Air-Quality Dispersion Modeling in Complex Terrain near the Umatilla Chemical Agent Disposal Facility, Hermiston, Oregon.

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May 11, 2000

Abstract:

Meteorological data at the Umatilla Chemical Agent Disposal Facility near Hermiston, Oregon, show a remarkable 58% of hours with stable air. A consequence of this will be many episodes with reduced efficiency for the dispersion of emissions.

Dispersion models suggest infrequent, but occasionally severe "garden-hose" impacts on the neighboring communities of Hermiston, Umatilla, Plymouth, Irrigon, and Boardman, with short-term concentrations several hundred times the annual averages at these sites. Attention should therefore be paid to non-linear effects on the exposed populations and to off-design emissions during stable conditions.

I. Introduction

The US Army, contracting with the Raytheon Demilitarization Company, is constructing an incinerator complex at the US Army's Chemical Agent Disposal Facility [UMCDF], located near Hermiston, Oregon. Many studies support this effort, including a Pre-Trial Burn Risk Assessment [ref.1], prepared for the Oregon Department of Environmental Quality [ODEQ], which reports use of on-site meteorological data from several months of 1994 and the Environmental Protection Agency's [EPA] Industrial Complex Short Term model [ISCST-3] to estimate annually averaged wet and dry depositions, and near-surface tracer concentrations. A central conclusion of this effort was that the principal impacts were expected to be short-range and that the maxima of air-quality degradations would likely remain on-site.

Meteorological measurements have continued to be collected at the UMCDF site since 1994, specifically including hourly temperatures, wind speeds and directions at 10 and 30 meters, together with the standard deviations of wind directions, and the solar radiation, precipitation, and atmospheric pressure [ref. 1].

Conspicuous among these data is an exceptional frequency of statically stable air, in 58% of 29,967 non-default hours between mid 1994 and the end of 1998. A consequence of this stability will be a frequent occurrence of "garden-hose" plumes that snake out close to the ground for relatively long distances, with little mixing. Owing to their narrow lateral dispersions, these plumes may be expected to miss the neighboring communities, most of the time, but occasionally to hose them with effluent concentrations many times higher than the annual averages at these communities.

For this reason I have undertaken additional modeling efforts to estimate potential impacts from shorter-term events in the Umatilla airshed, at longer ranges. In the following sections of this report I briefly describe WPUFF, a time-dependent, Lagrangian-puff, air-quality dispersion model, the meteorological data, stabilities, the terrain and modeled domain, emissions, and the results of simulations. I compare these results with those of a simple Gaussian-plume model, and I discuss their implications. I conclude with suggestions for on-line, real-time modeling of the UMCDF plume, with special attention to air-quality management during upsets.

II. WPUFF

For many years air-quality modeling studies have relied heavily on a set of "guideline" models recommended by the US Environmental Protection Agency. Most of these models, including ISCST-3, are variants of "Gaussian Plumes", as described by Turner's classical workbook [ref.2]. These guideline models have a long track record that enables useful comparisons among different sites, emission geometries, and meteorological conditions, and they serve usefully for preliminary "scoping" studies to estimate relatively long-term averages of concentrations and depositions of emitted tracers.

A major approximation of Gaussian-plume models is that winds are assumed to be steady over times that are long compared with a tracer's transit across the modeled field .. roughly an hour or more. As wind data are often not available more frequently than once an hour, this approximation is often not unreasonable. It has been increasingly appreciated, however, that tracer-parcel trajectories deviate greatly from steady states in time scales that are less than one hour, especially at low wind velocities and over complex terrain. Under these conditions .. which frequently obtain in the Umatilla airshed .. steady-state air-quality models such as ISCST-3 may be expected to generate significant errors with shorter-term, higher-concentration episodes.

Responding to these and other concerns, the national EPA and the California Air Resources Board [CARB] are encouraging the development and use of time-dependent air-quality models. One sensible effort in this direction is to simulate a series of emitted puffs that are allowed to expand and disperse while driven by the model's best perception of the wind fields. CALPUFF [ref.3] is an example of this approach. WPUFF is Another [Appendix A].

The two models share many common features but are distinguished by different ways to estimate those wind fields. CALPUFF usually employs CALMET [ref.3] to interpolate off-site meteorological soundings to estimate the winds in the local field and terrain. WPUFF assumes one or more on-site, near-surface wind measurements, and applies a mass-conserving algorithm to minimize near-surface convergences driven by complex terrain. That is, WPUFF constrains the tracer puffs from blowing through hills, and biases the winds to deflect around them, when the air is stable.

Both models are useful, and their approaches to estimating the local winds should converge, with perfect data. As good, local meteorological [Met] data are available at the UMCDF site [ref.1], and for other advantages of convenience and display, WPUFF was selected for this present study. A further discussion of WPUFF is deferred to Appendix A.

III. Meteorological Data

As I have mentioned above, exceptionally complete meteorological measurements have been collected at the UMCDF site since 1994 [ref.1]. From these data it is straightforward to estimate both vertical and horizontal diffusivities, vertical stabilities, and the vertical gradients of the near-surface wind velocities, temperatures, and directions; all contribute to sensible air-quality simulations. [Appendix A].

For the present dispersion studies I have selected the complete years 1995-1998, with a total of 35064 hourly records.

Default data entries [approximately 0.5% of all records] were treated as if persistent by repeating the nearest preceding non-default entries.

IV. About Stabilities[1]

As a central theme of this report is the exceptional incidence of very stable air in the Umatilla airshed, it is appropriate to discuss stability a little further.

When a parcel of dry air is lifted from the surface it expands and cools. The air outside that parcel also cools with height above the surface. If the rising parcel cools more rapidly than the air around it, that parcel becomes more dense than the ambient air, its buoyancy diminishes, and its rise is slowed, and then reversed. This condition defines "statically stable air"[1].

Quantitatively, the ambient air is statically stable[1] when

$$d\Theta v/dz = dTv/dz + 0.01 > 0 \qquad \text{[eqn.1]}$$

[degC / meter]

The "Tv" in equation 1 is the ambient "virtual temperature",the physical temperature corrected slightly for the ambient air's water-vapor content. "Θv" is called the "virtual potential temperature". Often the "virtual" is omitted in ordinary conversation, and the simple temperature, T, is substituted for Tv. In desert air, as in Umatilla, the difference is usually small.

The meteorological data at the Umatilla site include temperatures at both 2 and 30 meters above the surface, from which it is straightforward to calculate the potential temperature gradients. As I have stated above, the incidence of positive potential temperature gradients .. that is, statically stable air .. is exceptional at Umatilla: 58% of 29,967 non-default hours were stable between mid 1994 and the end of 1998. Over 90% of hours between 8 PM [PST] and 6 AM were stable [fig.1]. Stable air is more common in winter, but present in all seasons [fig.2]. In

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[1] In this note the expressions “stable air” and “stability” are used interchangably with “statically stable air”, and “static stability”, with units of degC/meter.. These stabilities should be distinguished from the common usage of “Pasquill-Gifford Stability Classes” [A, B, C, ..], which are discussed briefly in Appendix A. Static stabilities are appropriate to discussions of plume buoyancies and near-surface transport.

more than 23% of all hours [41% of stable hours] the near-surface potential temperature gradients, dΘv/dz, exceed +0.06 degC/m, which is very stable indeed. [Appendix A, p24, Table VII]

In consequence of this exceptional stability, initially buoyant plumes emitted at the Umatilla facility are expected often to limit their rise and subsequently to be transported as if squirted from "garden hoses", relatively close to the surface, snaking out for relatively longer distances, with little dispersion.

A further discussion of stabilities, as they interact with vertical diffusivities, is deferred to Appendix A.

