Procurement and Use						
a. Site license	+	?	+	+	?	+
b. Right to modify	+	?	+	+	?	?
c. modularity	+	?	+	+	?	+
d. Technical support	?	?	+	+	?	+
e. Right to upgrades	+	?	+	+	+	+
f. hard/software cost including transition from current system	low	low?	low	low	low	?
g. validation time/cost	?	?	?	low	?	?
h. Time to operation	?	?	?	short	?	?
i. training time/cost	?	?	?	?	?	?
j. time to obsolescence	long	short	mid?	long	?	-/+
3. Hard/Software issues						
a. hardware demands	high	low	mid	low	?	mid?
b. hardware obsolescence	low	low	low	low	?	low
c. Computer language	Fortran	Fortran	Fortran	Fortran	?	Fortran
d. portability,	+	+	+	+	?	+
e. programming ease	?	?	+	+	?	?
f. GUI	-	+	-	+	-	+
g. I/O constraints	?	?	-	?	?	?
h. Run time adequacy	-/+	+/?	+/?	+/+	?/+	+
windflow	~5min/hr at 15mips 5km grid	~2 min at 15mips 500m grid	~3min at 15mips 500m grid	<30sec at 15mips 500m grid		<1 minute 40 mips same grid
dispersion	~40sec/hr for same	?	~1min/hr for same?	~1 min/hr for same		<1 minute 40 mips
i. planned operations	+	+	+	+	+	+
j. emergency response	-	+	+	+	?	+
4. Input Data						
format						
NCDC TD3240 precip	opt	-	-	-	-	-
free-form precip	opt	opt	-	opt	-	?

CD144 surface obs	opt	-	-	-	-	-
free-form surface obs	opt	opt	opt	opt	?	-
fill-in missing	opt	-	-	-	-	-
TD5600 upper air	opt	-	-	-	-	-
TD6201 upper air	opt	-	-	-	-	-
non-standard sounding	opt	opt	opt	opt	opt	opt
upper air extrapolate	-	-	-	-	-	-
a. Surface Hourly obs	req	req	req	req	req	req
WS	req	req	req	req	req	req
WD	req	req	req	req	req	req
Temp.	req	?	req	req	req	-
Stability category	-	req	-	req	req	req
lapse rate category	-	req	-	-	-	-
CC	req	opt	opt	opt	-	-
Ceiling height	req	-	-	-	-	-
Surface pressure	req	req	req	-	-	-
relative humidity	req	opt	-	-	-	-
precip type rate	opt	-	-	opt	-	-
precip type code	opt	req	-	opt	-	-
Solar	-	-	opt	opt	-	-
Longwave	-	-	opt	opt	-	-
a. Towers	opt	opt	opt	req	req	req
b. Sodar	opt	opt	opt	opt	?	opt
Radar	opt	opt	opt	opt	?	opt
Upper Air						
WS	req	opt	opt	opt	req	opt
WD	req	opt	opt	opt	req	opt
temperature	req	opt	req	opt	req	-
pressure	-	-	opt	-	-	-
pressure tendency	-	-	opt	-	-	-
elevation	req	opt	opt	opt	?	opt
NWS upper air	opt	opt	opt	-	-	-
Zi		req	-	req	?	req
e. Overwater bucy						
Air/sea δT	opt	opt	-	-	-	-
Marine air T	opt	opt	req	-	-	-
Marine air R.H.	opt	opt	-	-	-	-
Marine BL height	opt	opt	-	-	-	opt
shipboard obs	opt	opt	opt	opt	-	opt

h. Gridded geophysical						
terrain MSL " resolution	req	req	req	req	req	req
sub-grid terrain features	opt	opt	-	-	-	-
receptor coords	req	req	req	req	req	req
gridded land use	req	req	opt?	-	-	-
z0	opt	req	opt?	req	-	req
albedo	opt	-	opt?	opt	-	-
Bowen ratio	req	-	-	-	-	-
soil heat flux	opt	-	-	-	-	-
anthro heat flux	opt	-	-	-	-	-
veg leaf area index	opt	-	-	-	-	-
5. Domain issues						
a. 50x50km	+	+	+	+	?	+
b. 500m Grid spacing	-	-	+	+	?	+
c. max grid elements	?	50x50x9	?x10	120x120x5	?	?
c. Surface boundary	energy balance	profile	energy bal	energy bal	-	profile
d. Lateral boundary	open	open	open	periodic	open	closed?
e. Top boundary	w=0, opt	rigid lid	rigid lid	w=0	open	rigid lid
f. grid type	terrain //	terrain //	curvilinear	terrain //	terrain //	rectangular
g. coordinates		UTM & lat/long	UTM	UTM	?	UTM
Source						
Strength	input req	input req	input req	input req	input req	input req
Chemistry	air quality	none	none	none	none	none
Release types						
surface point	+	+	+	+	+	+
elevated point	+	+	+	+	+	+
area	+	?	+	+	?	+
Data input						
Consistency checks	+	?	-	-	?	+
Met data extractor	+	+	+	+	?	+
precip data	+	+	-	opt	-	+
Objective analysis	-	+	+	+	?	+
smoothing	-	-	-	-	-	-
Windflow						
diagnostic						
slope flow	+	-	-	-	-	-
seabreeze	-	-	-	-	-	-

return flow	-	-	-	-	-	-
kinematic terrain	$V\cdot\nabla h\ e^{-kz}$	-	-	$U_0(1+(h/L)e^{-z/L}-e^{-k2/\ell})$	-	
terrain blocking	Froude	-	Froude	-	$V=f(\alpha)$	-
micromet	+	-	+	+	?	+
overland	energy balance	-	energy bal	energy bal	-	profile
overwater	profile	-	-	-	-	
	$u_*=uC_{dn}$ $z_0 = 2E-6u^{2.5}$			$u_*=uC_{dn}$ $z_0=10e^{(-12.6/\sqrt{(1+0.07U)})}$	-	
BL height	Carson, Venkatram	data	-	data	-	data
moisture	for CSUMM	-	-	-	-	-
clouds	" "	-	-	obs	-	-
Domain mean wind	upper air interp & CSUMM(old RAMS)	-	-	obj analysis	?	-
w =	$V\cdot\nabla h\ e^{-kz}$ and	-	$V\cdot\nabla h$	$V\cdot\nabla h$	$\nabla\cdot U_i=0$	$\nabla\cdot U_i=0$
wl =	$w-u\partial h/\partial x - v\partial h/\partial y$	-	-	-		
or opt	$w=w_1-(z/z_{top})w_{1,top}$					
Temperature	adiabatic to zi, $1/r^2$ profile above	-	profile req	similarity	profile	-
Objective analysis	refined $1/r^2$	$1/r^2$	$1/r^n$	modified $1/R^2$ $R=(a+(b-a)\lvert\sin\phi\rvert)r$	?	-
smoothing	opt	-	-	-	-	-
divergence minimize	$u_{adj}=u-Div\Delta x/2$ $\partial u_i/\partial x_i < \epsilon$	$\nabla\cdot U_i < \epsilon$ consistent	$\nabla\cdot U_i < \epsilon$	$\nabla\cdot U_i < \epsilon$	$\nabla\cdot U_i < \epsilon$	$\nabla\cdot U_i < \epsilon$
prognostic	CSUMM w/ $1/r^2$	-	-	-	-	-
Turbulence closure	1st order	-	-	1st order	-	-
vertical velocity	H	-	-	-	-	-
seabreeze	+	-	-	-	-	-
slope-valley	+	-	-	-	-	-
differential heating	+	-	-	-	-	-
complex terrain	+	-	-	-	-	-
Moisture	+	-	-	-	-	-
Grid solver	finite diff	-	-	spectral	?	-
Diffusion						
Chemical removal	NA	+	-	-	-	-
Photochemistry	CALGRID	-	-	-	-	-
horizontal advection	+	-	-	-	-	-
vertical advection	+	-	-	-	-	-
dry deposition	+	+	-	+	?	+
gases & particulates	+	+	-	-	?	+

diurnal cycle	+	?	-	-	?	-
space/time varying	+	+	-	+	?	-
fumigation	+	-	-	-	?	-
Elevated inversion	+	+	+	+	+	+
Wet deposition	+	+	-	+	?	+
scavenging coefficient	+	+	-	+	?	+
precip dependent	+	+	-	+	?	+
Complex terrain	+	+	+	+	+	+
dividing streamline	+	+	+	-	+	-
Building wakes	+	+	-	-	?	-
Overwater transport	+	-	-	-	?	-
Coastal interaction	+	-	-	-	?	-
Dispersion coefficients						
direct measurement	horiz	horiz	-	horiz	-	-
similarity	opt	-	-	-	-	+
Pasquill-Gifford	rural	-	+	vert	+	vert
Briggs	urban	+	-	-	+	-
Plume rise	+	+	+	+	+	+
basic Briggs eqns	+	+	+	+	+	+
stable stratification	+	+	+	+	+	+
partial penetration	+	-	+	-	?	-
vertical shear above stack	+	-	-	-	?	-
momentum & buoyant rise	+	-	+	+	+	+
increased lateral spread due to vertical shear	+	-	+	+	?	+
building downwash	+	+	-	-	?	-
explosive cloud rise	-	-	-	-	-	+
Type						
Gaussian plume	-	-	-	-	-	-
Gaussian puff	CALPUFF	MESOI	Adaptive	RIMPUFF	CITPUFF	-
near-field deformation	+	-	+	-	-	-
integrated puff	+	+	+	+	+	-
puff splitting	+	+	-	+	-	-
time/space filtered σ	-	-	-	+	-	-
Lagrangian particle	+	-	-	-	-	+
Postprocess met display	+	+	+	+	?	+
Postprocess diffusion display	+	+	+	+	?	+
Fire/explosion	-	-	-	-	-	+
blast overpressure	-	-	-	-	-	-
fireball	-	-	-	-	-	+
Back calculate source	-	-	-	-	-	-
Risk assessment	-	-	-	-	-	-

VANDENBERG AFB SPECIFIC REQUIREMENTS

MANDATORY REQUIREMENTS:	CALMET/ CALPUFF	PGEMS	WOCSS/ Adaptive/ MACHWIND	LINCOM/ RIMPUFF/ HEAVYPUF	NUATMOS CITPUFF	MATHEW/ ADPIC
a. Treats complex terrain	3	3	3	3	3	3
b. Gives surface footprints	3	3	3	3	3	3
c. Includes all met data	3	3	3	3	?	3
d. Handles 50x50km domain	3	3	3	3	?	3
e. Modeled winds near measured	3	3	3	3	?	3
f. Handles gas/liq puff/plumes	0	0	0	1	0	1
g. " surface/elevated sources	3	3	3	3	3	3
h. " spills by weight, volume, wetted area, & flow rate	0	0	0	0	0	0
i. " dense gas & VBG chemistry	0	0	0	1	0	2
j. " on-line data & gives THCs	3	3	3	3	0	3
k. " multiple THCs	3	3	0	3	?	3
l. Outputs THCs w/i 5 min.	0	3	3	3	?	3
m. Allows user overrides in GUI	0	1.5	0	3	?	3
SIGNIFICANT REQUIREMENTS:						
a. Adequate grid resolution	0	0	2	2	?	2
b. Treats variable Zi	2	2	2	1	?	1
c. " all PGFs & stagnation	2	2	2	1	2	1
d. " wet and dry deposition	2	2	0	2	?	2
e. Graphical & tabular output	2	2	2	2	?	2
f. Multi-level output	2	2	2	2	2	2
g. Treats vector shear	2	2	2	2	?	2
h. Source code, docs available	2	2	2	2	?	2
i. Site license & mod rights	2	2	2	2	?	1
DESIRED REQUIREMENTS:						
a. Modular code	1	1	1	1	?	1
b. MARSS compatible	1	1	1	1	1	1
c. Flexible chem module	1	0.5	0	0	0	0
d. Treats coastline & cloud/ clear interfaces	0	0	0	0	?	0
e. Operates w/i current MARSS	0	0	0	0	0	0
f. building wake effects	1	1	0	0	0	0
Total score	**44**	**48**	**42**	**50**	**?**	**50**

out of 63 **possible points**

CAVEAT: Detailed decisions compel hard thinking which cannot be distilled into a simple score. That the above scores are mainly congruent with our basic impressions is largely fortuitous. From the above comparison (allowing up to 3 points for mandatory features, 2 for significant, and 1 for desirable, and fractional scores for partial fulfillment), it seems that LINCOM/RIMPUFF and MATHEW/ADPIC display the most elements desired for a Vandenberg atmospheric dispersion model. Actually, since windflow and diffusion are usually separable, a combination of LINCOM, MACHWIND, and ADPIC, or either RIMPUFF or CALPUFF may be the optimal overall choice, if obtainable. For our specific reasons, see the following text. We also do not feel that PGEMS comes as close to the top models as is indicated by its score.

COMMENTS ON FIGURES

The following figures are intended to illustrate the cost of increasing grid resolution for dispersion models in terms of computer hardware as projected for calendar year, 1993. Figure 1 compares the cost of state-of-the-art representative PCs, workstations, mainframes, and supercomputers against their computational speed, measured in units of (MFLOPS) one million floating point (real number) instructions per second. Four points may be made. 1) The sample older installed systems at Vandenberg are less cost effective by one to two orders of magnitude than state-of-the-art systems. 2) The speed/cost ratio increases by perhaps an order of magnitude as modern systems get smaller, due to simplifications in job control scheduling, peripherals designed for smaller numbers of users, and efficiencies of production scale. 3) Workstation and PC systems are about to drop below $1,000 per MFLOP. 4) The ultimate potential of massively parallel systems exceeds other approaches, but current combinations such as Intel's 128 i860 CPUs have not broken away yet from the overall curve, nor are they yet as fast on real world problems as older vector supercomputer designs such as the CRAY C-90. This may be due to immaturity in hard/software systems and compiler design, as well as inadequate communications bandwidths between processors.

Figure 2 illustrates the effects of computer speed on allowed model resolution for sample operational diagnostic and prognostic dispersion models, as well as a sample research grade large eddy simulation (LES) windflow model. We see that 1) Diagnostic models require less computer power than prognostic ones, while LES models are very computer intensive. 2) The speed/resolution slope is steeper for prognostic models because for prognostic models greater spatial resolution also requires greater time resolution, while diagnostic models disregard time variations entirely.

Figure 3 combines figs. 1 and 2 to suggest the hardware cost of resolution for the same sample models. Diagnostic models can or at least should run effectively on systems in the one to ten megaflop speed range. This means that efficient operationally oriented diagnostics models should be able to run effectively on workstations priced at $10,000 to $60,000 and available now; while for the forseeable future LES models will still require the resources of vector or massively parallel supercomputers above the $1,000,000 price point and will remain research tools. This suggests that emergency response systems no longer need to depend on tenuous linkages with remote supercomputers. A second point can be illustrated in more detail by inspecting the computational configuration ASTeR has suggested for operational use of RAMS at Cape Canaveral (Lyons, et al., 1992)

GRID NO.	X		Y		Z	ΔX(km)	TIME STEP(sec)	GRID PTS
1	38	x	38	x	25	60	90	36,100
2	34	x	38	x	25	15	30	32,300
3	37	x	37	x	18	3	12	24,600
							TOTAL	93,000

Since the spatial nesting ratios are already quite strained within this configuration, running such a model at 500 meter resolution over Vandenberg might require more than one additional level of grid nesting. To account for local vertical accelerations in terrain, at least the inner two grids must operate non-hydrostatically, perhaps with second order turbulence closures, while the inner grid uses a 2 - 3 second time step. Such modifications would require more than an order of magnitude more computer power than is now available on workstations. The cost of computing power has dropped by about a factor of two every two years for the past decade. So it seems for Vandenberg that operational fine scale prognostic modeling on workstations may be some years away. Massively parallel systems may eventually accelerate computer power gains, but the timing does not seem near term and beyond that is difficult to gauge.

In the interim and perhaps beyond it, there exists a niche for fine scale diagnostic models. In fact a hybrid solution consisting of a prognostic model which supplies coarse resolution mean winds to a fine scale diagnostic model is quite defensible and could be tuned to run in seconds. Such a hybrid could conceivably supply 250 meter resolution winds based on currently available hardware. As available computer power increases, the resolution of such a hybrid may fall to the 100 meter level where some believe the point of diminishing returns begins.

COMPUTER COST vs SPEED (1993 $)

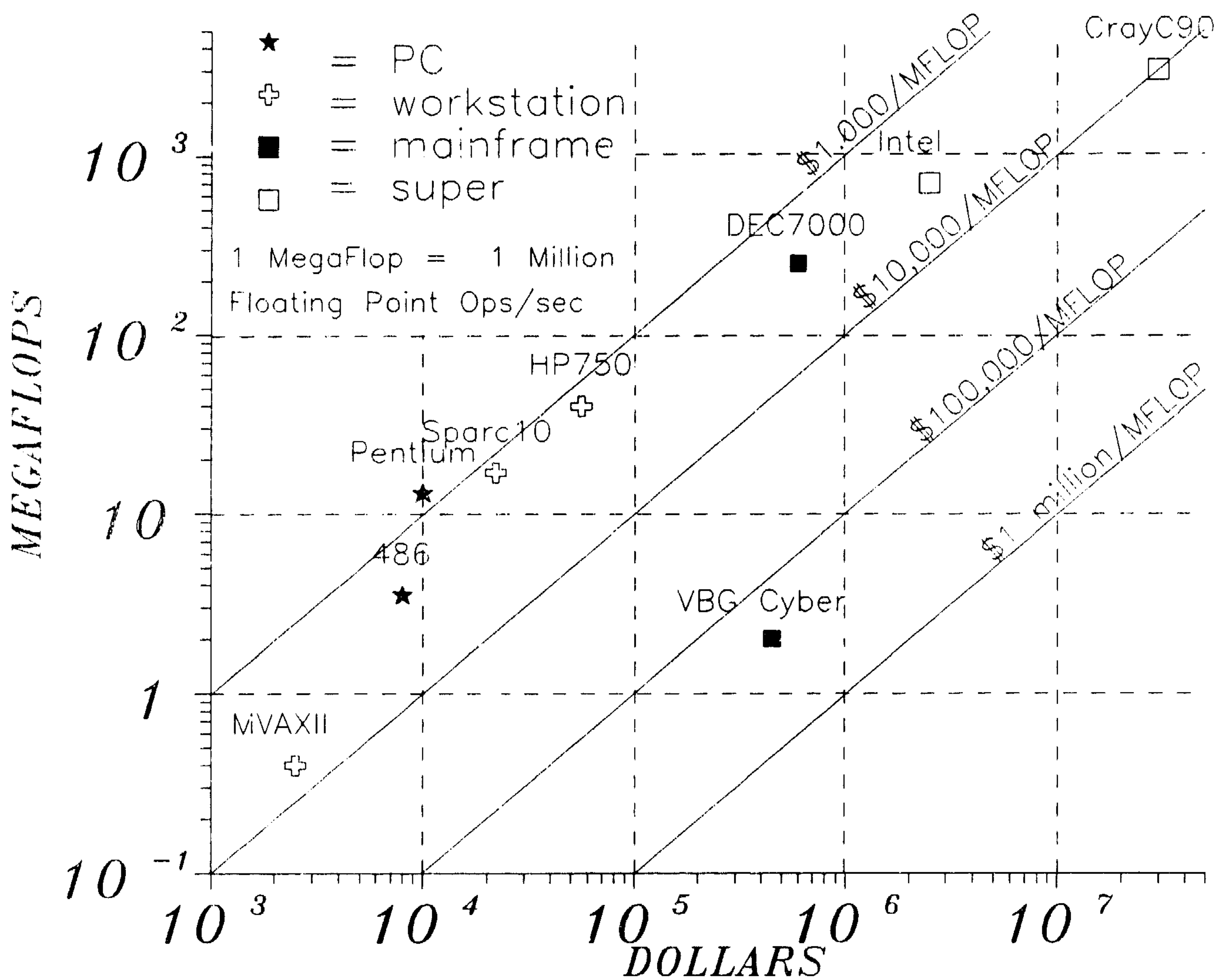

FIG. 1

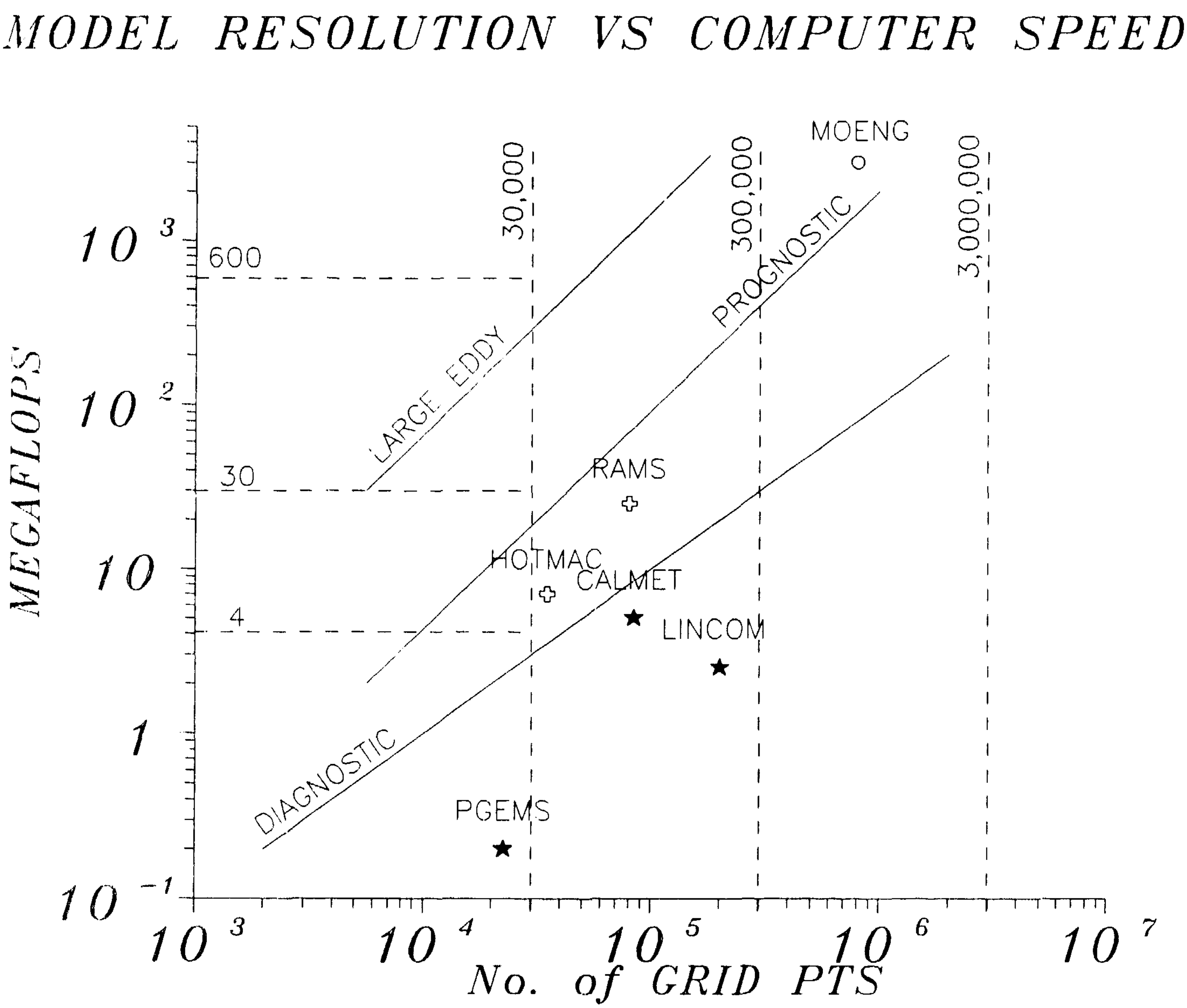
MODEL RESOLUTION VS COMPUTER SPEED
MEGAFLOPS
No. of GRID PTS
10^{-1}
1
10
10^2
10^3
10^3
10^4
10^5
10^6
10^7
600
30
4
30,000
300,000
3,000,000
LARGE EDDY
PROGNOSTIC
DIAGNOSTIC
MOENG
RAMS
HOTMAC
CALMET
LINCOM
PGEMS

FIG. 2

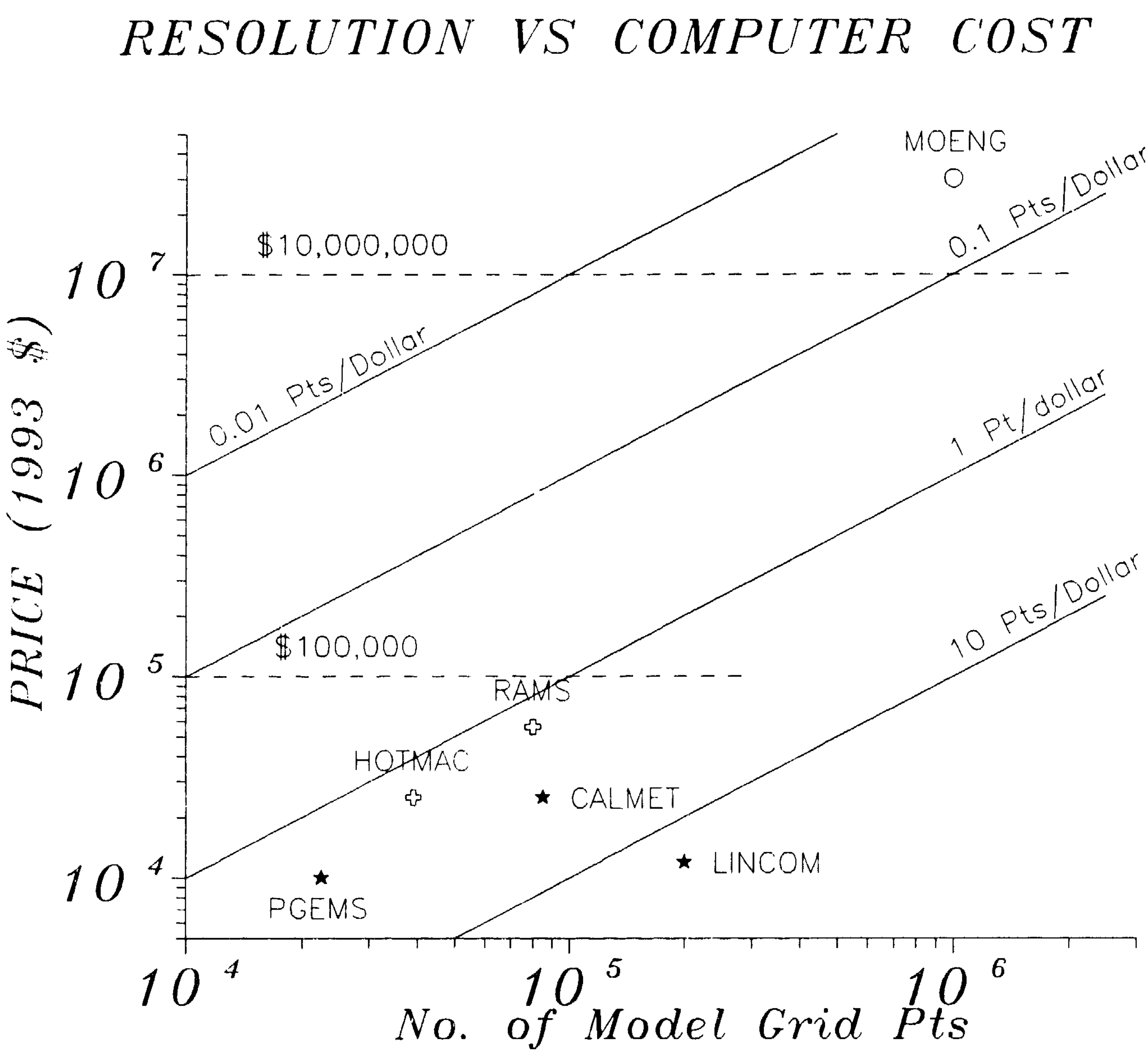
RESOLUTION VS COMPUTER COST
PRICE (1993 $)
No. of Model Grid Pts
$10,000,000
$100,000
0.01 Pts/Dollar
0.1 Pts/Dollar
1 Pt/dollar
10 Pts/Dollar
MOENG
RAMS
HOTMAC
CALMET
LINCOM
PGEMS
10 7
10 6
10 5
10 4
10 4
10 5
10 6

FIG. 3

Note that the immediately following CALMET/CALPUFF review based on the user's manuals #AO25-1,2 and personal communications with the Calif. Air Resources Board and University of Calif. at Davis is lengthier than reviews of some of the other models. If the critique seems more detailed, it is often because the comments also apply to many of the other models and diagnostic models in general.

CALMET/CALPUFF (J.S. Scire, et al.):

INTRO:

CALMET/CALPUFF combines either a diagnostic or prognostic wind flow model with fairly sophisticated puff dispersion. The output is now tabular, but UC Davis is under contract with the California Air Resources Board (CARB) to evaluate CALMET/CALPUFF and apparently also provide an output format using NCAR graphics. A full graphical user interface is not planned. A DEC VMS version of the Fortran code exists and CALMET/CALPUFF has been run on a MicroVax II, as well as DEC 3000/200 and 5000/200 Stations, so MARSS compatibility is probably not an issue. CALMET/CALPUFF has a limited number of user override options.

INPUT:

In its current form CALMET proceeds from domain average winds which can be specified from a sounding. It also uses surface tower data, and a single domain-wide vertically averaged temperature lapse rate. CALMET evaluations in progress at UC Davis indicate that the model needs to be altered to accept conditions where data is missing or when the available sounding does not reach the specified top of the domain (default 1200 meters).

PHYSICS:

CALMET computes step 1 and step 2 wind fields with step 1 having options, a or b. In option a, the time interpolated sounding or user specified domain average wind is adjusted empirically for terrain effects due to kinematics, slope flow, and blocking. The blocking occurs according to a critical streamline height (CSH) defined by a local Froude number criterion, $Fr \equiv U/N\Delta h < 1$, (See WOCSS review for more detail). Here U is local wind speed, Δh is the difference between local terrain height and the highest height within the local area. The Brunt-Vaisala frequency is defined as, $N \equiv [(g/\theta)(\partial\theta/\partial z)]^{1/2}$, where g is gravitational acceleration and $\theta \equiv T(p_0/p)^{R/C_p}$ is potential temperature. p and p_0 are pressure and surface pressure, R is the gas constant and C_p is the heat capacity of air. The significance of the CSH is that below it, flow is thought to diverge tangentially around the hill, while above it flow proceeds over the hill. The Froude criterion can be applied straightforwardly to an isolated hill but may be ambiguous in general complex terrain. The code should be inspected carefully to assure that the Froude concept will apply in a reasonable manner for the possible wind conditions and Vandenberg terrain.

In practice the CSH concept is widely accepted and used in most diagnostic models which operate for stable conditions. It is consistent with the results of laboratory experiments, using a number of hill shapes (Hunt et al. 1988b; Meroney, 1990). The CSH is based on the assumption of a kinetic versus potential energy balance. I.e., an air parcel completely converts kinetic to potential energy in rising to some maximum attainable height indicated by the critical streamline. Though the values calculated for CSH have been consistent with data, the underlying Froude concept is itself **physically suspect**. For one thing it implies a zero windspeed at the CSH, as well as local minimums atop hills; both of these features are contrary to all experimental data. The Froude number criterion ignores the role of horizontal pressure gradients on windspeeds. By considering hydrostatic and Bernoulli constraints on flow in a Lagrangian frame, Smith (1990) has shown that pressure gradients, rather than potential energy, control wind speeds and these gradients vary with hill steepness and aspect ratio. So the success of the Froude criterion may be fortuitous.

Eventually, we would prefer to see models for stable conditions which are consistent with Smith's more physically realistic basis. In particular, Smith has shown through linear approximation that there will be two regions of minimum windspeed, one above the hill top at height, $z \simeq 4.0\ U/N$, and one near the hill surface along the upwind slope. The height, Δh, of the near-surface velocity minimum varies from roughly U/N to $3U/N$, as the hill aspect ratio varies from flow perpendicular to a thin ridge to flow over a two-dimensional hill. For a radially symmetric hill the height estimate is $\Delta h \simeq 1.3U/N$. So for hills which are long and narrow in the flow direction, the height of the near-surface velocity minimum differs greatly from that predicted by the Froude criterion. Since neither of the two velocity minima need equal zero, a CSH is not defined and layer partitioning cannot proceed in such a straight forward manner. Instead, it appears that momentum equations which include pressure gradient forces may also be required to account for the added flow complexities (see LINCOM-T discussion).

Moving on to other issues, in CALMET horizontal divergence is minimized after kinematically adjusting the vertical velocities. In option b another model, usually CSUMM, an old hydrostatic version of CSU RAMS, provides step 1. In step 2 CALMET includes a $1/r^2$ objective analysis and smooths the resulting field. Mass conservation supplies vertical velocity, w, through the standard shallow convection form of the continuity equation, $\partial u_i/\partial x_i = 0$, or if the model top is subsequently forced to the condition, $w = 0$, divergence is minimized once again.

The kinematic and slope flow adjustments seem quick but ad hoc.

The slope flow adjustment requires that the domain mean wind be defined. Studies in the Los Angeles basin suggest that when the domain mean wind is difficult to specify, as is often the case for complex regional scale terrain, CALMET's slope flow and CSH adjustments may indicate wind directions quite opposite those measured; so the step 1 wind field at times does not even resemble the tower winds (CARB and UC Davis, personal communications). However, specifying a domain mean wind is less problematic for smaller domains such as Vandenberg. And the objective analysis included in the step 2 adjustment will re-align the winds with the available tower vectors.