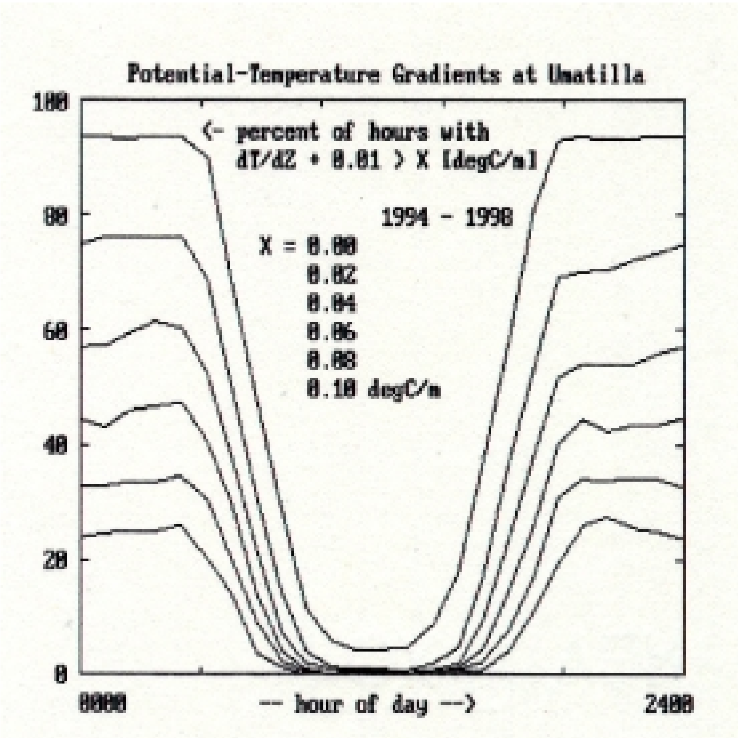

Figure 1.

Diurnal wave of stabilities. Note that over 90% of nighttime hours are stable. In 23% of all hours, [41% of stable hours], the near-surface potential temperature gradients exceed +0.06 degC/meter.

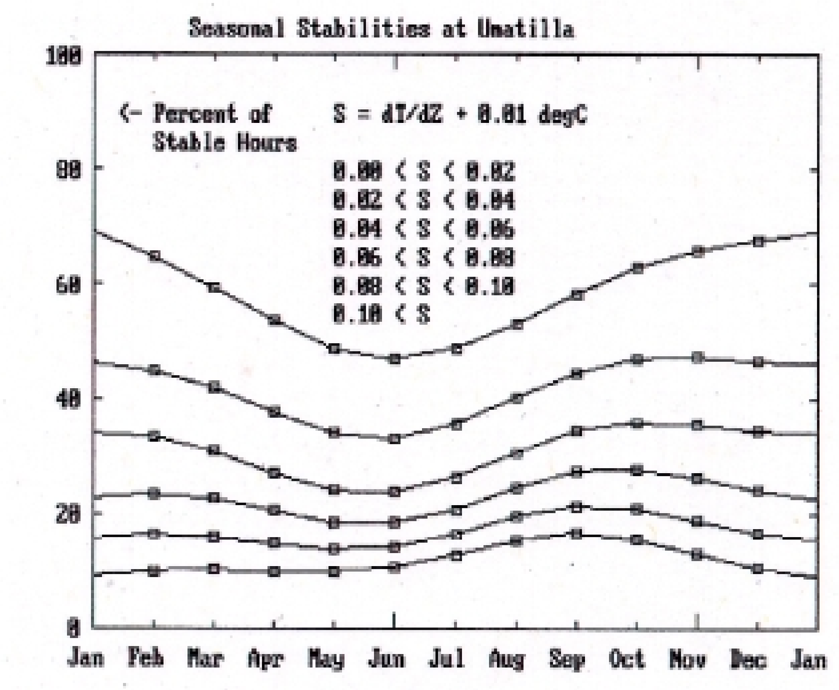

Figure 2.

Annual wave of stabilities. Note the summer minima and fall-to-winter maxima, with an interesting leading phase shift of the latter, with increasing stabilities. [These curves have been smoothed by a low-pass binomial filter.]

V. Terrain

WPUFF adjusts near-surface wind speeds and directions for effects of local terrain. Topographic elevation data to accomplish these adjustments are taken from the US Geological Survey's data base at 30 arc-seconds, which resolves grid elements approximately 0.9 km north-south, by 0.6 km east-west, at the latitude of the Umatilla facility [45.9 N.Lat], with a vertical resolution of 6 meters. As WPUFF's algorithm involves gradients of the terrain, which must be computed with finite differences, I have smoothed the topographic data slightly to an effective resolution near 2.5 km in both axes. An isometric projection of this smoothed topography under the Umatilla airshed is shown in figure 3, and a stippled topographic contour map of the same domain is shown in figure 4, which also locates some of the roads, streams, and the surrounding communities of Hermiston, Umatilla, Plymouth, Irrigon, and Boardman.

Within this domain, further defined in the next section, the mean terrain altitude above sea level is 144 meters, the standard deviation is 37 meters, the radial autocorrelation length is 7 km, and the root-mean-square [rms] gradient is 2 percent.

VI. The Domain

For these studies WPUFF was gridded in a domain of 44 [N-S] by 61 [E-W] cells, between 44.8083 and 44.9917 N.Lat, and 119.2766 and 119.6362 W.Lng, as shown in figures 3 and 4. This domain encompasses the UMCDF facility and the five nearby communities of Hermiston, Umatilla, Plymouth [WA], Irrigon, and Boardman.

Each of the 2684 cells are 0.46 km on a side, with some distortion owing to a coordinate transform from a spherical earth to a planar model. These cell dimensions set the resolution of tracer-concentration averages, and the outer scale of the modeled domain [20 km N-S x 28 km E-W].

VII. Emissions

All emissions were assumed to be 1 gram/sec of a generic, conservative tracer. Separate simulations were performed for "fugitive" emissions, assumed to be emitted at 10 meters, and for "stack" emissions, assumed initially at 60 meters. Note that the physical stack will be half this height. An extra 30 meters of initial plume height were added to approximate a prompt, near-field thermal and kinetic plume rise. As the puffs evolve their later heights are affected by the atmospheric stabilities, vertical diffusivities, and convergence or divergence owing to flows over complex terrain.

All simulations emitted puffs at one-minute intervals. This rate sums to 2.1 million puffs over 4 years, for each of the two cases, fugitive and stack. Every puff was followed until it was advected out of the modeled domain. Between 20 and 400 puffs were typically current during any "snapshot" [fig.4].

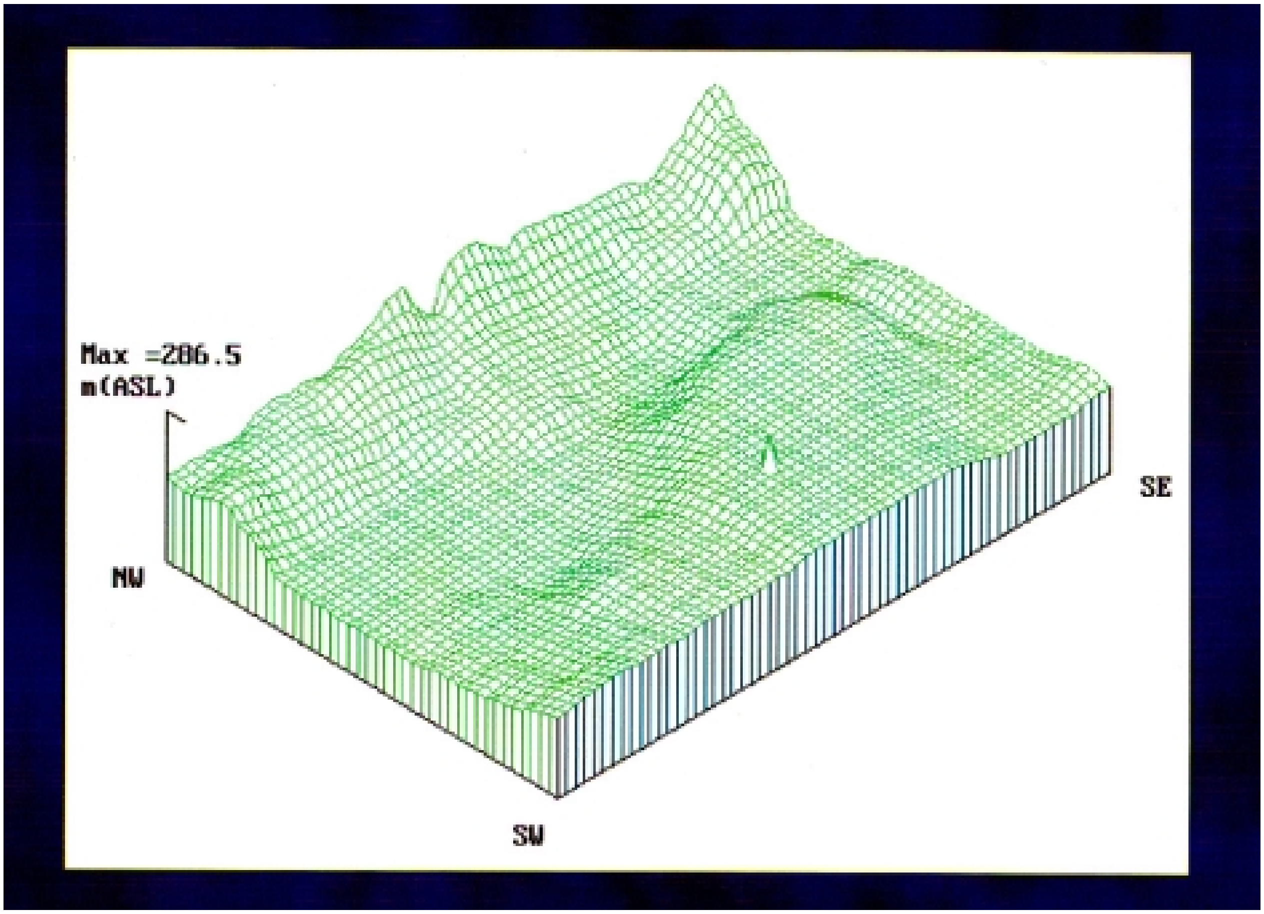

Figure 3.

Isometric projection of the topographic relief. The triangular spike locates the 30 meter UMCDF stack plus 30 meters of prompt plume rise. The Columbia river valley flows from upper right to lower left. Hermiston and Umatilla are located on the plateau to to the east and northeast of the stack.

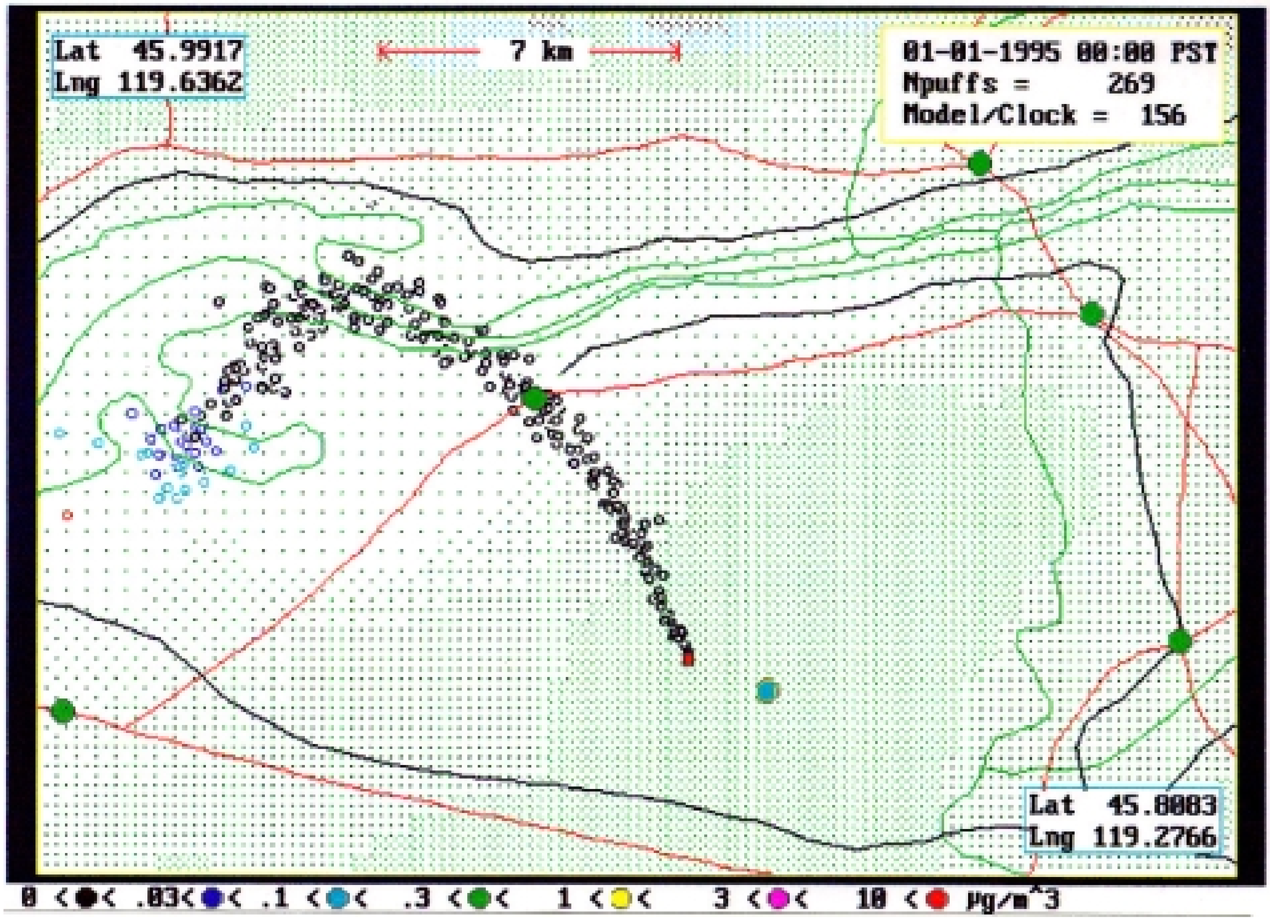

Figure 4.

A stippled-contour map of the modeled domain, with denser green stippling at higher elevations. The UMCDF stack is located at the small red square. The Met tower is about 1 km to the southeast. Red lines are roads, black are railroads, and green are streams and rivers, with the Columbia running east to west across the top, with an extra green line showing the state boundary. Towns are green circles, with Hermiston to the east of the stack and Umatilla, Plymouth [WA], Irrigon, and Boardman in a counter-clockwise arc. The current "snapshot" shows 269 puffs flowing towards the northwest, across Irrigon. The wind has recently veered by about 40 degrees.

VIII. Results

Results of these simulations are summarized in figures 5-9 and tabulated in Tables I-VI, [pages 17-21].

To help orient you to my discussion in the following section, please look for a minute at Table I-A, which summarizes simulations of stack emissions, using the WPUFF model.

TABLE I-A WPUFF Stack Emissions [60 m]

MetTower	Hermiston	Umatilla	Plymouth	Irrigon	Boardman	Parameter
12.417	7.051	10.694	5.973	5.833	3.426	Percent non-zero
7.609	4.245	3.858	2.382	3.368	2.891	Highest 1-hr
5.988	3.143	2.634	2.182	2.406	1.564	2nd High 1-hr
1.918	0.790	1.093	0.641	0.787	0.483	Highest 8-hr
1.718	0.705	0.910	0.511	0.696	0.413	2nd High 8-hr
0.704	0.306	0.404	0.240	0.343	0.179	Highest 24-hr
0.692	0.269	0.390	0.223	0.313	0.150	2nd High 24-hr
0.075	0.025	0.028	0.014	0.012	0.007	Average [all hrs]
0.375	0.159	0.138	0.094	0.103	0.068	SD
0.004	0.002	0.001	0.001	0.001	0.001	SE
5.064	6.266	4.905	6.715	8.673	9.816	SD/Avg

Except for the first and last lines of this table, all entries are of concentrations at the specified sites, per unit of emission. That is, their units are micrograms/cubic meter at the surface, per gram/sec of emissions, hereafter abbreviated as μg/m^3/g/s.

The vertical columns in Table I-A identify the "target" sites [MetTower, Hermiston, Umatilla, Plymouth, Irrigon, and Boardman] at which are assumed to be located instruments to detect and quantify emissions from the Chemical Weapons Demilitarization Facility [UMCDF]. The first of these, "MetTower", is located approximately 1 km southwest of the principal incinerator stack [fig.4].

The horizontal rows in Table I-A contain successively:

1. The percent of hours with non-zero concentrations of tracer concentrations, derived from stack emissions at the facility. Note immediately that these are small [3 - 10 %].

Thus:

* **Most of the time, the plume misses populated targets.**

2. The second row lists the averages of the four highest one-hour [that is, averaged over 60 one-minute simulation steps] tracer-concentrations, as simulated by WPUFF, one in each year [1995, 1996, 1997, 1998]. These numbers range from 2.4 [μg/m^3/g/s] at Plymouth, to 7.6 [μg/m^3/g/s] at the MetTower.