CALMET does use different approaches for surface energy balance, and hence heat flux and stability, depending on overwater or overland conditions. But at the same time, as in all dry diagnostic models, the effect of the land/sea and cloud/clear interfaces is not explicitly addressed in its entirety. The edge of the Pacific coast stratus deck hovers chronically over Vandenberg much of the year. Plume dispersion usually changes dramatically across the edge of stratus decks, due to pressure induced wind accelerations and secondary circulations, sudden jumps in inversion height, and increased turbulence on the sunny side. At the cloud edge the secondary circulation seems to involve vigorous boundary layer scale motions which may lead to much more rapid vertical mixing. This is consistent with the results of the Lompoc Valley Diffusion Experiment (Skupniewicz et al. 1992) which showed essentially complete vertical mixing within the boundary just beyond the stratus edge. Though stability changes which drive the puff model can partly account for some of these effects, the CALMET wind fields are subject to layer-segregated divergence minimization. So the model cannot effectively treat boundary layer scale vertical motions encountered across the stratus edge. Changes across the coastline itself are similar but less dramatic (Skupniewicz et al. 1991b).

With regard to other issues, the assumed exponential decay of vertical velocity in the kinematic adjustment does not account for the effects of the strong low subsidence inversions endemic to Vandenberg. During daytime, these inversions tend to be terrain parallel more than flat, resulting in substantial vertical velocities at the top of as well as within the boundary layer (Kamada et al. 1990a, b and Skupniewicz et al. 1991b). In CALMET vertical velocity does not appear to be readjusted after making the slope flow and blocking adjustments to the horizontal winds. This is mildly puzzling but perhaps peripheral, since the horizontal winds are what are really desired.

CALMET introduces spatio/temporal variability of the inversion height, but the inversion-height-change-with-time estimate (eqn. 2-42) might be revised, since it applies to entrainment-induced rather than subsidence inversions. Vandenberg's typical temperature jumps of 10 - 15°C across the subsidence inversion will make the square root term in eqn. 2-42 imaginary. Perhaps Ψ_I in the denominator should be reinterpreted as the lapse rate within rather than above the inversion zone. Alternatives are considered in Kamada (1988a,b) and Kamada et al. (1989, 1990a,b, 1992a). With regard to eqn. 2-44, Arya's (1982) study of neutral boundary layer inversion height formulae conclude that typical errors are on the order of 50 - 100%. Another possibility is Troen and Mahrt's (1986) single formula which applies to all stabilities. CALMET supplies another ad hoc form, eqn. 2-45, for advective changes. But by now we suspect that a single prognostic inversion height equation which includes heating, subsidence, and advection might be preferable. An example implementation is given in Glendening et al. (1986).

For other particulars, in eqn. 2-11 it is unclear how upslope flow is generated (S > 0), for negative temperature lapse rates near the surface, since this makes the square root imaginary. The surface energy balance is based on Holtslag and van Ulden, (1982) and supplies CALMET's initial surface layer wind and temperature profile. However, the user's guide provides no description for obtaining the required incoming and outgoing long-wave radiation in eqn. 2-29. We assume that this is also taken from Holtslag and van Ulden. More sophisticated radiation schemes are also presented in Kamada and Flocchini (1984a,b and 1986). Long-wave radiation is a strong function of cloud cover. Our own experience with eqn. 2-39 is that it is too crude to be useful in estimating stability for dispersion purposes, sometimes leads to non-convergence in L, the Obukhov length, and requires the coefficient to be tuned for the particular site. As an alternative, we suggest the energy balance method given in Appendix A of Skupniewicz et al. (1992). Also, the Deardorff convective velocity scale in eqn. 2-48 may not apply as well as the shear inclusive velocity scale given in Kamada (1992b) to Vandenberg's usual moderately convective, strongly baroclinic conditions.

RUN-TIME:

We suspect that most of CALMET's rather lengthy time is spent with objective analysis and iterative divergence minimization. We cannot determine from the description whether the divergence minimization is fully three-dimensional (see MATHEW review for equations), or uses the faster pseudo-two-dimensional equation over several flow surfaces, such as in WOCSS and MACHWIND (reviewed below). Apparently run-time is also a strong function of the number of surface stations involved in the analysis (CARB, personal communication, 1992). For a 30x30x5 (4,500 grid point) domain at 4 kilometer resolution using 14 surface stations, UC Davis reports about ten minutes for execution time on a VAX 3200 workstation, a ~12 MIPS machine. Suppose three of the five minutes allotted for THC output is available to compute the windfield. Vandenberg's requirements are for a 50km x 50km domain at 500m resolution with at least four levels (40,000 grid points) incorporating 30 towers and five SODAR. For this configuration we expect emergency response using CALMET to require a 400 MIPS computer (perhaps available in 3 years for under $50K). Currently available workstations priced less than $50K run at speeds of 50 - 120 MIPS and perhaps 5 - 30 MFLOPS (million floating point instructions per second) as fig. 1 indicates. Thus, for now it appears that CALMET/CALPUFF is really a regional air quality model intended for ~200km x 300km domains with a 4 km mesh, rather than a high resolution local scale emergency response model. Some sub-grid scale terrain effects can be included in CALPUFF, rather than CALMET, by modeling sub-grid scale hills as ellipsoids. This may be useful for regional air quality studies, but we question whether, in lieu of 500 meter resolution, this approach is adequate for Vandenberg.

For one thing, 4 km resolution of the coastal interface (either land/sea or cloudy/clear) is probably inadequate. Much of the Vandenberg coastline terrain consists of abrupt bluffs rather than smooth beach; so it is kinematically and mechanically quite disruptive of the near surface flow. The Hypergolic Stockpile and Storage Facility (HSSF) and other potential "cold spill" sites lie within two kilometers of the coastline. For roughly 6 months of the year the seabreeze blows the stratus deck inland, while solar heating burns it back to within a few kilometers of the coast. So for local scale dispersion, these large near-coastal changes probably compel 1 km accuracy in locating the coastal and stratus edge interfaces, as well as paramtrizations specific to the cloud edge. Skupniewicz et al. (1992) describe such a two-zone convective scaling procedure and algorithms for high resolution specification of the cloudy/clear interface from GOES and AVHRR satellite images.

CALPUFF:

INTRO:

CALPUFF seems to be a sophisticated, fairly inclusive, puff model which features multiple puffs and alterations due to building down-wash near the source, transitional plume rise, vertical wind shear and subgrid-scale terrain interactions. It also includes wet and dry deposition, air quality oriented chemistry, overwater transport, coastal interaction, some options for dispersion coefficients, and near-field puff stretching. Puff splitting is also included to allow for wind shear and plume bifurcation in complex terrain.

PHYSICS:

CALPUFF's near-field puff elongation (slug mode) probably accrues large savings in CPU time for commensurate accuracy. That is, for standard puff models small puffs (< 100 meter radius) must be released frequently to maintain near-field accuracy in a time-varying windfield. So to avoid artificial concentration oscillations, the mean distance between puffs at the time of release should not exceed 1.5 puff radii.

CALPUFF has three options for dispersion coefficients: direct measurement of turbulence intensities, similarity expressions, and Pasquill-Gifford stability classes. Obtaining accurate direct measurements of vertical turbulence intensity is unlikely, so CALPUFF's default option is to use similarity based expressions. These are taken from Panofsky (1977), Hicks (1985), Arya (1984), Nieuwstadt (1984), Deardorff (1975), and the empirical interpolation formulae of Scire et al. (1990). Analyzing these options, we note that data under unstable conditions show that plumes from surface releases tend to lift rather quickly above ground in the near-field, leaving ground level concentrations much lower than is indicated by parametrizations using Pasquill-Gifford stability classes A and B (Willis and Deardorff, 1976, 1978; Lamb, 1978, 1979; Nieuwstadt, 1980; and Briggs, 1985, 1986). On the other hand, the congruence between data and Nieuwstadt's similarity expressions for stable cases has been questioned; the alternative scaling by Sorbjan (1989) may be more robust. For unstable to neutral cases, an alternative to empirical interpolation is the Kamada (1992b) scaling which 1) is physically derived and 2) also treats mechanical turbulence due to entrainment, baroclinicity, and surface layer shear.

Another issue is that CALPUFF lacks spectral filtering. Without spectral filtering, a puff model designed for use with a static wind field will over-estimate dispersion, if that wind field is frequently updated. The point is that eddies much larger than the puff dimension will induce meander rather than puff growth. If time-averaged $\sigma_{u,v}$ which include meander are used, then diffusion will be exaggerated. Since THCs must account for plume meander during the dispersion period, spectral filtering is not needed with fixed winds, provided the $\sigma_{u,v}$ averaging times and hazard dispersion periods are about equal. But for CSUMM's time-varying winds or for frequently updated met data, meander must be filtered from the puff model to avoid double counting it in both the windfield and puff. The band width for the required high-pass spectral filtering must also change with individual puff size. Stability and wind direction dependent velocity spectra for Vandenberg were presented for this purpose in Skupniewicz et al. (1989).

An issue already addressed in the CALMET review is that within one grid cell, the transition from marine to continental dispersion rates can be complicated by the presence of both the coastline, as well as cloud/clear interfaces (Skupniewicz et al. 1991b). Since much of south Vandenberg's hilly terrain simply extends into the sea, the coastline discontinuuity is quite disruptive of the near surface flow. Not only is there mean flow acceleration but also augmented turbulence due to large velocity gradients and significant turbulence anisotropy, all initiated ~ 1 - 2 km upwind of the potential release sites. This may occur together with even more dramatic flow disruptions across a stratus edge which often lies at or just beyond the release site. The stability indices and sub-grid procedures in CALPUFF must account to some degree for these features, but again this seems to demand high resolution and specific validation for Vandenberg. Current data is most valuable, so maintenance of tower 057 next to the HSSF and the SODAR and tower at Building 900 is critical for HSSF releases. But bear in mind that the horizontal dispersion coefficients, σ_u and σ_v, obtained from SODARS have been considered unreliable (Neff, 1986).

Again, CALPUFF's CSH algorithm is consistent with theories of stratified flow by Hunt (1978) and Carruthers and Hunt (1990). These have achieved some empirical but not theoretical confirmation (Smith, 1990). Allowance for entrainment and internal boundary layer growth implies that downwind fumigation can be treated. The chemistry model is interesting but not quite relevant, since the pollutants of general air quality concern are different from the propellants and oxidizers used near the launch complexes. Relevant chemistry must be installed in CALPUFF, perhaps from the REED-M and AFTOX chemistry modules. On the other hand, many of the reviewed diffusion models lack any treatment of downwind chemistry. So CALPUFF may have some advantage in this regard.

CALMET/CALPUFF SUMMARY:

Apart from CALPUFF's technical merit in the context of a static wind field, a major strength of CALMET/CALPUFF seems to be that it is a fairly comprehensive, modular, and operational system maintained by an interested public agency, the California Air Resources Board (CARB). The entire code and documentation is available free from EPA electronic bulletin boards or through CARB. and is undergoing an extensive review for regional air quality purposes at the University of California at Davis. Apparently, no site license is required, nor are there any special restrictions on local modification. On-line technical support may be available. However, this issue always awaits de facto confirmation. Since the code is actively supported by a large local agency and widely available, the climate for general acceptance may be good, time to obsolescence relatively long, and life-cycle costs commensurately low. CARB also plans validation studies using its Los Angeles Air Basin (1987) and San Joaquin Valley (1990) tracer data sets (CARB, personal communication). Such studies should be regarded as supplementary to, rather than a substitute for studies specific to Vandenberg, since the domain scale, station densities, and terrain differ enough to effect qualitative as well as quantitative changes in model performance. Suitably tailored for Vandenberg's needs, the cost, time, and training involved in procurement, testing, validation, and operational installation should be similar to that of other models not specifically tailored for the MARSS system. For most models, installation of Vandenberg data bases and appropriate sizing and resolution of the grid is likely to be considerably more time consuming than the relatively minor effort involved in porting a Fortran based model to MARSS.

Compared to an ideal Vandenberg model, chief weaknesses and omissions seem to be near-field dense gas effects, liquid spill source term assessment, CALMET's slow speed, inadequate grid resolution, ad hoc physics, incomplete coastal and cloud/clear interface parametrizations, and lack of Vandenberg tracer validation. In particular CALMET's slowness makes it unsuitable for Vandenberg emergency response. However, for the step 1 CALMET wind field, option b allows substitution with another wind field model. If CALPUFF is chosen, we recommend substituting CALMET with a faster, higher resolution model, such as LINCOM and MACHWIND. If CALPUFF is installed, we also suggest that it be retrofitted to use filtered velocity spectra for its dispersion coefficients. This may be a difficult task requiring fundamental changes to puff model's physical assumptions as well as coding. Perhaps the AFTOX or REED-M source term modules could also be modified for inclusion in CALPUFF or any of the other reviewed models, since they all seem to lack this feature.

PGEMS, MELSAR/MESOI (Allwine, Ramsdell, et al.):

INTRO:

The PGEMS model is slated to become operational at the Diablo Canyon nuclear power plant. The core of the modeling system consists of the wind field portion of MELSAR and the MESOI puff diffusion model (both developed by Battelle Labs). The Diablo Canyon domain is quite similar to south Vandenberg's. Prominent features are a turning coastline, rugged coastal hills with peaks up to ~ 400 meters, a number of intervening canyons, and a broad series of valleys surrounding the coastal hills from the northwest Morro Bay region to the southeast Avila Beach region. Since a validation study was undertaken for this area, one initial hope was to avoid the expense of a separate study for Vandenberg, should PGEMS be seriously considered. We discuss this possibility below.

MELSAR wind field (K.J. Allwine and C.D. Whiteman):

PHYSICS:

Following a Cartesian to terrain following grid transformation, mass consistency is based on the standard shallow convection form of the continuity equation. Some explanation seems missing for eqns. 2-12 to 2-16 of the MELSAR technical documentation (PNL-5460 Vol.1 UC-1), since units are not in agreement for the left and right hand sides. These equations dictate grid transforms for the wind field. Nine vertical levels are specifiable. However, we cannot reasonably interpret the sentence on p. 2-20, "These input upper-air observations at each gamma level are then spatially interpolated using a $1/r^2$ weighting to each surface weather station, with the ground level interpolated winds being replaced by the surface-wind observations". The remainder of this part of the description is equally murky, but a reasonable interpretation would be that the objectively analyzed vertical winds are held fixed, while the continuity equation is used to adjust the horizontal winds to be divergence free. The wind field for each surface is represented as sums of amplitude functions multiplied by fifth degree orthonormal Chebyshev polynomial basis functions, according to an undescribed non-linear least squares technique. The purpose is to greatly reduce memory storage requirements. The solution technique assumes that there are no domain scale horizontal wind gradients and no general subsidence or lifting. These are not good assumptions for Vandenberg. Again, layer-segregated mass continuity does not adequately describe non-terrain induced, boundary layer scale vertical motions in unstable atmospheres, convective clouds, or at the stratus cloud edges which are endemic to the Vandenberg domain.

A CSH is computed to determine terrain induced flow distortion under stable conditions, but details are puzzling. Temperature lapse rates for the hill Froude number, $F_H \equiv U_0H/N \leq 1$ (see CALMET review for more detail), are determined from input temperature/pressure soundings and surface observations. As shown by Hanna (1987) and specifically for Vandenberg by Skupniewicz et al. (1992), energy balance methods are more accurate than actual surface observations in estimating surface layer lapse rates. Though the treatment of temporal variation in lapse rate seems reasonable, the description of averaged surface and obstacle height lapse rates from soundings is not clear or convincing.

The mixing height is assumed to be the maximum of the mechanical and convective mixing heights. The mechanical mixing height is given as 0.0053 Ug, where Ug is the free stream velocity (m/s). Obviously, the constant is in error. Convective mixing heights are estimated by drawing a vertical line from the current surface potential temperature up to where it intersects the morning sounding. So this assumes that surface heating variations perturb the otherwise flat boundary layer top. Lapse rates and mixing heights are interpolated from sounding and surface station sites to a 10 x 10 grid spanning the domain. Upon reaching the strong subsidence inversion, this method implies that boundary layer heights become more uniform, i.e., less than terrain following, contrary to the day-time studies of Kamada, et al. (1990a,b).