3. The next row lists the similar averages of the second-highest one-hour concentrations. These range from 1.6 to 6.0 [μg/m^3/g/s].

4. The fourth row lists the highest 8-hour averaged concentrations, which range from 0.5 to 1.9 [μg/m^3/g/s]. These eight hours are continuous, may start at any hour, and may continue over midnight into a following day.

5-8. Rows 5 through 8 similarly list the second-highest 8-hr, the highest and second-highest 24-hr [midnight to midnight], and the grand averages of all hourly simulations. Note that the grand averages [Avg] span from 0.007 to 0.08 [μg/m^3/g/s], very much less than the similar averages over shorter periods. I shall further discuss this important point in the next section.

9-11. The last three rows respectively list the standard deviations [SD] of the grand-averaged hourly measure-ments"[Avg], the standard errors [SE] of the grand averages [also μg/m^3/g/s], and the coefficients of variation [SD/Avg, dimensionless]. Note that the latter ratios range from 4.9 to 9.8, with the larger ratios at the more distant sites. More about this, later.

Tables II-A, III-A, and IV-A [collected with other tables, below, beginning on page 17] have similar formats, respectively for fugitive emissions simulated by WPUFF, and stack- and fugitive emissions simulated by a steady-state Gaussian model.

Figures 5a,b show simulated "strip-charts" of hourly averaged concentrations, at Hermiston.

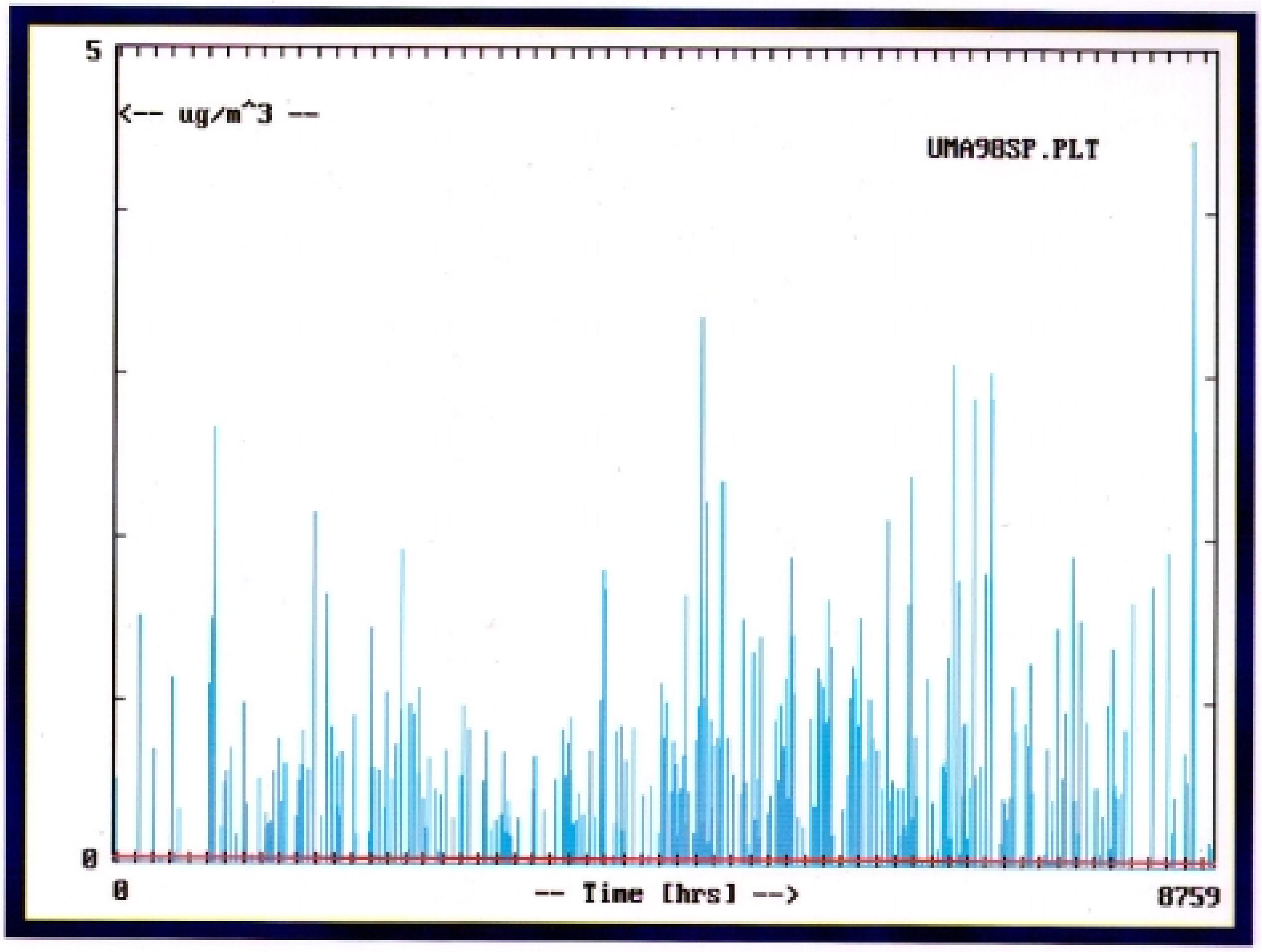

Figure 5a

A "stripchart" recording of one year's hourly averaged concentrations at Hermiston [1998], simulated by WPUFF. The red line near the abcissa shows the annual average. Owing to superpositions, this plot somewhat exaggerates the puff densities.

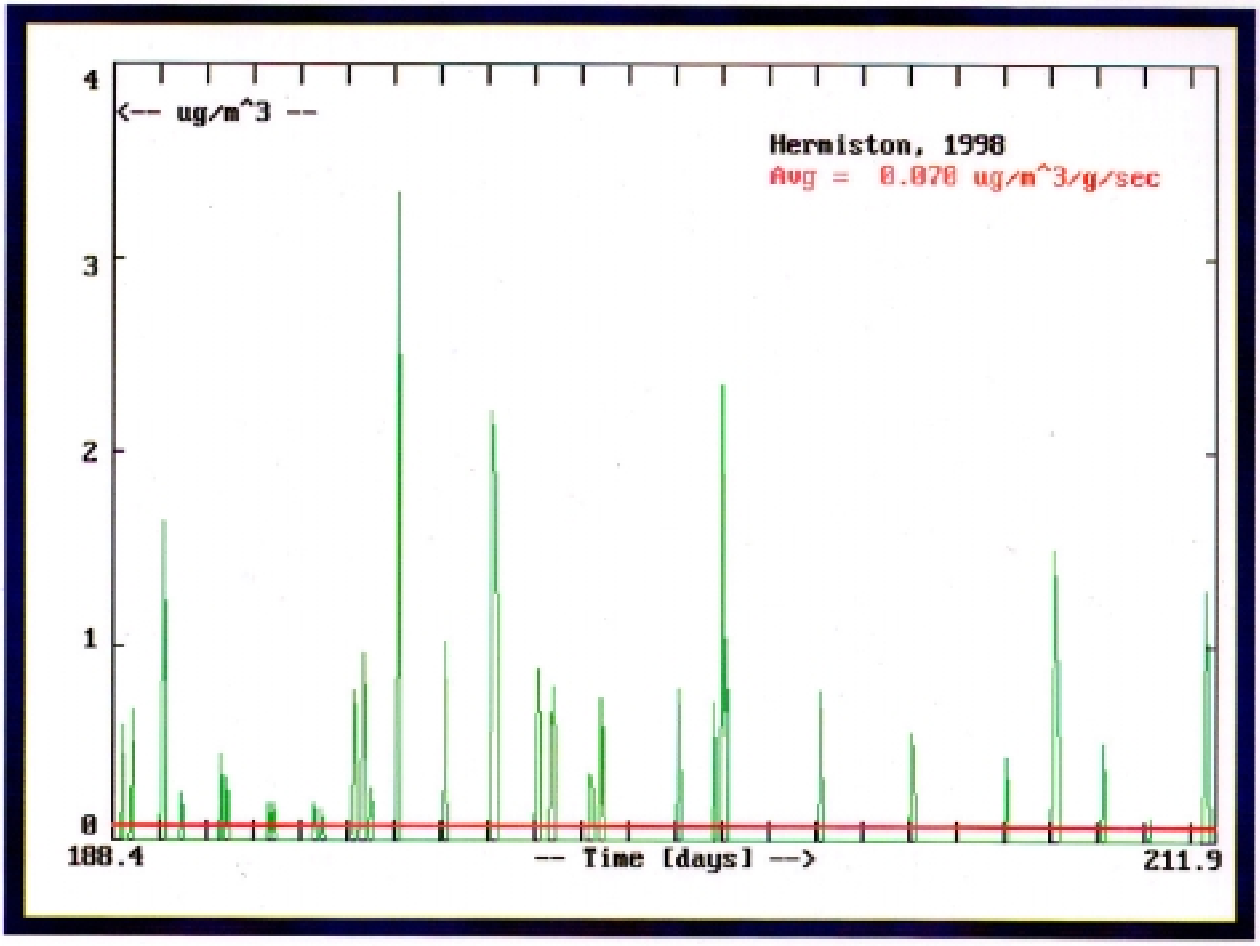

Figure 5b

A similar stripchart showing a section of the same data, with all puffs resolved. The red line averages these puffs, only.

Figures 6-9 respectively show annual averages of surface-concentration contours with stack- and fugitive emissions, as simulated by WPUFF and the Gaussian model.

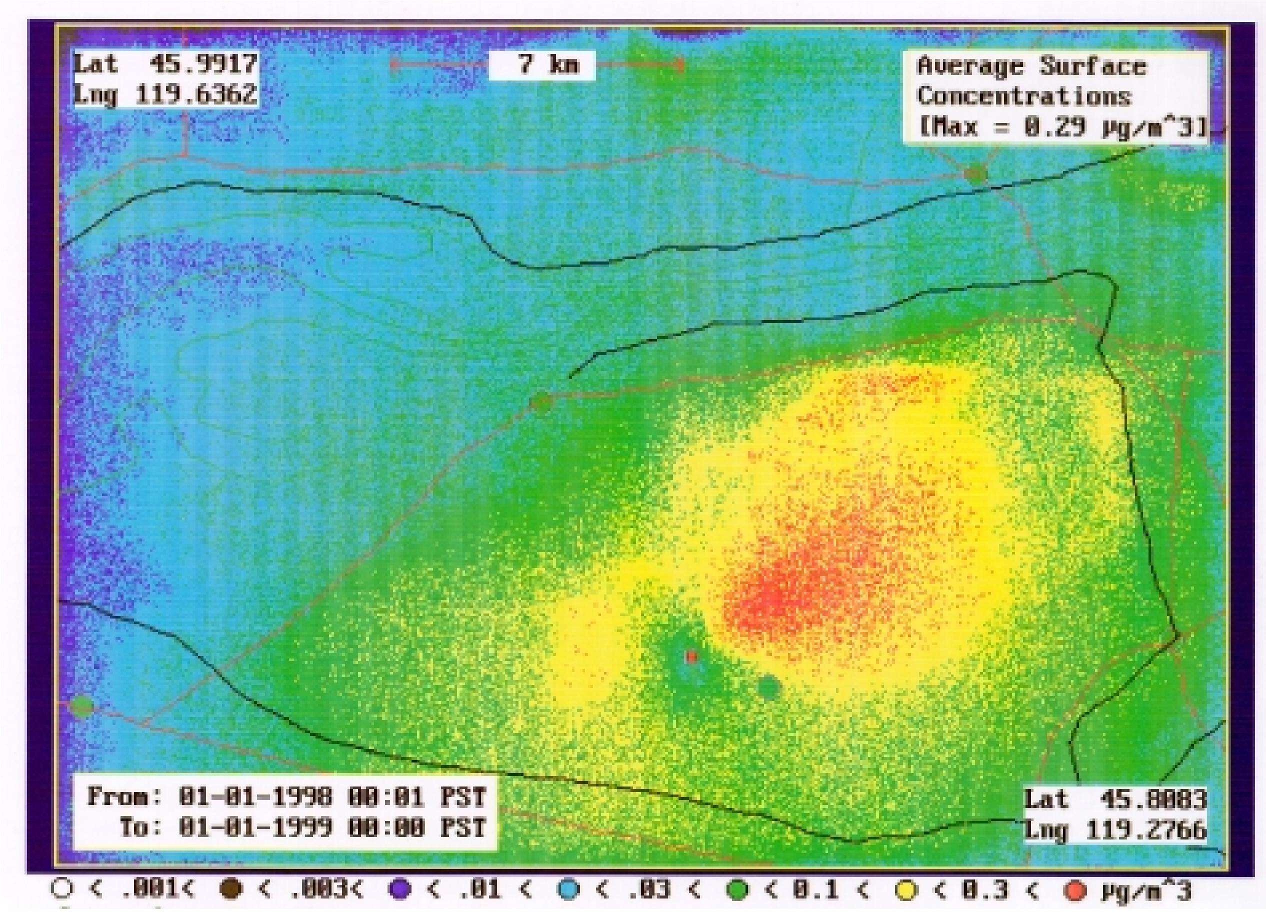

Figure 6a.

Annually averaged surface concentrations from stack emissions, as simulated by WPUFF [1998].

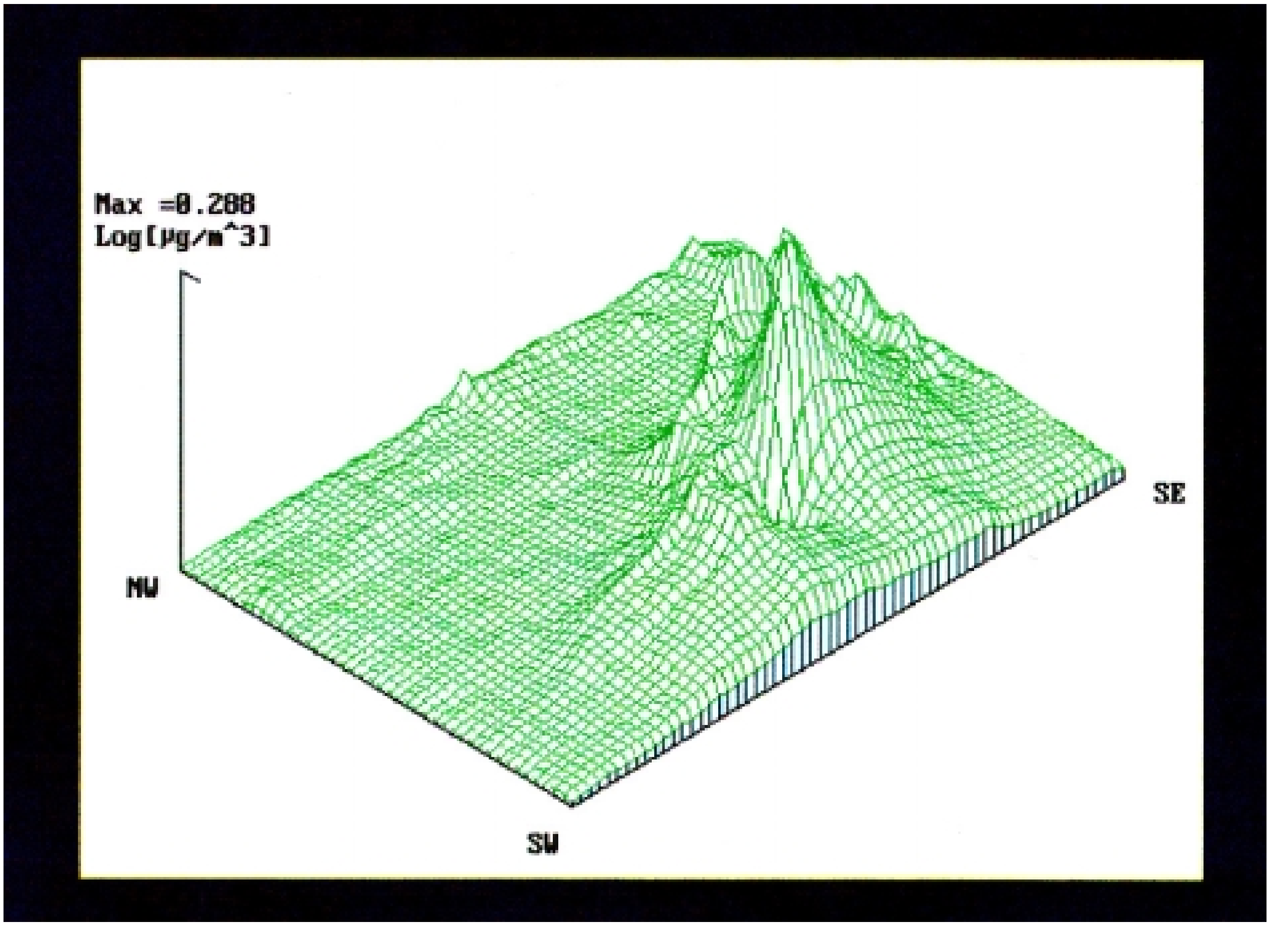

Figure 6b

Annually averaged surface concentrations from stack emissions, as simulated by WPUFF [1998]. These are the same data as figure 6a, in isometric projection. [Note the logarithmic scale.] The cover of this report shows the same figure, rotated and smoothed,