Pasquill-Gifford stability class is estimated for each gridpoint and hour according to wind speed and convective mixing height. A thermodynamic method is presented which includes a topographic amplification factor (TAF) to estimate coupling between valley and ambient flows. Equations, 2-23 to 2-26 prognose the convective boundary layer height and inversion top height. Together these define the inversion depth within a valley. They are in turn used to define an hourly flow coupling coefficient. At Vandenberg's required fine grid resolutions, this may not be needed for the Lompoc Valley. However, for the given inland heating and distance from the coastline or stratus cloud edge, Lompoc measurements show inversions much lower than expected (Skupniewicz et al., 1990, 1992). This may stem from 1) an inversion deepened by cold nocturnal drainage into Lompoc Valley, and 2) subsidence in the valley center which compensates for day-time upslope flow along the sides, effects included in eqns. 2-23 to 2-26. The method is based on studies involving topographical features much larger than south Vandenberg's canyons. Since pressure gradient driven slope flows increase as the square of the horizontal scale over which the gradient applies, flows over short slopes may be limited (Mikkelsen and Kamada, unpublished). This would reduce the method's quantitative accuracy for Honda and other local canyons. Yet a number of cases during the Mt. Iron tracer study showed flow decoupling over Honda Canyon (Kamada et al. 1992c,d). So the MELSAR method invites further scrutiny for both the Lompoc Valley case and sub-grid scale canyon flows.

The physical basis of the MELSAR wind model is much simpler than CALMET, LINCOM, or even WOCSS. In the context of computer power available or soon to be available at Vandenberg, the question is whether the presumed speed advantage offsets the presumed accuracy loss. Tower/SODAR data density and the quality of objective analysis are more critical in assuring the accuracy of output wind fields when using less physically based models such as MELSAR. Improved objective analyses are available as in LINCOM. But bear in mind that most of Vandenberg's many met sensors are sited near the coast. The NOAA buoys, oil platforms, and Santa Barbara Air Quality Management towers are not included in the on-line data stream. We have not found discussions of run-time in the available PGEMS documentation for the complete model. Glantz and Burk (1990) mention that computation of just the wind field alone requires ~ 30 seconds per hour of simulation on a MicroVax II. Porting MELSAR to a current 486 PC might reduce run-time to less than one second. However, for Vandenberg's purposes, enhanced accuracy is probably more important than run-times much below 30 seconds.

VALIDATION:

A wind model verification project is described in Appendix E of Phase I of the PGEMS technical document, referred to as Appendix A of Volume I of Phase III of the PG&E Report 009.5-88.4 (Thullier et al. 1988). Seventeen hourly wind fields were used from nine surface stations and two SODAR sites for 5:00 to 21:00 June 11, 1985. The approach was to compare wind fields with/without data from a given site and with/without the critical streamline height (CSH) option. Only two stations were tested, the San Luis Obispo APC site and VC Doppler station. Results for the six runs were decidedly mixed with disagreement between modeled and measured winds ranging from 5° and 0.3m/s to 41° and 1.1m/s. Use of the CSH alternately improved and degraded agreement. Separation distance between stations was rather large by Vandenberg standards, on the order of a ten to twenty kilometerss. For Vandenberg this test was too cursory to validate the wind flow model. Little was said about the local terrain surrounding the two station sites in question, so it was not possible to evaluate the strength of the flow model on this basis. Congruent with these thoughts the evaluation portion of the report (Phase III, pps. 24 - 27) suggests that the wind field relies strongly on interpolations from individual site measurements and notes that "mass consistent adjustments are of limited value in the absence of measurements" and that "the diagnostic model is simply an interpolative scheme that attempts to flesh out the details of the wind field in a manner consistent with the principle of mass continuity" (p. 62). A look at fig. 8, p. 25 of the report suggests that without the CSH option the model will ignore most terrain effects beyond that objectively analyzed from station data. So high tower and SODAR density are critical to MELSAR's use in complex terrain. The absence of towers along the northwestern promontory and in See Canyon meant that terrain channeling and strong upslope flow in those areas were not predicted. Thus, major discrepancies appeared in the dispersion predictions on some occasions. On the other hand, towers may be aliased by local terrain, resulting in local flows not indicative of larger scales. This was seen in the Mt. Iron vs. LINCOM/RIMPUFF results for flow over Vandenberg's Honda Canyon (Kamada et al. 1992c,d). This highlights the need for inclusion of as much physics in wind flow models as possible, within the available time and computer power constraints.

A more extensive tracer study took place from the power plant and Morro Bay for seven non-consecutive days during the period August 31 to September 15, 1986. Releases occurred from 0800 to 1600 LDT and sampling from 0700 to 1900 LDT. This sampling period and schedule is quite comparable to the 1989 Lompoc Valley Diffusion Study for releases from the HSSF and the mouth of the Lompoc Valley at south Vandenberg. However, the range of wind patterns from the power plant were considerably more diverse than seen from the HSSF. The two modeled Diablo Canyon domains, northwesterly and southeasterly, were both 50 x 50 km at 1 km grid spacing and were offset from each other by 10 km along the north/south axis and 12 km in the east/west. The northwesterly domain was used to model southeasterly flow from the releases at the power plant, while the southeasterly domain was used for northwesterly flows. Three SODAR, eighteen surface stations, and about 150 bag samplers were employed in the study. The CSH option was not employed for the windfield model runs. Twelve puffs were released per hour. The model computes concentrations on a 31 x 30 grid encompassing the domain and at up to 25 receptor sites, so eleven separate modeling runs were employed for each release to treat the 150 receptors. A terrain parallel upper boundary at 1200 m AGL was employed. Wind fields were updated at 15 minute intervals. In an updated PGEMS v. 1.1 the list has been expanded to include 250 receptor sites, so separate runs are no longer necessary.

Graphical results do not immediately appear as congruent as the Vandenberg Mt. Iron vs. LINCOM/RIMPUFF set. But this may be misleading because Diablo Canyon involved much longer ranges, along with a lower relative density of wind measurements. In contrast to the rather cursory wind field analysis, the report gives a lengthy statistical and graphical analysis to show the considerable disparity between near-field modeled and measured concentrations. The report assumes that building down-wash and misleading wind direction fluctuation statistics (sigma θ) from the release site tower lead to more stable PG diffusion classes than were effective downwind or above the surface layer. Apparently, a building down-wash algorithm has since been installed in the puff model. However, as noted above, the remaining issue is that surface releases tend to loft quickly in unstable conditions. So it is well-established that PG classes A and B will overpredict near-field ground level doses. We recommend deriving dispersion coefficients from surface energy balance and similarity theory, rather than tower wind/temperature profiles such as in PGEMS, if stability and wind dependent velocity spectra are unavailable at the release site and for each tower.

We are puzzled that results from some runs using the CSH option were not presented. However, most of the releases occurred for atmospheric stabilities too weak to warrant its use. The report makes the general comment that the windfield agreement with data tended to degrade near the domain boundaries.

Far-field results were rather poor, but comparable to other complex terrain studies. "Correlations between predicted and observed values were generally insignificant (p.74)". A distinct bias toward overprediction of concentrations appeared, perhaps partly due to the lack of filtered wind velocity spectra for dispersion coefficients (corrected in v. 1.1). MESOI's lack of puff splitting or much physics in the wind field may be partly responsible also. Vertical and horizontal puff splitting were also added to PGEMS v. 1.1. So improvements have been made, but there remains some necessary disagreement between predicted and observed results stemming from the stochastic nature of atmospheric turbulence. So a high degree of far-field correlation cannot be expected, particularly in complex terrain. However, the Diablo Canyon study results do not warrant acceptance of the MELSAR wind flow model for operational use at Vandenberg without additional on-site studies.

MESOI PUFF MODEL (J.V. Ramsdell, G.F. Athey, C.S. Glantz):

INTRO:

Information for this review comes from an NRC report published by the above authors in 1983. We suspect that further work must have proceeded on this model in the interim. Installation of certain improvements were surmised from comments in other MELSAR documentation. There perhaps are others which we have not detected. Be that as it may, from our best information MESOI seems to be a standard puff diffusion model which fairly mature in the sense that itt also incorporates puff-splitting, plume rise, building down-wash, wet and dry deposition, and half-life decay rates for radioactive materials and chemicals.

PHYSICS:

Plume rise is computed from the standard effective stack height equations of Briggs. These equations are not recommended if the release does not occur through a stack. For puff centers the resulting effective release height parallels the terrain. Away from puff centers the effective release height remains fixed or matches terrain height, if the terrain height happens to exceed it. Terrain height is computed by interpolating gridded terrain data. The inversion is set to be terrain parallel. Total reflection from the inversion is assumed, so partial puff penetration is not allowed. However, if the release occurs above the mixing layer, downward penetration is allowed.

Diffusion coefficients are based on several data sets obtained in the 1960's and categorized by Pasquill stability classes. We repeat that conservative tracers were not available before the advent of SF_6 ~ 1970 and that the A and B Pasquill stability classes do not account for near-field plume lofting associated with convective conditions. So these features need updating, if this has not already been done.

A second option for diffusion coefficients in MESOI is to use current local turbulence data. σ_y is derived from, σ_v/U, the ratio of the standard deviation of cross wind turbulence, to mean wind speed. σ_z is obtained from σ_ϕ, the standard deviation of the wind elevation angle (in radians). This is probably a better method for horizontal turbulence. However, for vertical turbulence we suspect that σ_ϕ, if derived from bivanes not sonic anemometers, probably does not reliably measure vertical wind fluctuations. Of course Vandenberg towers cannot normally be outfitted with expensive sonics. As in the CALMET/CALPUFF reviews, we again suggest as a practical matter that vertical turbulence be estimated from surface energy balance computations and boundary layer similarity theory, perhaps in conjunction with solar and net radiometer readings.

A technique of computing virtual source distances is used to avoid sudden changes in puff dimensions with stability class. The spectral filtering caveat, described in the above CALPUFF review also applies, so MESOI may over-estimate diffusion, if the wind field is frequently updated and puff meander is double-counted.

Downwind chemistry may be included within MESOI with assumed half-lives for species. MESOI can also account for the creation of toxic intermediate species, as well as final inert species in a two stage process which assumes exponential decay and creation rates, ala radioactive processes. For the puff level of modeling, this seems appropriate. Complete computation of downwind chemistry would be computationally prohibitive in an emergency response context.

Dry deposition is estimated using the standard source depletion method, assuming that the deposition velocity is 0.01 ms^{-1} regardless of position or material. Wet deposition is treated as washout, wherein mass loss from the puffs is proportional to precipitation rate and in-puff mass concentrations. Such estimates are probably useful to within an order of magnitude.

PGEMS SUMMARY:

In summary we are left with the impression that MELSAR was developed some years earlier than CALMET/CALPUFF for efficient use on computers from that era. Inexpensive computer power has increased by two to three orders of magnitude in the interim. Hence, some of the simplifications used, particularly in the MELSAR windfield are no longer necessary, nor are they all appropriate for Vandenberg. MESOI appears to be a viable puff model which includes computationally simple downwind chemistry capability based on a half-life approach, as well as many of the add-ons necessary for practical dispersion estimates. Unfortunately, the chemical base does not include the types of rocket propellents of interest to Vandenberg. As with CALPUFF, the lack of spectral filtering registers a caveat, if MESOI is piggy-backed to a frequently updated wind field, as is expected at Vandenberg.

Also, we find that errors in the MELSAR windfield documentation available to us have not been updated consistently. We do not understand some portions of the wind field model description. The valley flow theory developed by Battelle Laboratory personnel is excellent. However, it is meant to apply for grid resolutions that are too coarse for Vandenberg use. Again, other weaknesses are the lack of accounting for near-field dense gas effects and source terms for liquid spills.

On the other hand we expect that MELSAR is already adapted to DEC MicroVax II computers using the VMS operating system and Techtronix graphics display terminals; it is installed in this configuration at the Diablo Canyon nuclear power plant. We understand that it and WCCSS also have been validated for Diablo Canyon in similar coastal terrain less than 100 km north of Vandenberg and that the delivered Battelle model featured a domain which could be varied between ten and several hundred kilometers on a side. If so, we suspect that the MELSAR documentation available to us may be somewhat out of date, while an improved version of the model may exist. Perhaps further contact with Battelle Labs could clarify this issue. At the same time the downwind range of nuclear plume THCs certainly exceeds that of any conceivable chemical plume emitted from Vandenberg. So the emphasis on far-field dispersion and coarse grids may be entirely appropriate for Diablo Canyon but not for Vandenberg. If so, we suggest that while the code may be as accessible as CALMET/CALPUFF and the installation effort minimal, so might obsolescence time for such a model. So the overall life cycle cost of this modeling system may be high, even if the initial installation costs are deceptively low.

NUATMOS/CITPUFF (D.G. Ross and D.G. Fox)

NUATMOS (D.G. Ross et al.):

NUATMOS employs terrain following coordinates and variable vertical grid spacing. Like CALMET, MELSAR, WOCSS, MACHWIND, and MATHEW, it is a mass conservative windflow model. It differs from these other in that it seeks to include dynamic speed-up and stability effects by apportioning the adjustment between horizontal and vertical flow during iterative divergence minimization. In this process the error functional,

$$E(u,v,w) = \iiint\left[(u-u_0) + (v-v_0) + \alpha^{-2}(w-w_0)^2\right]dV \quad , \qquad (1)$$

is minimized by the variational method, subject to the standard shallow convection continuity constraint (see MATHEW review for general description). Energy conservation arguments and laboratory data suggested to the authors of NUATMOS that the tuning parameter for vertical velocity adjustments, α^{-2}, is well characterized by the form,

$$\alpha^{-2} = 1 + \frac{3}{(S^2-1)\,Fr^2} \quad . \qquad (2)$$

Here S is the amount of speedup over terrain beyond the initial upstream velocity, U_0, and $Fr = U_0/NH$ is the hill Froude number based on the Brunt Vaisala frequency, $N = [(g/\theta)(\partial\theta/\partial z)]^{1/2}$, and the hill height, H (Ross et al. 1991) (See CALMET and MATHEW reviews for more detail). Earlier test forms for α, based on physical arguments did not agree well with data. So the actual forms used for α and S are empirically based. However, the basic physical reasoning for the stability parameterization is as follows. In the lower limit as α approaches zero, flow adjustments at each level become two dimensional (as in WOCSS). This limit is physically consistent with very strong stability. In the upper limit as α approaches unity, the solution becomes consistent with solutions for potential flow. So the purview of NUATMOS seems to be for neutral to stable cases. Indeed, for $\alpha = 1$ NUATMOS was found to agree closely with exact, analytic potential flow solutions which are available for idealized perturbations such as hemispheres, half-cylinders, ellipsoids, and polynomial hills imbedded within an otherwise featureless horizontal plane (Ross et al. 1988). Such solutions do not include adjustments due to thermal effects or turbulent drag. NUATMOS also does not include upslope flow adjustments, ad hoc or otherwise.

Dispersion from the puff model CITPUFF with the flow field supplied by NUATMOS was also tested against data from the Cinder Cone Butte study (Ross et al. 1991). Cinder Cone Butte is a lone roughly axisymmetric hill rising from an otherwise nearly flat plain.

The available documentation is not clear on this issue. However, in principle NUATMOS seems to demand an initially uniform undisturbed flow field upon which to make its stability and terrain based adjustments. Isolated hills such as Cinder Cone Butte are ideally suited to meet such a demand. However, obtaining a pristine upstream vector may be difficult in Vandenberg's highly complex terrain. A tower averaged wind vector will include myriad terrain effects. Overwater vectors from NOAA buoys do not include the effects of surface roughness, stability, or boundary layer height changes seen over neighboring but otherwise uniform land surfaces. The only tower in a low region, 009, is subject to Lompoc Valley winds which are often not representative of the remainder of the flow over south Vandenberg. An objectively analyzed windfield supplied from tower and SODAR data would already contain flow adjustments which would be repeated in NUATMOS. The net result might be exaggeration or distortion of certain flow features. Tests against Vandenberg tower winds would be required to make a proper evaluation of NUATMOS. We cannot suggest that the Cinder Cone Butte data are sufficient for validation purposes.

CITPUFF:

The following analysis is based on a 1985 publication which may be somewhat out of date. An updated analysis is in order, if more recent references become available. CITPUFF appears to be a standard puff model which includes three options for calculating puff dispersion: PG stability classes or Briggs functions for $\sigma_{y,z}$ as functions of stability class and downwind distance, or a simple 22.5° arc assumption. Briggs-type formulas are used for plume rise and effective stack height. The available CITPUFF documentation makes no mention of the many add-on features demanded of operational diffusion models, such as: partial inversion penetration, puff-splitting, near-field deformation, building down-wash, vertical shear effects, wet/dry deposition, multiple sources, source strength calculations, dense gas treatment, chemistry, graphical user interfaces, graphical output, computer hardware requirements, or CPU run-time information on various systems. Thus, many features including MARSS compatibility and current state of support for this model are unknown. Some speculation on the effect of terrain induced streamline distortion on puff diffusion is given, but has no immediate bearing on CITPUFF, which uses flat terrain assumptions.