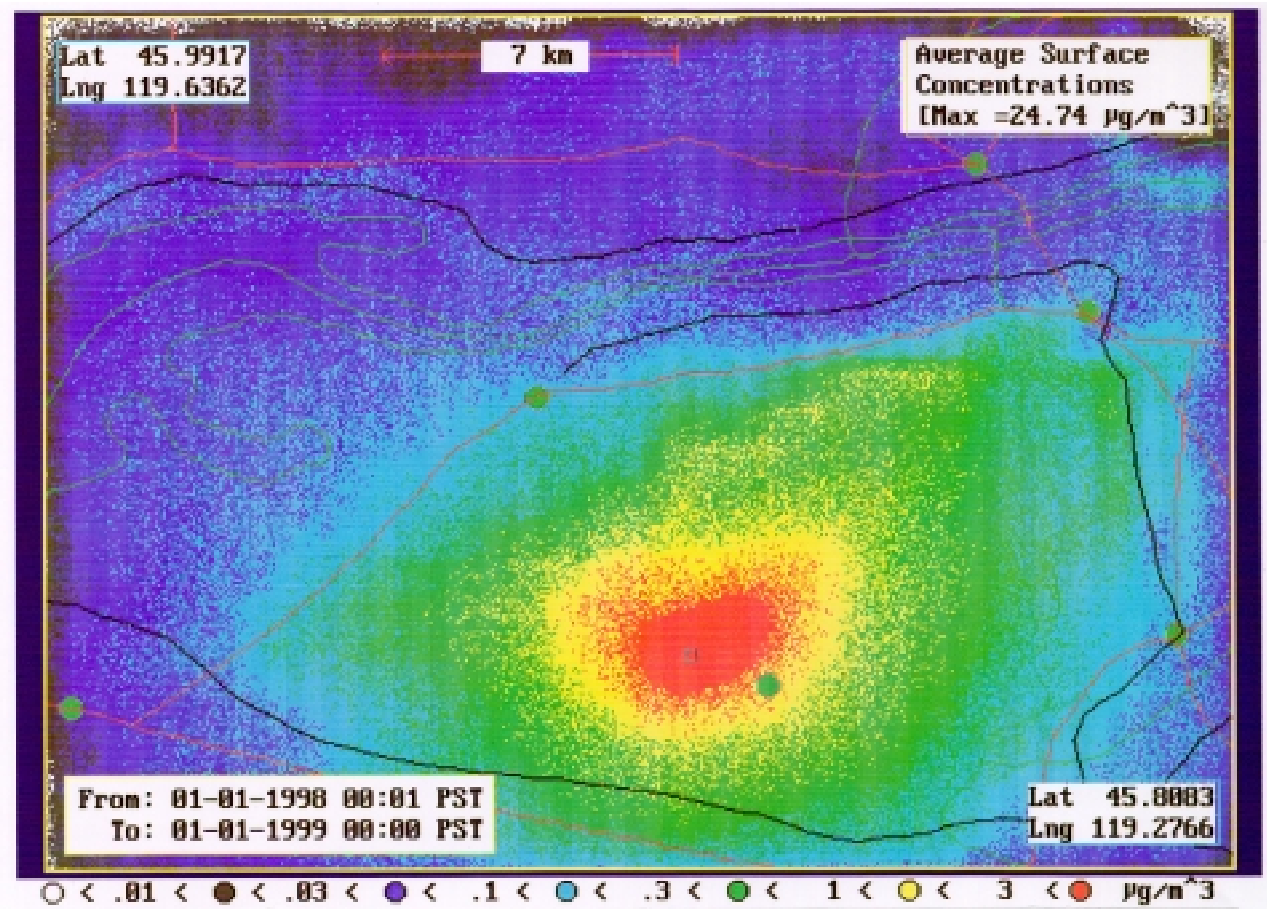

Figure 7.

Annually averaged surface concentrations from fugitive emissions, as simulated by WPUFF [1998].

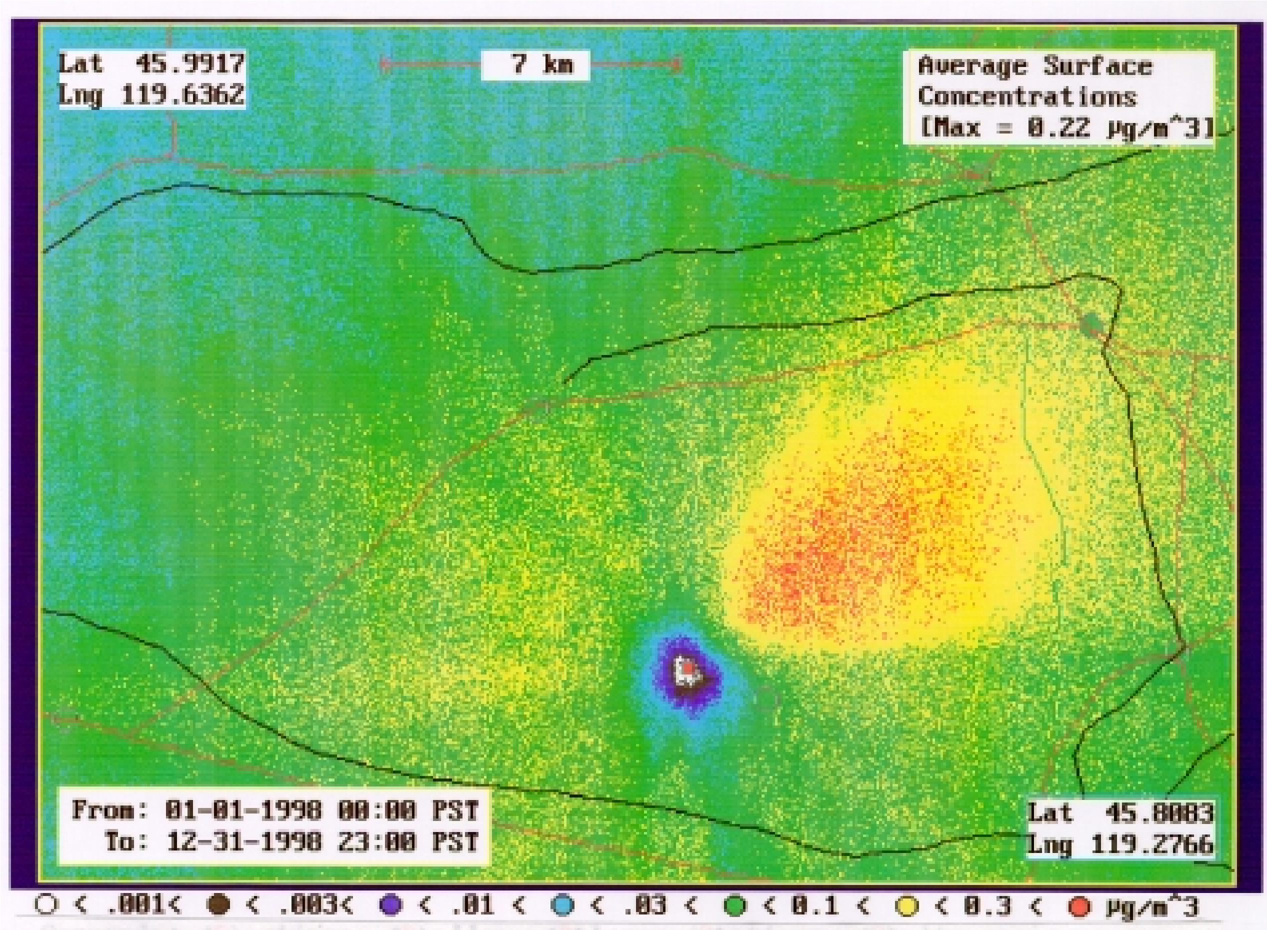

Figure 8.
Annually averaged surface concentrations from stack emissions, as simulated by a Gaussian model [1998].

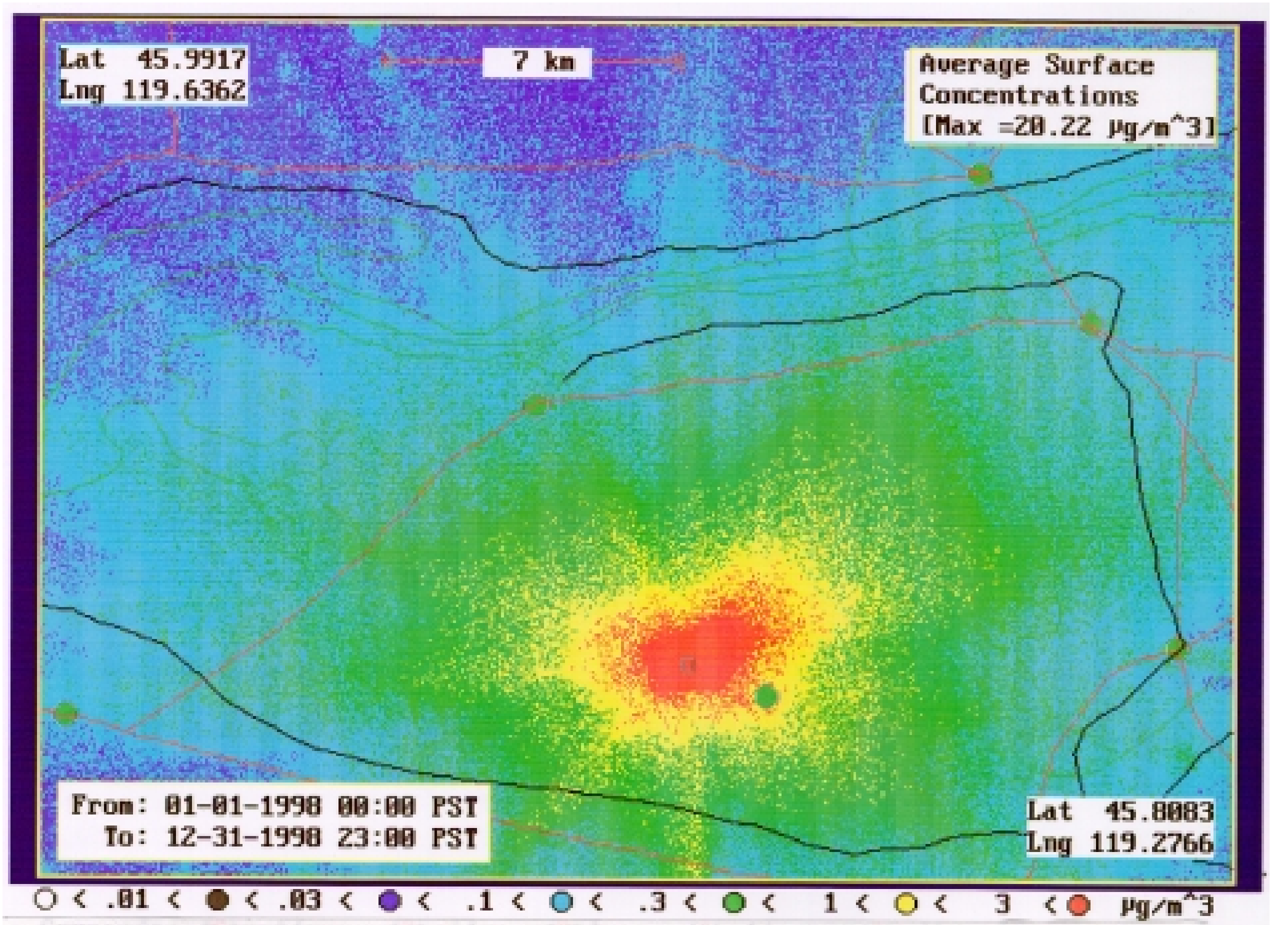

Figure 9.

Annually averaged surface concentrations from fugitive emissions, as simulated by a Gaussian model [1998].

IX. Discussion

Both WPUFF and the Gaussian models simulate tracer concentrations without arbitrary scaling factors [though with several adjustable dispersion coefficients and other assumptions]. The modeler's art is still imprecise, however, owing largely to imprecision of data, and errors of 2X or more are commonly discovered in those relatively rare cases where good observations are available to keep the modelers honest.

In the present case, with the demilitarization facility still under construction [Jan. 1, 2000], neither emission data, nor measurements of tracer concentrations, are yet available. The absolute numbers of Tables I-A through IV-A are therefore not very useful, and their peculiar units [μg/m^3/g/s] may obscure the underlying physics of the dispersion processes. Insights into what is really happening can more easily be extracted after normalizing the numbers into appropriate dimensionless ratios.

I have attempted this in several ways:

In Tables I-B through IV-B all the concentrations at each site are divided by the long-term averages at that site, listed in the last rows:

TABLE I-B WPUFF Stack Emissions [60 m]

MetTower	Hermiston	Umatilla	Plymouth	Irrigon	Boardman	Parameter
102.141	166.480	137.768	170.161	269.480	413.000	Highest 1-hr
80.379	123.245	94.062	155.857	192.500	223.393	2nd High 1-hr
25.742	30.971	39.045	45.750	62.980	68.964	Highest 8-hr
23.064	27.647	32.500	36.500	55.680	59.036	2nd High 8-hr
9.453	11.990	14.420	17.143	27.440	25.536	Highest 24-hr
9.292	10.559	13.920	15.964	25.060	21.500	2nd High 24-hr
1.000	1.000	1.000	1.000	1.000	1.000	Average [all hrs]

In Tables I-C though IV-C the concentrations at the several sites are divided by those at the MetTower [Column 1].

TABLE I-C WPUFF Stack Emissions [60 m]

MetTower	Hermiston	Umatilla	Plymouth	Irrigon	Boardman	Parameter
1.000	0.558	0.507	0.313	0.443	0.380	Highest 1-hr
1.000	0.525	0.440	0.364	0.402	0.261	2nd High 1-hr
1.000	0.412	0.570	0.334	0.411	0.252	Highest 8-hr
1.000	0.410	0.530	0.297	0.405	0.241	2nd High 8-hr
1.000	0.434	0.573	0.341	0.487	0.254	Highest 24-hr
1.000	0.389	0.563	0.323	0.453	0.217	2nd High 24-hr
1.000	0.342	0.376	0.188	0.168	0.094	Average [all hrs]

Tables V-A,B [collected below, beginning on page 22] list the ratios of surface concentrations, as simulated by the WPUFF model, to those computed by the Gaussian Model, respectively for emissions from the stack [at 60 meters] to fugitive emissions at 10 meters]. Tables VI-A,B [page 22] similarly ratio the Fugitive/Stack concentrations, respectively, for the WPUFF and Gaussian models.

From these tables and figures let me now try to extract a few insights: ["The purpose of computation is insight. Often, the purpose of computation is not in sight". Anon.]

1. Firstly, note immediately from figures 5a,b and the first and last lines of Tables I-A and III-A that strip-chart sequences of concentrations are exceptionally noisy, and that:

> *** Citing annual averages of tracer concentrations, only, obscures the extreme variations of the transport processes.**

That is, figures such as 6-9 are not as informative as one would hope. Time resolutions of 10's of minutes or less are necessary to capture direct hits from the sinuous garden hose of a meandering plume, when the winds are light, and the air is stable.

2. Equivalently, please note from Tables I-B through IV-B that at every site, with both models, for both fugitive and stack emissions:

> *** The expected highest episodes, averaged over shorter intervals, greatly exceed the annual averages.**

Thus, just to grind this point in firmly:

> *** Short episodes dominate the potential for damage in the Umatilla airshed.**

3. Thirdly, note from Tables VI-A and VI-B that, per unit of emission, both models suggest that fugitive sources will produce 4-10x higher near-surface concentrations at *all* the sites, than do emissions from the stack. That is:

> * Stacks work.