CITPUFF was compared with the COMPLEX I and COMPLEX II models for idealized flat terrain and isolated hill cases. Since in this comparison CITPUFF used a flow model other than NUATMOS, little of relevance can be inferred from this study. However, the Cinder Cone Butte study compared NUATMOS/CITPUFF against models such as NEUTRAL and LIFT for flow above the CSH, and IMPINGEMENT and WRAP for flow below. LIFT and WRAP (Venkatram, 1988) were developed as improvements to the NEUTRAL and IMPINGEMENT models, respectively. In turn these are variants of the well known CTDM and CTDM+ modeling systems (Strimaitis et al. 1983, 1987). With respect to scatterplots of predicted versus observed concentrations, NUATMOS/CITPUFF appeared to be at least as accurate as the best of the other models, namely, NEUTRAL and WRAP. In fact NUATMOS/CITPUFF showed no statistically significant fractional bias and a normalized mean square error significantly smaller than WRAP in these tests. Inclusion of the α adjustment factor in NUATMOS caused a large improvement in results. The authors also note that NEUTRAL performed much better than its supposed improvement, LIFT. However, as in the NUATMOS review, we do not recommend applying results from an isolated hill like Cinder Cone Butte to Vandenberg, one problem being specification of a true background mean wind in the context of complex terrain. NUATMOS seems to be particularly sensitive to this issue. Results from a forthcoming Tracy power plant study using NUATMOS/CITPUFF may be more relevant.

SUMMARY:

In summary NUATMOS provides a simple way to include the effects of stability and dynamic wind speed-up in an otherwise purely mass conserving model. Yet, the algorithm is empirical because attempts to base the α tuning parameter on physical considerations were not successful. Being a recent development, NUATMOS does not appear to be fully mature. Validation studies in truly complex terrain are not yet available in the literature and NUATMOS still lacks many niceties found in operational versions of diagnostic models. CITPUFF appears to be a standard puff model with all the typical issues including the puff/plume averaging time and spectral filtering problem mentioned a number of times above. If CITPUFF also has not been updated yet to include a number of desired operational features, we cannot recommend further evaluation of this model until more relevant validation studies and better documentation are available. This may occur too late for the Vandenberg modeling itinerary.

WOCSS/Adaptive Plume (F.L. Ludwig, et al., SRI Int.)

INTRO:

WOCSS (winds on critical streamline surfaces) is a windflow model from SRI International which employs critical streamline heights and mass conservation but no dynamics, i.e., no momentum conservation. An initial guess windfield is supplied by available combinations of tower, SODAR, rawinsonde, and National Weather Service based wind data. These are $1/R^n$ interpolated to the grid. n is a user-specifiable variable, usually between one and three. The coordinate system follows flow surfaces defined curvilinearly by critical streamlines. Flow is partitioned into several non-interacting layers, each of which are assumed to have constant temperature lapse rates. Because the surfaces are decoupled, recirculations from slope winds, valley winds, and seabreezes which depend on vertical flow cannot be modeled. This also applies to the typical secondary circulation around stratus cloud edges as discussed in the CALMET review.

PHYSICS:

The local height of each surface is defined by,

$$z_j = z_{j,0} + (z_{j,\max} - z_{j,0}) f \left(\frac{H - H_{\min}}{H_{\max} - H_{\min}} \right) , \qquad (3)$$

where $z_{j,0}$ is the height of the bottom of the jth flow surface taken over the lowest terrain in the domain. H, H_{max}, and H_{min} are the local terrain height and the highest and lowest terrain heights in the domain, respectively; f is an adjustable function. Using the standard Froude number concept, the maximum height of the flow surface in the domain is given by

$$z_{j,\max} = z_{j,0} + V_{j,0} \left(\frac{g}{T_0} \frac{\partial \theta_j}{\partial z_{j,0}} \right)^{-1/2} . \qquad (4)$$

$V_{j,0}$ is the windspeed for level j at the lowest point in the domain. In some locations we may have the condition, $z < H$, so the coordinate system defined by the flow surfaces will then intersect the terrain. With divergence minimization, this forces the wind to flow around some terrain obstacles under stable conditions because it lacks the kinetic energy to surmount obstacles taller than $z_{j,max}$.

As with the other CSH based models, the underlying Froude criterion is **physically suspect**, since contrary to data it implies zero windspeed at the CSH and local minimums atop hills. Smith (1990) showed that pressure, not potential energy variations, control wind speeds. Yet, perhaps fortuitously, applications of the streamline concept are still in reasonable agreement with data (see CALMET review for more detail).

Also, specifying $V_{j,0}$ may be a problem for Vandenberg, since the lowest lying towers are in the Santa Ynez River Valley. The valley towers, in particular, tower 009, are subject to channeled down-valley drainage winds under stable conditions which may be quite different from the domain scale flow.

Unlike the primitive 3-D continuity equation used in CALMET, WOCSS accelerates the computation by integrating the vertical divergence across finite layers whose local thicknesses, Φ_j, are defined as fixed fractions of the local CSH. That is, the primitive 3-D continuity equation can be re-arranged as,

$$\frac{\partial w}{\partial z} = -\left[\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right] \quad . \tag{5}$$

From (5) we obtain the vertical velocity change, Δw, across a layer by parsing the vertical divergence and layer integrating to give,

$$\Delta w = w_{z_{j+1}} - w_{z_j} = -\int_{z_j}^{z_{j+1}} \left[\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right] \partial z \simeq -\Phi_j \left[\overline{\frac{\partial u}{\partial x}} + \overline{\frac{\partial v}{\partial y}}\right] \quad . \tag{6}$$

Note that eqn. (6) uses layer averaged velocity gradients. We can also obtain the same vertical velocity change as in eqn. (6) by subtracting a vertical velocity equation applied at the bottom of the layer from a similar one applied at the top,

$$
\begin{array}{rcl}
w_{z_{j+1}} & = & \dfrac{\partial z_{j+1}}{\partial t} + u\dfrac{\partial z_{j+1}}{\partial x} + v\dfrac{\partial z_{j+1}}{\partial y} \\
- \; w_{z_j} & = & \dfrac{\partial z_j}{\partial t} + u\dfrac{\partial z_j}{\partial x} + v\dfrac{\partial z_j}{\partial y} \\
\hline
\Delta w & = & \dfrac{\partial \Phi_j}{\partial t} + u\dfrac{\partial \Phi_j}{\partial x} + v\dfrac{\partial \Phi_j}{\partial y} \quad .
\end{array}
\tag{7}
$$

If we equate the two expressions for vertical velocity change and re-arrange, we obtain,

$$\frac{\partial \Phi_j}{\partial t} + u\frac{\partial \Phi_j}{\partial x} + \Phi_j\frac{\partial u}{\partial x} + v\frac{\partial \Phi_j}{\partial y} + \Phi_j\frac{\partial v}{\partial y} = 0 \quad . \tag{8}$$

Employing the inverse of the chain rule for differentiation gives,

$$\frac{\partial \Phi_j}{\partial t} + \frac{\partial (u\Phi_j)}{\partial x} + \frac{\partial (v\Phi_j)}{\partial y} = 0 \quad . \tag{9}$$

This reduces to

$$\frac{\partial (u\Phi_j)}{\partial x} + \frac{\partial (v\Phi_j)}{\partial y} = 0 \quad , \tag{10}$$

if the layer thickness, Φ_j, does not change with time. So a fixed Φ_j replaces iterative computation of the vertical divergence, $\partial w/\partial z$, resulting in a considerable savings in computer time.

As a further approximation, WOCSS defines the variables,

$$u^* = u\Delta z \quad , \; and \quad v^* = v\Delta z \quad , \tag{11}$$

where, instead of Φ_j Δz, the average separation distance between adjacent surfaces is used. The assumption is that, if the slopes of the flow surfaces are not too large, the continuity constraint can then be approximated by,

$$\frac{\partial u^*}{\partial x} + \frac{\partial v^*}{\partial y} = 0 \quad . \tag{12}$$

Even so, the divergence minimization procedure is still **the** time-bottleneck. But with the approximations used, tests indicate that on new workstations WOCSS can probably meet the emergency response time, resolution, and domain size requirements stipulated for Vandenberg.

In WOCSS continuity should accelerate winds over high terrain where the layers are thinner. This is consistent with tests which show speedup over or around hills under stable conditions. But, the CSH concept upon which WOCSS is based is physically suspect, so it is not surprising that there are qualitative differences. That is, for vertically uniform stable stratification, linear diagnostic models also produce a speedup over hills which are driven by stress interactions with local pressure gradients rather than continuity of flow through thinning layers. Unlike WOCSS, such linear models show a secondary downwind speed maximum which eventually overwhelms the hilltop maximum, as stability increases. Stagnation at the upstream base of the hill is also augmented (Carruthers and Hunt, 1990).

Though there is no explicit moisture in WOCSS, optional cloud cover data can be used to estimate net radiation at the surface and hence PG stability class. WOCSS also estimates turbulence kinetic energy (tke) and Richardson number. However, they are not yet used in the Adaptive plume computations.

SUMMARY:

WOCSS takes a more sophisticated approach to mass conservation than MELSAR and MATHEW by parsing divergence minimization into discrete layers so that a pseudo-2-D equation can be used. This results in large computational savings. However, the parsing is done in terms of the critical streamline height concept, long in vogue, but recently shown to be physically suspect. It also lacks the momentum conservation of LINCOM or empirical approaches for dealing with dynamical momentum effects and slope flows found in CALMET. On the other hand, we have found that it does run at 500 meter resolution for a 25 x 40 km grid on a 386 PC within ~four minutes using four levels. So on a faster machine, we expect that WOCSS will comply with the suggested time constraints, while we doubt that CALMET can.

MACHWIND: (R.E. Meyers, U.S. Army Atmospheric Sciences Lab)

MACHWIND is a derivative of the WOCSS diagnostic windflow model which has been adapted for use at Vandenberg. MACHWIND improves computationally upon the original WOCSS version by using a three-nested grid method to reduce the time required for divergence minimization, the most time-consuming step. The coarse and medium grids are set at 1/4 and 1/2 the fine grid resolution, respectively. From an initial objective analysis, a minimally divergent windfield is then computed on the coarse grid. Respecting the fixed winds represented by the tower sites, this field is interpolated to the medium grid and becomes the initial field for divergence minimization on the medium grid. The process is repeated for the fine grid. The multi-grid procedure reduces the number of iterations required overall by eliminating the coarser scale divergences first.

Among the Vandenberg adaptations are the use of SODAR and tower data to produce non-uniform inversion base heights. The MACHWIND inversion height at a given grid point is based on the terrain height averaged over a ten kilometer radius, plus a $1/r^2$ interpolation of boundary layer depths taken from the four coastal SODARs. So the modeled inversion would be basically flat, if the inversion base height is derived from one SODAR measurement plus a terrain height averaged over a very large radius. On the other hand, if the radius were quite small, then the inversion base would become essentially terrain following. The default ten kilometer terrain averaging radius is an optimization based on the following consideration. If tower based temperatures match those within the subsidence inversion (as indicated by rawinsondes) it is likely that the inversion intersects the terrain at such sites. It was found that a ten kilometer averaging radius placed the maximum number of such towers within the inversion. We find this procedure somewhat ad hoc but perhaps serviceable. Kamada et al. 1989 and 1990, showed for the summer day-time period that the highest correlations with mobile SODAR data at Vandenberg were obtained assuming a terrain parallel inversion height. Semi-parallel inversion height assumptions showed slightly lower correlations.

Already planned for future versions of MACHWIND is an estimate of the local temperature lapse rates to improve both the windspeed interpolation between vertical levels (now assumed logarithmic) and to also allow the sigma surfaces to be based on hydrostatic iso-pressure surfaces, rather than terrain. We agree with Hanna in Venkatram and Wyngaard, 1988, that better lapse rates are likely to be obtained from surface energy balance methods than tower data. The thermister accuracy required for the tower method requires calibrations too frequent and detailed for routine operational use. A sample surface energy balance method is given in Appendix A of the LINCOM/RIMPUFF Mt. Iron Comparison (Kamada, 1992).

To accelerate the incorporation of tower data in the divergence minimization process, a time transient velocity equation has been suggested which includes advection and a pseudo-pressure gradient force based on the divergence. One suggested form of the pressure gradient force is based on the deep convection form of the continuity equation which includes density changes. Even with time tendencies of density, sound waves will not arise, since the time tendency of vertical velocity is not included. The deep convection continuity equation is used in prognostic models such as RAMS to simulate cumulus circulations which involve large fractions of the troposphere. The second suggested form for the pseudo-pressure gradient force involves a large coefficient times the divergence of the velocity divergence. These suggested forms seem rather involved, considering that the purpose seems to be to simply diffuse data induced divergence efficiently. Moreover, the use of time dependent equations demands considerably more computer power. We question whether such a set can meet Vandenberg's emergency response constraints on currently available workstations.

SUMMARY:

MACHWIND is a derivative of the above reviewed WOCSS model which has been adapted to use at Vandenberg. The main advantages over WOCSS seem to be the faster divergence minimization scheme and non-uniform inversion base heights. Also planned are a conversion to hydrostatic sigma surfaces and the use of time transient truncated Navier-Stokes equations to facilitate the diffusion of data induced divergence into the windfield. The latter would make MACHWIND a considerably different model from WOCSS. However, we question the latter implementation for Vandenberg emergency response, given currently available workstation speeds. With appropriate lapse rate estimates, it appears that MACHWIND may be the most suitable of the current models designed for stable flow conditions, as well as the one nearest to operational status at Vandenberg.

Adaptive Plume Model:

PHYSICS:

Rather than a spherical puff, the adaptive plume model describes a Lagrangian volume using five different points in the vertical with an initial separation of three meters. All material within the puff lies between the highest and lowest points. The fraction of total material between any two of the five points is assumed to be given by a piecewise Gaussian function. The resulting nearly five-fold increase in computational demands is somewhat offset by an attempt to merge puffs within a distance of $\sigma_y/2$ as well as purge puffs which have exited the domain. The purpose of the five points is to allow for vertical differences in advection and diffusion presented by the windfield model which may be more complex than that given by standard similarity profiles. Thus, vertical shear, plume rise, and the effect of growing internal boundary layers all may be treated within the model. The very small initial separation between points suggests that the near-field slug/puff adaptation used by CALPUFF is not necessary for the Adaptive plume model. However, the need to release small puffs frequently does increase computational cost.

Plume rise is handled via adjustments of the standard Briggs equations applied separately to each of the five points. 100 receptor sites may be specified. At present vertical dispersion is based on PG stability classes, which we noted above tend to underestimate near-field vertical diffusion for surface releases under convective conditions. Complete specular reflection is assumed at the surface, such that deposition effects are not computed. Puffs are not allowed to split and there is no provision for treating multiple sources within a single run. As with CALPUFF there do not appear to be provisions for spectral filtering of the dispersion coefficients. So adjustments would be required when using this model with a prognostic or frequently updated diagnostic wind field. Graphical output is now available in one version of the model and it has been run on MARSS compatible DEC systems.

VALIDATION:

The model was tested against LIDAR data collected on May 5 and 15, 1980 from the EPRI project at the Kincaid power plant in Illinois. Good topological agreement was obtained between the model and vertically oriented 2-D frames from the LIDAR. Thus far, comparisons of surface footprint data from other studies are not available.

WOCSS/Adaptive Plume SUMMARY:

The adaptive plume concept appears to have some merit and invites further study. However, the model is in research level, proof-of-concept status rather than in a fully operational system mode which includes all features necessary for dispersion calculations. Like the other reviewed models, relevant chemistry, source terms for liquid spills, and options for treating dense gases are not available. Near-field building down-wash, multiple sources, overwater transport, and wet/dry deposition effects are also not implemented.

Both WOCSS and the Adaptive plume models are in the public domain, although some restrictions apply. The code is modular and modifiable. Technical support is available from SRI, but is not likely to come gratis. Versions exist in VMS Fortran, so MARSS compatibility is probably not an issue. In fact, most of the reviewed models have been written in ANSI F77 standard Fortran. Thus, portability should be a trivial matter in most cases. A graphical output format is being developed at San Jose State , but there are no current plans for a full graphical user interface (F.L. Ludwig, personal communication, 1992).

For satisfactory operation at Vandenberg, the Adaptive plume model would probably require extensive additions to the basic algorithms to include the many add-on features required of operational models. Given the right personnel, this might be done in less than one man-year. However, we suggest that other more mature models be studied before attempting such an undertaking.

LINCOM-RIMPUFF: (Troen, Mikkelsen, et al., RISO National Labs, Denmark)

LINCOM (I. Troen et al.):

INTRO:

LINCOM belongs to the only class of diagnostic model which retains both mass **and** momentum conservation. The first proponents were Jackson and Hunt (1975), followed, e.g., by Mason and Sykes (1979), Walmsley et al. (1982), Taylor et al. (1983), Beljaars et al. (1987), and Hunt et al. (1988a). LINCOM uses linearized versions of the perturbation momentum equation with first order turbulent diffusion, the standard shallow convection form of mass continuity, and equation of state. Thus, to first order, LINCOM conserves momentum as well as mass by treating the effects of pressure force dynamics, turbulent stress, advection, coriolis, and continuity, Currently, the thermodynamic energy or temperature equation is neglected. So, buoyancy induced, non-neutral conditions are not treated explicitly in the governing equations. (A thermal version of LINCOM, LINCOM-T is under development.)

Actually, in version 1.0 a post-process objective analysis anchors the wind field to match the tower vectors exactly. However, in this process true mass conservation is lost. The objective analysis uses a terrain modified $1/R^2$ interpolation, wherein each tower's circle of influence is warped into ovals matching the aspect ratio of the local terrain contours surrounding the tower site. This should be an improvement over the standard Barnes technique. If only surface data is supplied, LINCOM extrapolates vertically on the basis of similarity theory to obtain a mean background wind. Version 1.0b is significantly different in that it retains mass conservation by using a fitting techique which does not attempt an exact match to tower wind vectors. Moreover, for a given domain, orthogonal basis functions for the wind vectors are pre-computed and stored on hard disk. So assembly of the final wind field only involves a non-iterative variational search for the domain mean wind vector, which when added to the pre-computed perturbation field, provides the best fit to the available data. Thus, this model may be one to two orders of magnitude faster than the other windfield models reviewed here.

PHYSICS:

Both LINCOM versions solve the equations by Fourier transforming the terrain as well as the flow. For each wave number in the spectral domain, pre-calculated analytical solutions are available for linearized equations. Unlike the divergence minimization schemes, time-consuming iterative numerical procedures are not involved. Analytic solutions could also be obtained for individual grid points in finite difference mode. The reason for the transformation from grid points to wave numbers is that only ~1/3 as many wave numbers are required as grid points in each dimension. This reduces computational requirements by an order of magnitude for a 2-D transform (minus the relatively small time involved in computing the transform and inverse transform).

Though useful in setting up a domain, in LINCOM version 1.0 the speed gained by using Fourier transforms is actually academic because for operational purposes the solutions are pre-calculated. Thus, version 1.0 stores 72 pre-calculated solutions for the terrain induced perturbations for a given domain on hard disk in three degree increments around 360° of arc for reference 1 ms^{-1} mean background winds. Version 1.0 then retrieves a stored perturbation windfield based on the mean wind direction supplied by that tower. Since flow above the surface layer is assumed to be frictionless, the perturbation field vectors are simply multiplied by the tower wind magnitude and added to the mean vector to produce the final field based on that particular tower. Version 1.0 then combines separate fields obtained for each tower, using the terrain modified $1/R^2$ interpolation. Since the perturbations are constrained to be zero at each tower site, the final field provides an exact match to the tower winds, while allowing a dynamically based interpolation scheme between towers. This accounts for the well validated wind "speed-up" in the surface layer over hills. Although the individual perturbation fields are mass conservative, mass conservation is lost in the combinatory process. Version 1.0 was used for the Mt. Iron tracer study.

Another aspect of linear systems exploited in version 1.0b is that the total flow is expressible as a linear combination of orthogonal solutions of the perturbation flow field. This means that all the basic features of neutral flow can be expressed as a linear combination of just two fixed orthogonal fields which may be pre-calculated for any fixed set of terrain. So in practice two, rather than 72, perturbation fields are stored, based on 1 ms^{-1} due northerly and easterly mean winds, a 36-fold savings. Instead of combining multiple fields based on exact anchoring to the towers, a single field is obtained by variationally optimizing the fit to the horizontal tower winds. Thus, this procedure yields both momentum and mass conservation in a single non-iterative pass. And because the essential flow features are pre-stored rather than calculated, it is also very fast. On a 15 MIPS 486/33 PC, LINCOM/RIMPUFF required three minutes to simulate nine hours of continuous plume dispersion using windfields updated every ten minutes on a 200 x 200 x 5 grid at 50 meter resolution. So here LINCOM requires less than three seconds to formulate and output each of 54 wind fields.

In actual operation the input-to-output time for version 1.0b depends on the trivial fitting routine and hard-disk retrieval of pre-calculated results. Version 1.0 is generally somewhat slower.

Both versions have also been run on a DEC VAX 5000 workstation, so software compatibility with MARSS seems likely.

The complete linearity presumed in the pre-calculation method assumes that the flow is inviscid in the outer boundary layer, which is less reasonable within the inversion (which LINCOM assumes is terrain following). LINCOM also lacks time tendencies in the velocity, so terrain forced dynamics propagate instantly over the whole domain, rather than at some realistic set of phase speeds. This problem is shared by all diagnostic models. Linearization also means that higher order perturbation terms are neglected. In a prognostic scheme, such solutions would gradually diverge from reality. However, for a diagnostic model, where only the present time step is considered, this is not as significant an issue. Still, linear models cannot treat large non-linear synergisms. One example might be the south side of Honda Ridge during north-westerlies where roughness and stability changes occur along with flow separation.

The vertical velocity is basically assumed equal to the horizontal velocity at that site times the sine of the terrain slope. This only holds well for slopes of less than twenty degrees (Hunt, personal communication, 1990). However, ACTA's analysis of the Vandenberg terrain concludes that at 500 meter resolution, little of the terrain shows slopes exceeding twenty degrees (Conley et al., 1990).

Transformation of a limited mesoscale area to the spectral domain involves the assumption of periodic boundary conditions. So wave energy leaving one boundary immediately re-enters the domain from the opposite boundary. Thus, LINCOM employs a 10 km buffer zone over which terrain is gradually relaxed on all sides to sea level. This greatly damps wave motions, but not completely. Quantitative assessment of the influence of this effect on flow is not presently available.

Exact matching to tower winds is not always desirable, since tower winds may represent very local conditions which scarcely influence the bulk flow (see validation effort below). This can be regarded as a form of aliasing. LINCOM 1.0 also presumes that each tower contributes its version of the undisturbed mean flow vector. But the in-terrain towers are all influenced by the surrounding complex terrain and can hardly be considered representative of undisturbed background flow. For this reason Vandenberg tower 052, sited within a reasonably flat mesa portion of the domain, was used to represent background flow in the Mt. Iron comparison. LINCOM 1.0b places less importance on the meaning of the background wind by deriving it through empirical fitting. This seems more honest.

Version 1.0b also does not suffer the loss of mass conservation or the local aliasing problem. However, its tower fitting technique cannot yield local slope flows or stability effects, since they are not treated in the governing equations. Hence, the fitting technique in version 1.0b may produce poor results when such effects are important in determining local wind directions. Stability alters local winds strongly during drainage flows. So Froude balance models might be more appropriate than neutral LINCOM under strongly stable conditions. Real slope flow forcing increases as the square of the slope's length, so small scale slopes do not contribute much to slope flows. For example the Vandenberg seabreeze is often augmented significantly by a southwesterly up-slope flow. This flow is due to heating of the large scale slope, extending from the coast to the Santa Ynez ridge, about 75 to 100km. However, for LINCOM's purposes the domain mean background wind incorporates both this effect as well as the seabreeze.

Both LINCOM versions assume a terrain parallel inversion. This agrees generally with daytime data from the Vandenberg area studies of Kamada et al. (1990a, b). However, such an assumption may not be valid under strongly synoptic or stable conditions.

VALIDATION:

Version 1.0 has been tested together with RIMPUFF for eight representative cases from the 1966-67 Mt. Iron tracer study conducted by Battelle Corp. over south Vandenberg. In some cases modeled plumes tracked measured dosages quite well, due in part to "tower anchoring". In other cases, the real plume floated above the local canyon flow represented by towers. A simple improvement in version 1.0 would be to alter the $1/R^2$ dependence used in the objective analysis to $1/R^n$, where n depends on local terrain slope and stability. This would tend to limit the influence of highly localized effects on the overall wind field and also limit the degradation of mass conservation. However, this adjustment has not been implemented or tested as yet.

The surface-layer, ridge-top "speed-up" recognized in LINCOM's physics already tends to localize some tower influences. That is, many of the Vandenberg towers are sited along ridge tops rather than at the bottom of or along hills. Since ridge tops represent only a small fraction of the terrain, these towers often record atypically high winds. If a flow model is unaware that "speed-up" is confined to hill tops, then its objective analysis step will over-accelerate the rest of the flow to match the ridge top data. Such overly high speed estimates will lead to overly thin, overly long plume estimates. Unlike other models LINCOM should be able to avoid this effect during neutral and unstable conditions.

Since in operation pre-calculated solutions are used, the speed gained by finding wave number rather than grid point solutions is irrelevant. So it also seems that the periodic boundary condition problem could be avoided and nesting within larger scale models could be facilitated by instead storing finite difference grid point solutions with zero gradient lateral boundary conditions. This point is being considered in developing a thermal version of LINCOM, LINCOM-T.

SUMMARY:

Given the 500m resolution and 50x50 km domain size demonstrated for Vandenberg, LINCOM appears to be reasonably accurate, while also capable of running in near real-time. LINCOM can easily run using on-line data updated every minute. It is also considerably more sophisticated than MELSAR and less ad hoc than CALMET because it belongs to a class of linear models which treat neutral flow physics, including the turbulent drag and pressure gradients neglected in pure mass conservation/Froude number based models. I.e., LINCOM belongs to the only class of diagnostic models which includes both mass **and** momentum conservation. Since many Vandenberg towers are sited at ridge tops, a major practical advantage of such models is cognizance of "speed-up" over hills. In reality this "speed-up" occurs not only for neutral but also extends to both unstable and stable conditions. So in its objective analysis, LINCOM should avoid over-estimates of speed in lower terrain, i.e., the bulk of the domain.

Among the class of linear dynamics models the chief advantage of LINCOM is the pre-calculation of purely analytic solutions. This makes it many times faster than other models of this type (e.g., FLOWSTAR, 1988). The chief disadvantage is that any non-neutral physics is currently treated, not in the governing equations, but by objectively analyzed adjustment.

The basis for current work on extending LINCOM to LINCOM-T is that in principle it is possible to treat stable and unstable cases within the linear context analytically. Hunt maintains that this may be true provided that the hill Froude number, $F_H \equiv U_0H/N > 1$. Here U_0 is mean wind speed, H is hill height from 1/2 the hill width, and $N = [(g/\theta)(\partial\theta/\partial z)]^{1/2}$ is Brunt-Vaisala frequency. For $F_H \leq 1$, the Hunt group claims that air will tend to be blocked by or flow around a hill in which case Froude balance models are probably more appropriate (Carruthers and Hunt, 1990). However, as discussed in the CALMET review, Smith's recent work suggests that the kinetic/potential energy balance which forms the basis for the standard Froude number criterion is false (Smith, 1990). If so, LINCOM-T may apply eventually to all stability conditions.

Until LINCOM-T is developed, models such as MACHWIND may be the best currently available for such stable conditions. So for now, these two types of models could be woven easily into a selection system based on measured or estimated atmospheric stability. However, at Vandenberg strongly stable flows are not nearly as common as moderately stable, near-neutral, and unstable ones, due to the influence of the marine boundary layer, particularly during daytime when cold spill potential is higher due to operations. One exception is larger scale drainage out of the Santa Ynez valley. In winter such down-valley drainage may not reverse until mid-morning in the face of a weak seabreeze.

RIMPUFF (T. Mikkelsen et al.):

PHYSICS:

RIMPUFF employs the LINCOM flow field to advect contaminant puffs downstream. Puff growth is controlled by local turbulence level, using spectrally filtered relative diffusion in time and space. As discussed in the analysis of CALMET, the filtering is undertaken to eliminate eddy scales which contribute principally to puff meander rather than diffusion. However, if the mean flow is not updated frequently, RIMPUFF re-introduces the larger eddy scales to simulate stochastic meander of the puff centers of mass. This is particularly important when puff progeny are closely spaced shortly after puff splitting. RIMPUFF initializes 100m puffs and allows them to split horizontally when their diameter exceeds the 500m LINCOM grid spacing or vertically under shear conditions. The practical limit on PC based computers is several hundred puff progeny. Lateral diffusion depends on tower based parametrizations of the lateral dispersion coefficients, $\sigma_{u,v}$. These are a function of averaging time, stability, and wind direction. For vertical diffusion, RIMPUFF currently relies on PG stability classes modified for complex terrain. Note our above caveat on the use of PG classes for estimating plume behavior in the vertical under convective conditions.

Standard Briggs-type equations are used in the plume rise module. 100% reflection is assumed at a user specified inversion height which parallels the terrain. Dry deposition from the standard source depletion method and wet deposition with washout is included. Like the other reviewed models, relevant chemistry, source terms for liquid spills, and options for treating dense gases are not available. Near-field building down-wash is also not implemented. Graphical along with tabular output is provided, and a full graphical user interface is currently available for UNIX based workstations. The source code, written in ANSI F77 standard Fortran is available to Vandenberg, modular, and modifiable. RIMPUFF has been run on DEC computers as well as PCs and should thus be MARSS compatible. Typical run-times are on the order of one minute on a 486/33 PC.

VALIDATION:

Comparisons of LINCOM/RIMPUFF with eight representative cases from the Mt. Iron zinc sulfide tracer study (Kamada et al. 1992a, b) indicate fairly good agreement. However, modeled plumes were longer than measured in seven of the eight cases. This agrees with other modeling comparisons for Mt. Iron data (Kunkel and Izumi, 1990 and Kunkel, 1991) and results from the Vandenberg Lompoc Valley Diffusion Experiment using inert SF_6 tracer in 1989 (Skupniewicz et al. 1991a,c, 1992). Briggs (1988) suggests that, before the deployment of field GC detection equipment for SF_6

around 1970, all previously used tracer compounds had significant deposition velocities. Carruthers and Hunt (1990) suggest that surface concentrations should be independent of deposition velocity within a downwind range given by 5 $z_s U/u_*$. This is just a few hundred meters for Mt. Iron, since tracer was released from a height, z_s, of only twelve feet. So the range discrepancy seems due to a field study rather than modeling artifact.

Case 55 from Mt. Iron shows immediate lofting of the plume under convective conditions, wherein RIMPUFF's dependence on PG classes for vertical diffusion may be demonstrably in error. Unlike the Diablo Canyon study, the Mt. Iron isopleths were relatively short range, hardly extending beyond five kilometers. So better agreement is expected so long as the initial wind vector measured at the release site is itself accurate. Case 28 of the Mt. Iron study shows some discrepancy in this regard. Much of the disparity between the model and Mt. Iron data occurred in the very near field, due to the initial 100 meter puff radii. Much smaller puffs could have been used. However, small puffs must be released frequently to maintain accurate instantaneous concentrations, since the distance between successive puff releases must not exceed ~ 1.5 σ_y. This constraint can be relaxed substantially, if instantaneous concentrations are integrated to give dose exposures, **provided** the wind direction remains constant. In practice smaller initial puff radii often compel increased computer time. This trade-off applies generally to all puff models.

SUMMARY:

In summary RIMPUFF seems to be a fairly sophisticated model whose chief advantage is that it incorporates spectral filtering and averaging time dependent dispersion coefficients which are already tailored for Vandenberg. Thus, RIMPUFF can be run with either a static or frequently updated diagnostic wind field, or even a prognostic one. We suspect that additions to RIMPUFF to include the AFTOX and/or REED-M source terms and chemistry, as well as such items as building down-wash, and similarity based vertical diffusion coefficients would not be as difficult as modifying CALPUFF or MESOI for spectral filtering. RISO Laboratory does support HEAVYPUFF, a 1-D similarity based dense puff also driven by LINCOM (see following review). However, HEAVYPUFF has not as yet been coupled to RIMPUFF. So with respect to Vandenberg's needs the chief current disadvantages of RIMPUFF seem to be inaccuracy in the near-field due to PG based vertical diffusion, and the omission of algorithms for estimating source terms and downwind chemistry, building down-wash, cloud/clear interface, and dense gas effects. The LINCOM/RIMPUFF tandem is generally much faster than the other modeling systems. Nine hours of dispersion involving wind fields spaced every ten minutes (54 in total) required only three minutes on a 15 MIPS 486/33 PC for a 200 x 200 x5 grid at 500 meter resolution.

GENERAL DISCUSSION OF DENSE GASES:

We note that dense gas behavior may differ from that of trace or neutrally buoyant gases in a number of ways. For example, like water in air, the cloud's greater density will cause it to slump and spread laterally to produce a lower, broader cloud, as well as induce it to flow down hill. Greater entrainment will occur at the leading edge for down-slope flow due to the enhanced shear, if the cloud's speed exceeds ambient by a value greater than the friction velocity.

If the cloud is not cold relative to the surface over which it travels, its initial speed may only slowly shift to ambient values. That is, the large cloud/air density difference will suppress cloud top entrainment of ambient air. The strongly stratified in-cloud density gradient will also suppress in-cloud turbulence and thus any side entrainment.

On the other hand the material in question may be stored cryogenically or released upon rupture of a pressurized tank. Sudden expansion upon loss of tank pressure will cool the cloud. If the tank pressure used was sufficient to liquify the material, flashing, i.e., intense boiling and expansive release of a rapidly evaporating mist will occur, at the lower temperatures appropriate to ambient pressure. In any case the resulting cloud will be much colder than the underlying surface. If so, the surface will warm the cloud convectively, thus opposing the turbulence/entrainment suppression induced by density. Material dilution during flashing will also diminish any initial cloud/air speed differences.

If the release occurs in the wake of a building, rapid entrainment may terminate the slumping phase quite quickly. Then the cloud will grow much more rapidly until it is downwind of the wake or the mean cloud height is higher than surrounding buildings. In any event the cloud will eventually behave as a neutral gas due to sufficient dilution with ambient air.

Dense gas models seem to fall into three major categories of complexity: a) 1-D models which assume evenly distributed properties within a cylindrical box; b) intermediate models which assume similarity based vertical profiles of concentration and other properties in the cross-wind plane; and c) fully 3-D Monte Carlo models which diffuse many particle packets of concentration and other properties according to mean advection velocities supplied by the windflow model, plus a turbulence simulating, random component.

The simple box model, HEAVYPUFF, is associated with RIMPUFF, while ADPIC is representative of the more complex Monte Carlo approach. Both will be reviewed in light of the above differences between neutral and dense gas behavior.

HEAVYPUFF (N.O. Jenser, M. Nielsen, RISO National Labs, Denmark)

HEAVYPUFF is a simple PC based, dense puff model which is menu driven, interactive, and delivers graphical output. It requires release inputs such as spill size, storage temperature, wind speed, ambient air and surface temperatures, surface roughness, ambient Obukhov length, L_a, and whether the material is flashing from liquid phase. Initial puff aspect ratio, temperature, and air/gas mass ratio are also input. However, if flashing occurs, the temperature and mass ratio are coupled by enthalpy and cannot be specified independently, since the model computes the amount of air necessary to evaporate exactly all the material. Effectively complete evaporation may occur if depressurization is rapid, or if the heat lost by flashing freezes the surface of the remaining liquid and greatly reduces the subsequent release rate. Such a release will appear as a sudden puff followed by a greatly diminished plume. But the user must then estimate the actual effective spill size outside of HEAVYPUFF.

Left unspecified, the release temperature will default to the liquid's boiling point and the cloud height/radius aspect ratio, h/R, will default to 0.5. The integration time step is user specifiable or variably automatic. Outputs range over a list of 20 variables, including centerline concentrations and the area in which concentrations exceed user specified limits.

The physics in HEAVYPUFF treats heat convection from a warm surface to a cold cloud, using surface layer similarity theory. Ideally, this requires flat terrain and a cloud height much greater than the surface roughness, but much less than the atmospheric boundary layer inversion height. The puff is modeled as a cylindrical box with all properties evenly distributed. Indeed, over a much warmer surface, a cold cloud, once convective, may tend to even distributions due to vigorous turbulent mixing induced by the strong upward heat flux.

In HEAVYPUFF cloud volume and mass increase only by cloud-top entrainment. A parametrized, vertically averaged version of the turbulent kinetic energy (tke) equation, similar to that used for atmospheric boundary layer entrainment, is used to obtain the cloud-top entrainment rate. The heat from the warmer air and shear generated tke is used to entrain air against the resistance imposed by the negative cloud/air density gradient.

However, lateral spreading is driven solely by the cloud/air buoyancy deficit. The influence of ambient diffusion and side entrainment is ignored. Here, our initial thought is that the assumed vigorous unstable mixing seems to run counter to the neglect of side entrainment, even though h/R is small. Cloud height is determined by the rates of lateral spread and cloud-top entrainment. This allows the cloud to slump before growing. However, Jensen (1981) showed that though side entrainment hardly affects the cloud's horizontal spread rate, it may greatly reduce the initial slumping rate.

Since the authors believe that rapid mixing due to rupture of a pressurized tank is the most likely scenario, the puff advection velocity is set to equal the ambient wind speed at cloud top. Data from isothermal releases at Thorney island showed less early advection than HEAVYPUFF due to the initially stationary puff's inertia. The HEAVYPUFF equations are for convective turbulence which implies relatively rapid mixing. So even if the initial puff speed were other than ambient, HEAVYPUFF is not really designed to handle an initially stationary, quiescently turbulent puff, such as those released at Thorney Island.

Even for cases of rapid mixing over flat terrain, we suspect that cloud speeds may differ from ambient, since in-cloud and ambient Obukhov lengths, L_c and L_a will differ. I.e., cloud/ambient differences in stability should generate different vertical profiles of wind speed resulting in cloud-top shear. The computed speed difference might provide a basis for a more definite and larger value for shear induced cloud-top entrainment than the form, Cu_*^3/h, now assumed in HEAVYPUFF's tke equation. As diffusion proceeds and cloud-top shear and surface heat flux decay, use of such an algorithm should allow L_c values and hence cloud-top speeds to approach ambient levels smoothly.

Down-slope flow is neglected; thus, so is lead edge entrainment. This probably makes the current model unsuitable, since Vandenberg's Hypergolic Stockpile and Storage facility sits on a mesa often just upwind of the steep slope to the Santa Ynez River Valley. Jensen (1981) has suggested a number of first order adjustments for terrain slope, side entrainment, building wake effects, above ground releases, and the modeling of dense plumes rather than puffs, all of which may be suitable for eventual inclusion in HEAVYPUFF. More recently, Kukkonen and Nikmo (1992) have installed down slope components in a cylindrical box model. The model's simplicity allows for fast runtimes and coupling to RIMPUFF should also be fairly straight forward. However, source term mechanics and chemistry and engineering/probability estimates for flashing/non-flashing scenarios are still required.

(MATHEW/ADPIC M. Dickerson, R. Lange, D.L. Ermak,
Lawrence Livermore Labs)

MATHEW: (M. Dickerson, C.S. Sherman)

MATHEW is a wind flow model used to drive ADPIC. MATHEW makes minimal adjustments to an objectively analyzed wind field by variationally minimizing the 3-D divergence to ensure mass consistency. Unlike LINCOM, MATHEW does not include momentum balance in its interpolative adjustment. The description given in the MATHEW/ADPIC user's guide is highly mathematical and optimized for vector computer performance. But the main concepts can be taken from an earlier description by Sherman (1978). In essence the operative error functional to be minimized is,

$$E(u,v,w) = \iiint [\alpha_1^2(u-u_0) + \alpha_1^2(v-v_0) + \alpha_2^2(w-w_0)^2 + \lambda\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}\right)] dxdydz \quad . \tag{13}$$

where u_0, v_0, w_0, are the objectively analyzed variables; $\lambda(x,y,z)$ is the Lagrange multiplier; and the α_i are Gauss precision moduli taken to be $\alpha_i^2 \equiv 1/2\ \sigma_i^2$. The σ_i are deviations of the objective from the adjusted field. This model is unlike WOCSS or MACHWIND, where vertical divergence is parsed over layers defined by a CSH to produce a pseudo-2-D divergence equation, as in eqns. (6-12). Unlike NUATMOS, the vertical Gauss modulus, α_2, does not try to include the effect of speed-up over hills, but the code does have stability dependent divergence parsing. At any rate, minimization of eqn. (13) requires the solution of

$$\begin{aligned} u &= u_o + \frac{1}{2\alpha_1^2}\frac{\partial\lambda}{\partial x} \\ v &= v_o + \frac{1}{2\alpha_1^2}\frac{\partial\lambda}{\partial y} \\ w &= w_o + \frac{1}{2\alpha_2^2}\frac{\partial\lambda}{\partial z} \\ &\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \quad , \end{aligned} \tag{14}$$

subject to the x, y, and z boundary conditions,

$$n_x \lambda \, \delta(u) = 0$$

$$n_y \lambda \, \delta(v) = 0 \qquad \textbf{(15)}$$

$$n_z \lambda \, \delta(w) = 0 \ .$$

$\delta(\ )$ gives the first variation in the bracketed quantity and the n_i are the positive outward unit normals on the boundaries. λ is obtained by differentiating eqns. (14a,b, and c) and substituting into eqn. (14d) to give

$$\frac{\partial^2\lambda}{\partial x^2} + \frac{\partial^2\lambda}{\partial y2} + \left(\frac{\alpha_1^2}{\alpha_2^2}\right)\frac{\partial^2\lambda}{\partial z^2} = -\,2\alpha_1^2\left[\frac{\partial u_o}{\partial x} + \frac{\partial v_o}{\partial y} + \frac{\partial w_o}{\partial z}\right] \ . \qquad \textbf{(16)}$$

Eqn. (16) is solved with the boundary conditions from eqn. (15) and the adjusted velocity field is obtained from eqn. (13).

Aside from being a purely mass conservative model, perhaps the main limitation of MATHEW is the approximation of terrain features as rectangular blocks at the resolution of the Eulerian grid. This can lead to excessive flow blockage when the terrain is steep. When used with the dense gas version of ADPIC, the imposed stair-stepped approximation to terrain slopes can also produce distortions in cloud shape, since dense gas clouds may be on the order of one grid cell high (see ADPIC review below). A change to terrain following coordinates might be useful, provided all conserved quantities can be maintained.

ADPIC: (R. Lange, D.L. Ermak)

To depict material concentrations the dense gas version of ADPIC allows Lagrangian particles to diffuse in Monte Carlo fashion within a 3-D Eulerian grid composed of rectangular cells. This is somewhat different from the original neutral ADPIC which used a down-gradient diffusion model for turbulence to solve the flux conservation equation,

$$\frac{\partial C}{\partial t} + \nabla\cdot(C\bar{U}_p) = 0 \ . \qquad \textbf{(17)}$$

Here C is concentration and $\bar{U}_p$ is a pseudo-transport velocity. $\bar{U}_p$ includes a mean advection velocity, $\bar{U}_a$, from MATHEW, and a diffusion velocity, $\bar{U}_d$, both interpolated to each particle's position. In dense ADPIC $\bar{U}_d$ is not imposed as being proportional to the concentration gradient. Instead, it arises from the aggregate of random and independent particle motions. This point is not always clear and both versions of ADPIC are rather different from the above-reviewed puff models. So it may be useful to analyze the main equations in some detail. In discussing the original ADPIC, if we use a vector identity, eqn. (17) is equivalent to

$$\frac{\partial C}{\partial t} + \bar{U}_p \cdot \nabla C + C \nabla \cdot \bar{U}_p = 0 \quad . \tag{18}$$

Since

$$\bar{U}_p = \bar{U}_a + \bar{U}_d \quad , \tag{19}$$

we have,

$$\frac{\partial C}{\partial t} + (\bar{U}_a + \bar{U}_d) \cdot \nabla C + C \nabla \cdot (\bar{U}_a + \bar{U}_d) = 0 \quad . \tag{20}$$

MATHEW has already arranged $\bar{U}_a$ to be non-divergent, i.e.,

$$\nabla \cdot \bar{U}_a = \frac{\partial \bar{U}_a}{\partial x} + \frac{\partial \bar{U}_a}{\partial y} + \frac{\partial \bar{U}_a}{\partial z} = 0 \quad . \tag{21}$$

So eqn. (20) becomes

$$\frac{\partial C}{\partial t} + \bar{U}_a \cdot \nabla C = -\bar{U}_d \cdot \nabla C - C \nabla \cdot \bar{U}_d \quad . \tag{22}$$

Reversing the above vector identity now gives,

$$\frac{\partial C}{\partial t} + \bar{U}_a \cdot \nabla C = -\nabla \cdot (C \bar{U}_d) \quad , \tag{23}$$

In dense ADPIC the particles move independently and randomly. But the original neutral ADPIC assumes that diffusion velocity is proportional to the material concentration gradient determined at the grid points,

$$\vec{U}_d = -K\cdot\nabla C/C \quad , \tag{24}$$

where K is a diffusion coefficient appropriate for the ambient conditions. The material concentration gradient is equated with the aggregate particle density gradient. Each particle's diffusion velocity is obtained by interpolating the values at the grid to the individual particle positions. In this way eqn. (23) becomes,

$$\frac{\partial C}{\partial t} + \vec{U}_a\cdot\nabla C = \nabla\cdot(K\nabla C) \quad . \tag{25}$$

Using non-divergence and the vector identity again,

$$\nabla\cdot(C\vec{U}_a) = \vec{U}_a\cdot\nabla C + C\nabla\cdot\vec{U}_a = \vec{U}_a\cdot\nabla C \quad . \tag{26}$$

This leaves the flux conservation equation in the pseudo-velocity form,

$$\frac{\partial C}{\partial t} + \nabla\cdot\left[C(\vec{U}_a - \frac{K}{C}\nabla C)\right] = \frac{\partial C}{\partial t} + \nabla\cdot(C\vec{U}_p) = 0 \quad . \tag{27}$$

The particles move within the cells but advection velocities: U, V, W, and also K, $\vec{U}_a$, and C are defined only at the grid points. C is obtained for each grid point from a weighted sum of the mass within the eight surrounding cells. This is done simply to smooth stochastically induced unevenness in the distribution.

The dense gas version of ADPIC adds an in-cloud gravity flow component,

$$\vec{U} = \vec{U}_a + \vec{U}_g\cdot g_i(z) \quad , \tag{28}$$

to the ambient velocity field, $\vec{U}_a$, supplied by MATHEW. Here U_g is the vertically averaged perturbation of the horizontal wind due to gravity. $g_i(z)$ is a vertical profile function. The subscript, i, may be horizontal, h, or vertical, v. Thus, the down-slope flows are simulated by deterministic advective components which include gravity. For the diffusive component, rather than the original strict down-gradient fashion of eqn. (24), in dense ADPIC the adjusted velocity field is used to displace the Lagrangian particles stochastically in random Monte Carlo style, so that,

$$
\begin{aligned}
x_{t+1} &= x_t + \bar{U}\Delta t + R_x(\Delta t) \\
y_{t+1} &= y_t + \bar{V}\Delta t + R_y(\Delta t) \\
z_{t+1} &= z_t + \bar{W}\Delta t + R_z(\Delta t) + \upsilon_o\Delta t \quad .
\end{aligned}
\tag{29}
$$

U, V, and W are the local velocity components, interpolated from the grid to the individual particle positions, and R_x, R_y, and R_z are independent, normally distributed (Gaussian) random displacement components. The R_i are specified as having zero means and the following mean square (< >) properties,

$$
\begin{aligned}
\langle R_x^2 \rangle &= 2K_x\Delta t \\
\langle R_y^2 \rangle &= 2K_y\Delta t \\
\langle R_z^2 \rangle &= 2K_z(z(t))\Delta t + \upsilon_o^2\Delta t^2 \quad .
\end{aligned}
\tag{30}
$$

The horizontal and vertical diffusivities for momentum, K_i, are derived from similarity theories and $\upsilon_0 = \partial K_z/\partial z$ is a drift velocity correction. Drift correction is used to counter the tendency for particles to accumulate in low turbulence regions. The problem is that the near presence of a hard surface truncates the modeled turbulence scales and severely restricts particle motion, producing long residence times near the ground. So particles tend to accumulate. In ADPIC this effect is implied by K_z approaching zero as z approaches zero. In reality, turbulence tends to be positively skewed near the ground. So large but intermittent burst/sweep turbulence events will at times breach the quasi-laminar sub-layer and eject particles which would otherwise be trapped near the surface. Some models include such skewness explicitly (see Baerentsen and Berkowicz, 1984). However, this generates a modeling paradox, since particle reflection off the surface should reverse any skewness and in the aggregate make it difficult to maintain. So drift velocity is a standard ad hoc method used to avoid such complexities.

ADPIC equates drift velocity with the vertical momentum diffusivity gradient, $\upsilon_0 = \partial K_z/\partial z$. This form of drift velocity is non-local but computationally less expensive than the original form proposed by Legg and Raupach (1982) (installed in a third version of ADPIC) which requires that the local gradient of vertical velocity variance be computed instead. Since $\partial K_z/\partial z$ becomes large near the surface, the general effect is the same, to give near-surface particles an extra upward kick.

The vertical diffusivity is defined according to surface layer similarity theory by

$$K_z = \frac{ku_* z}{1 + \frac{5z}{L_c}} \quad , \tag{31}$$

where in-cloud and ambient Obukhov lengths, L_c and L_a, differ by

$$L_c^{-1} = L_a^{-1} + 2gk^2 \frac{(\rho - \rho_a)}{\rho u_*^2} \tag{32}$$

and u_* is friction velocity. ρ and ρ_a represent the vertically averaged in-cloud and ambient densities.

Simple bulk transfer is used to account for the ground flux of heat, J_g, into a cold, dense cloud,

$$J_g = \rho C_p V_h (T_g - T) \quad . \tag{33}$$

Rather than employing a more involved surface energy balance, T_g, the ground temperature has thus far been equated with ambient air temperature, T_a. T and C_p are local layer averaged cloud temperature and heat capacity, and V_h is a bulk heat transfer coefficient.

In inspecting eqns. (31-32), we note that standard similarity theory defines L_a in terms of the friction velocity and kinematic heat flux, $\overline{w'\theta'}$, i.e.,

$$L_a \equiv -\frac{u_*^3 \theta}{gk\overline{w'\theta'}} \quad . \tag{34}$$

So in eqn. (32) for $L^{-1} = 0$ (neutral stability) we see that the fractional density surplus in the ADPIC cloud is given by

$$\frac{\rho - \rho_a}{\rho} = \frac{\overline{w'\theta'}}{k u_* \theta} \quad . \tag{35}$$

For cold releases due to cryogenic storage or pressure drops following rupture of a pressurized tank, $\overline{w'\theta'}$ may be of order 1 ms^{-1}°K or larger. $k \approx 0.4$, ambient u_* may be ~ 0.1 - 0.2ms^{-1}, and $\theta \approx$ 300°K. So the equations seem to allow the cloud to become unstable ($L_c < 0$) at density differences of ~ 4% or larger, i.e., well before reaching ambient density. If so, both the form used for V_h and the denominator in eqn. (31) (given above only in the standard similarity form for stable conditions) must change to reflect unstable conditions. In turn this should increase the vertical diffusivity, expand the cloud, and speed its approach to neutral gas behavior. In unstable ambient conditions the feedback loop appears positive because the cloud will also tend toward instability as the cloud/air density difference decreases. If so, accurate timing of stable/unstable transitions may be significant generally in modeling surface-heated cloud development.

The authors respond that the above u_* is actually an in-cloud term which varies with L_c, such that cloud instability is unlikely; in any event cloud growth is not affected much by in-cloud stability. On the other hand, HEAVYPUFF assumes that a surface-heated cloud is essentially unstable. So a convective velocity like w_* can be used to help scale the cloud-top entrainment rate. Clearly, the difference in physical assumptions suggests more scrutiny of both models, as well as the timing and effect of real cloud stabilities.

Above the surface layer, K_z is computed by the empirical form,

$$K_z = C U_* z e^{-z/z_i} \quad , \tag{36}$$

where C is an empirically derived coefficient and z_i is boundary layer height. Equation (31) could be replaced by more modern, stability dependent forms, such as those of Sorbjan (1989).

In ADPIC U_g arises from a balance between gravitational forces, dissipative cloud-top entrainment, and ground friction, after assuming steady state gravity flow and hydrostatic balance. This yields, for the gravity induced component of the horizontal wind,

$$\rho\omega_e U_g = -\frac{d}{dx}[0.5g(\rho - \rho_a)h^2] - g(\rho - \rho_a)h\frac{dH}{dx} - \rho u_f U_g \quad ,$$

$$\rho\omega_e V_g = -\frac{d}{dy}[0.5g(\rho - \rho_a)h^2] - g(\rho - \rho_a)h\frac{dH}{dy} - \rho u_f V_g \quad , \tag{37}$$

where ω_e is the cloud-top entrainment rate, g is gravitational acceleration, h is cloud height above the terrain, H is terrain height, and u_f is the surface friction coefficient. ω_e is taken to be proportional to $K_z(h)/h$. Since the densities are vertically averaged, this gravity component does not seem to be height dependent.

The gravity induced component of the vertical wind does appear to be height dependent and is given by,

$$W_g \cdot g_v(z) = -\left[\frac{\partial U_g}{\partial x} + \frac{\partial V_g}{\partial y}\right] \cdot \int_0^z dz\ g_h(z) \quad . \tag{38}$$

Save for the $g_h(z)$ and $g_v(z)$ adjustments, eqn. (38) looks like the one for which a detailed derivation was given in the review of WOCSS and MACHWIND (eqn. 4). But here the gravity flow field, a sub-set of the total velocity field, is assumed to be non-divergent in itself. We question this and also wonder whether the hydrostatic balance assumed in eqn. (37) applies to such small scales. The current cloud-top entrainment term also seems to neglect the resistance provided by the negative density gradient across the cloud/air interface and also assumes that the cloud is stable. As discussed above, parametrized tke budgets are an alternative approach to cloud-top entrainment which can be used for both stable and unstable conditions.

Gravity flow should allow the initial slumping phase to occur for isothermal cases and the Monte Carlo diffusion should model the side entrainment. However, since shear is currently neglected, the extra lead edge entrainment expected during down-slope flow does not appear to be modeled in dense ADPIC.

In ADPIC, an energy deficit, ϵ_i, induced by the cloud/air enthalpy (heat content at constant pressure) difference is used to treat the effect of ground heating. Starting from an initial value of unity, at each time step, ϵ_i decreases slightly by the inverse geometric factor, $1/(1 + \lambda)$, where $\lambda = \Delta t V_h/h$. Since the time step, Δt, and heat transfer coefficient, V_h, are fixed, this rate varies only with cloud height, h. Since dense clouds are typically much wider than they are tall, ADPIC assumes reasonably that cloud expansion due to surface heating occurs solely in the vertical direction. Thus, changes in cloud height and temperature due to surface heating are directly proportional. This implies that the energy deficit reduction rate is largely regulated by the vertically averaged cloud temperature, T. Conversely, the vertically averaged energy deficit defines T which in turn controls the vertically averaged density, ρ, which in turn helps regulate the ground heat flux and gravity flow.

Advection/diffusion effects are included by tagging each Lagrangian particle with an individual energy deficit. Thus, Monte Carlo diffusion transports the enthalpy in all directions, while aggregate displacements affecting cloud height feed back to the energy deficit reduction rate. Without deeper analysis we cannot say yet whether this energy deficit approach properly couples and represents both dispersion and heating effects.

Some further algebra, plus the approximation that thermal expansion occurs only vertically, leads to an equation for the additional particle displacement due to surface heating,

$$\Delta z_H = \frac{\lambda(\frac{T_a}{T_o} - 1)}{1 + \lambda} z_o \quad . \tag{39}$$

So for each particle Δz_H is added at each time step to the vertical displacement obtained from eqn. (29). Also at each time step, all the dispersive computations are executed separately from the thermodynamical ones in order to simplify the equations.

ADPIC is a mature model in the sense that many features of operational interest have been added to the basic scheme. The model includes graphical user interfaces, dry and wet deposition, plume rise, and explosive cloud rise. This last feature may be of particular interest to Vandenberg and should be analyzed in detail in a later study.

Building wake effects are not included yet in ADPIC, but model structure does not seem to preclude the necessary local adjustments to the diffusivity profiles. The rectangular Eulerian grid used in MATHEW creates a stair-step surface along slopes which can lead to significant flow artifacts for low-lying dense gases. An ADPIC upgrade, scheduled for mid-1993, will replace the stair stepping with an improved piece-wise continuous, linear interpolation from grid point to grid point. However, MATHEW will probably retain the stair-stepping beyond 1993. As with the other models, additional source term chemistry and mechanics are also needed to determine proper input values and potential scenarios such as flashing.

The model compared quite closely with results from two cases of 111.7 °K (boiling point) methane released into an atmosphere at 298 °K. ADPIC's equations have exact analytic solutions for these two idealized cases. In both cases advection occurred only in the x direction. The first case was isothermal and only vertical diffusion was allowed. Vertical diffusion was turned off in the second case, while surface heating was turned on. This indicates that numerical errors and errors due to the finite number of particles (5000) were quite minimal (~1%) over the time span of the comparisons (36 seconds).

Further comparisons against experimental data would be required to analyze the quality of ADPIC's new physics. In particular, we might suggest that ADPIC's thermodynamics be tested under more controlled conditions than can be achieved in the atmosphere. This might be possible by making comparisons against heated tank data involving two miscible fluids with different densities.

Execution time is a remaining question. For a demonstration 51 x 51 x 15 grid over a 35 km domain the objective analysis routine, MEDIC, executes together with MATHEW in less than one minute on a DEC 5000/200 workstation. In the same demo five hours of diffusion using K-theory ADPIC and 5000 particles took less than one minute. Monte Carlo versions should execute faster, since the aggregate particle concentration gradient does not need to be evaluated to obtain the grid point diffusion velocities which must then be interpolated back to the individual particle positions. Also, grid cells lacking particles can be ignored. So the main computational expense for Monte Carlo ADPIC is random number generation which is in the process of being made more efficient. This type of random displacement model appears to be considerably faster than the random velocity models used in most Lagrangian particle simulations. So the inclusion of ADPIC within an optimal diagnostic modeling suite is tempting, since it is designed to handle many of the dense gas scenarios one expects for large accidental releases at Vandenberg.

SUMMARY:

The new ADPIC is a quasi-3-D model which may be suitable for emergency response use at Vandenberg for puffs and plumes. It employs random Monte Carlo rather than down-gradient particle motions to model diffusion. Gravitational terms are added to treat dense gas behavior. ADPIC is designed to treat surface heating, cloud-top entrainment, and down-slope flow.

For surface heated dense gases the possible transition from stable to unstable cloud conditions may be of significance, since once the cloud is unstable the heating feedback loop becomes positive and mixing may increase considerably. We seek clarification of the non-divergence and hydrostatic assumptions used to obtain the gravity flow terms and also suggest an alternative tke approach to modeling the cloud-top entrainment. Extra lead-edge entrainment during down-slope flow does not seem to be included. The Lagrangian particles carry not only material mass but also individual energy deficits which are used to determine temperature changes and thermal expansion effects. We cannot say yet whether this energy deficit approach properly couples and represents both dispersion and heating effects.

Stair-stepped surfacing along slopes will be retained in MATHEW in the near term but is to be replaced shortly in ADPIC by straight line interpolation between grid points. This should be of considerable benefit to low-lying dense gas simulations. Building wake effects are not included, but the model structure does not seem to preclude the required adjustments. Comparisons with analytical results indicate accurate numerical execution for two idealized cases. Further tests against relevant experimental data may be required to assess ADPIC's underlying physics. Source term chemistry and mechanics are also needed to implement ADPIC operationally at Vandenberg. In general some of dense ADPIC's physics may not be fully mature or at least remains to be validated at this juncture. However, Monte Carlo deployment of thousands of Lagrangian particles in a manner which includes dense gas effects and is fast enough for emergency response makes ADPIC a strong candidate for installation at Vandenberg. Like most diffusion models ADPIC can probably be decoupled fairly readily from MATHEW.

OVERALL SUMMARY COMMENTS ON THE MODELS:

This summary is predicated on ready decoupling of the windflow and diffusion components of the modeling systems reviewed above. Based on the currently available documentation and perhaps in the following order, dense ADPIC, RIMPUFF, and CALMET appear to be the most viable diffusion models for Vandenberg applications at this time. ADPIC has the large advantage that it treats dense gases in Lagrangian particle fashion and yet seems fast enough for emergency response on current workstations. It also contains an explosive cloud rise module. At this point we retain some reservations regarding ADPIC's physics. Among the puff models CALPUFF seems to have the most inclusive features, while RIMPUFF has perhaps a more fundamentally sound basis. Changes would be required for either puff model to perform satisfactorily in the Vandenberg setting. Additions such as a graphical user interface and output, spectral filtering, relevant chemistry, source term specification, and dense gas effects would be required in CALPUFF. Chemistry, source terms, dense gas, improved vertical diffusion, and near-field characterization of items such as building down-wash would be required for both ADPIC and RIMPUFF. Some features might be provided by modules already contained in the ADAM, AFTOX, HEAVYPUFF, and ADPIC models. ADPIC and RIMPUFF already have UNIX based graphical user interfaces. Coupled to RIMPUFF, HEAVYPUFF, a simple cylindrical box model, may also be suitable for dense gas dispersion in relatively flat terrain, where the surface is heated, but would need adjustments for slope flow which are apparently manageable. All reviewed diffusion models could profit by the inclusion of diffusion and flow parametrizations specifically addressed to changes across the coastline and cloud/clear interfaces.

There is no undisputed winner among the diagnostic windflow models. A selection scheme using LINCOM for unstable to slightly stable conditions and MACHWIND for stable conditions may be most robust, as well as cost effective, since these two models are probably nearest to operational form for Vandenberg purposes.

Taken individually, each flow model displays limitations which leave cause for concern. Though in rough agreement with laboratory results, the physical basis of the Froude number criterion and models based on them such as WOCSS, CALMET, and MELSAR are suspect. At its present grid resolution, sub-grid parametrizations and speed, CALMET seems intended for regional rather than Vandenberg scales. According to preliminary results from CARB's Los Angeles Air Basin study, CALMET's windflow may deviate substantially from tower indicated winds when its slope flow adjustment scheme has difficulty defining a mean background wind in complex terrain. CALMET may also not be fast enough for emergency response on workstation class computers at the required 500 meter resolution over a 50x50 kilometer domain, while MELSAR, LINCOM, WOCSS, MATHEW, and MACHWIND clearly are. However, the MELSAR and MATHEW windflow schemes seem rather dated. According to available documentation MELSAR's maximum resolution over a 50 x 50 kilometer domain would be 1 kilometer, i.e., insufficient resolution. MATHEW also uses problematic rectangular rather than terrain following coordinates. The flow schemes in LINCOM, WOCSS, and MACHWIND are essentially terrain following. Information concerning the speed of NUATMOS has not been made available. We understand that NUATMOS was included in the test suite of models over Rocky Flats but documentation has not been received. In general the presumption that the background mean flow can be defined in the context of complex terrain is more viable over the Vandenberg domain than at larger regional scales. At this time LINCOM's major drawback is that its momentum budget treats only neutral flow physics. However, it is the only windflow model among those seriously reviewed which includes momentum as well as mass conservation equations.

Among the larger issues such as availability, portability, maintenance, validation, and total life-cycle cost, LINCOM/RIMPUFF seems to be the overall least expensive choice, since it has already been tested on a relevant Vandenberg data set. User support and the availability of future upgrades is also important and contingent upon the stability of support staff. Regarding these issues, CALMET/CALPUFF is available in its entirety from the EPA electronic bulletin board. WOCSS/Adaptive plume remains in the public domain. MELSAR/MESOI is presumed available from PG&E, as is NUATMOS/CITPUFF from the EPA. CALMET/CALPUFF and MELSAR/MESOI are supported by large public agencies. MATHEW/ADPIC is maintained by a large staff at Lawrence Livermore Labs. WOCSS/Adaptive plume is supported by SRI International but on a lesser scale. MACHWIND is maintained by U.S. Army Atmospheric Sciences Lab. LINCOM/RIMPUFF has been supported by the Naval Postgraduate School and RISO National Laboratory of Denmark. The current status of NUATMOS/CITPUFF has not been ascertained. Real installation costs and short term technical support are important issues which cannot be resolved prior to the fact. However, MACHWIND and LINCOM/RIMPUFF have both been run on Vandenberg terrain and conditions.

It is known that versions of all the above models, perhaps save for NUATMOS/CITPUFF, have been run on DEC computer systems. So MARSS compatibility is not expected to be a problem, provided hardware upgrades beyond the MicroVAX II (1 MIPS) level become available to Vandenberg. At this point it is difficult to imagine an overriding reason for operational use of a good diagnostic dispersion model on less than a 25 MIPS machine, i.e., a 486/50 PC. So this review has not been written with the constraint of MicroVAX II and VMS operating system compatibility in mind. If such a constraint were invoked, then PGEMS and LINCOM/RIMPUFF would likely be the only two remaining viable candidates. Of course, conversion to a GUI different from the 2-D graphics based MARSS and retraining of FSC staff involves some time, effort, and expense. This might be saved if the current hardware were replaced by DEC Alpha-chip based VMS systems. However, Yamada Science & Art is scheduled to deliver the prognostic HOTMAC/RAPTAD modeling system to Vandenberg on a UNIX workstation in late 1993. So conversion or at least inclusion of UNIX based systems appears to be inevitable. The potential also exists for faster, more accurate reality checks of dispersion results, if modern 3-D point-and-click GUIs are installed.

A number of other models were also considered. The FLOWSTAR flow model from Carruthers and Hunt's firm, Envirosoft, Cambridge, England, is among the most interesting, since it treats complex terrain physics for a variety of stabilities, albeit in a linear manner. However, due to its use of numerical solutions, it does not yet seem fast enough for Vandenberg emergency response, even on workstation class computers. Also briefly considered were TRAC from Rocky Flats, Colorado, the EPA CTDM and CTDM+ models, and the EPA Urban Airshed Model which is apparently a precursor to CALMET. HARM II from Oakridge Labs is reputed to feature dense gas, chemistry, and source term modules. However, the available documentation was not adequate to assess its merit.

We have yet to mention that none of the considered models contains modules for such items as: blast overpressure, back calculation of source strength from on-site receptor data, or overall risk assessment. Apparently, ACTA is working on a risk assessment model. The commercial model, SAFER, from Dupont also contains some of these modules. However, SAFER source code, documentation details, and modification rights are apparently not available, even though the working algorithms are all based on public domain EPA models. So this model was not seriously considered.

We presume that this evaluation of the technical and practical merit of several models will be considered along with others in making an initial determination of detailed study for a few of them. We hope these comments prove useful in furthering such an effort.

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