However:

> * High attention should be paid to off-design fugitive emissions that may .. even if rarely .. escape the demilitarization facility in non-buoyant plumes, near the surface.

3. Finally, please note from Tables I-C through IV-C that the fall-off in predicted surface concentrations with increasing range, with both stack and fugitive emissions, amounts to a factor of 10-20 for the annual averages, but only 2-3 for the higher concentrations seen at shorter averaging periods.

   Thus,

> * Stacks don't work as well to diminish brief maxima, as they do for longer averages.

X. More Discussion

In the bulleted assertions of the previous section I have tried to emphasize only those insights that appear robust to the choice of models: Puff or Gaussian. I now emphasize their differences.

Firstly and most obviously, please look at figure 8, where it is dramatically seen that this Gaussian model asserts a "blue hole" at the surface near the UMCDF site, from stack emissions. This is a well-noted and unphysical result with Gaussian models in their simplest form, and various fixes have been addressed to this artifact, as for example by increasing the near-field vertical mixing to account for "fumigation looping" and "building wakes". [ISCST-3 does the latter.]

With the present simulations I have neglected these effects. Note, however, that WPUFF partially fills in the near-field hole [fig.6a], though by different physics, as can be seen vividly during brief snapshots of the evolving simulations, when recirculating winds "slosh" old puffs back across the UMCDF site, near the surface.

Secondly, note in Tables V that the two models differ in their predicted concentrations at the various sites, by factors of two or more, with the WPUFF model mostly [but not always] lower at most sites, and the differences increasing with range, for both fugitive and stack emissions. The sense of these differences is consistent with effects from topography and from meandering winds that, in the WPUFF model, result in longer transit times from source to receptor, and consequently greater mixing and dilution, than with the Gaussian model. It is interesting .. at least to me .. that test comparisons of the two models with steady winds over flat terrain agree within relative differences between 4 and 16%, the higher difference calculated with an RMS scoring function weighted to emphasize the higher concentrations. [Appendix A. p-26]

Thus it appears that:

* **Effects of topography, meandering winds, and recirculating trajectories are significant in the Umatilla airshed, and are captured in some degree by WPUFF, but not by the Gaussian model.**

I must caution, however, that while WPUFF simulates additional physics that are not accounted for by the Gaussian model, and that it is therefore tempting to prefer it, real measurements are not available at this site, and no "winner" can yet be declared..

For this and other cautious reasons:

> * **We must presently accept no greater confidence in the absolute concentrations predicted by these models, than factors of two.**

XI. More Discussion: Probability Distributions

Please look again for a minute at figures 5a,b, which show WPUFF's simulations of concentration stripcharts at Hermiston, during 1998 What is dramatic in these figures is their extreme spikiness. The red lines close to the bases of these plots show time-averages that poorly represent the noisy events that exceed those averages, by factors up to several hundred. In figure 10 I have plotted a histogram of the non-zero concentrations at Hermiston [1995-1998], which can be seen to be distributed approximately exponentially, as:

$$P(C) \bullet dC = \{f / [Avg]\} \exp\{-C/[Avg]\} \bullet dC \qquad \text{[eqn. 2]}$$

In equation 2:

P(C) = the incremental probability of measuring a tracer concentration, C, between C and C+dC.

dC = an increment of C

f = the fraction of non-zero measurements. At Hermiston this was 0.071 [see Table I-A].

[Avg] = the average of C at the specified site. At Hermiston, this was 0.025 μg/m^3/g/s.

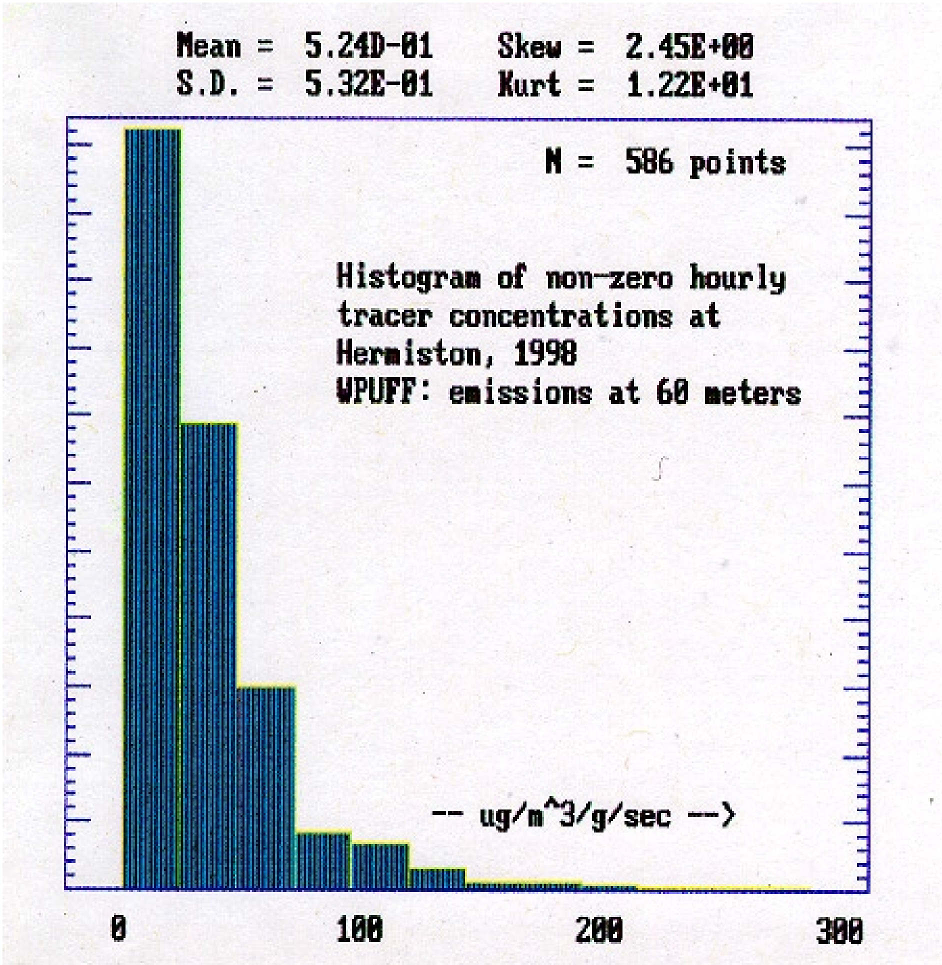

Figure 10.

Histogram of non-zero hourly concentrations at Hermiston, 1998, as simulated by WPUFF for stack emissions at 60 meters.

XII. Still More Discussion: Risks

In a series of memoranda [ref.5] I have elsewhere discussed the risks associated with toxic waste incineration and the Umatilla facility. In my judgment, these risks are dominated by the .. we hope ..relatively small probabilities of accidental releases of very toxic gases that have not passed through the incineration process. The highest fraction of these risks will be born by workers in the plant, a smaller fraction by the surrounding communities. The uncertainties in estimating these risks are very large .. many times larger than the risks themselves.

The relevance of this present study, if any, may be in the "management" .. if that is indeed possible .. of brief, accidental releases that escape the UMCDF site. It is for this reason that I have emphasized short-term exposures at longer ranges, and WPUFF as a tool that captures the physics that dominate brief events.

In my judgment, risks from cumulative exposures that may result from on-design stack effluents, as for example cancer risks from dioxins, are likely of lower order than risks from accidental release of toxic agents that escape the detoxification facility. For this reason the annually averaged exposures listed in Tables I-IV, and illustrated in figures 5-8, and the similar annual averages with ISCST-3 that were reported by SAIC [ref.1], are, I judge, substantially irrelevant. With risks at the Umatilla detoxification facility, my greatest concern is not with on-design operations, which good engineering can account for, but with off-design operations, exceptions, mixups, accidents, idiocies, and overt sabotage.

* At Umatilla it is not ordinary operations that should most concern us, but the potential for accidents.

XIII. Real-Time and Predictive Modeling

The emphasis of this study is upon transient effects at longer ranges, in stable air.

With the present data both models have been exercised retrospectively with physically real winds but synthetic emissions. When the UMCDF facility is operating, however, it will be possible to follow the plumes in current time, and .. with predictive wind-field models .. prospectively.

* **To support damage control of accidental and off-design emissions, I strongly recommend that skills be developed for fast-response and predictive modeling of tracer dispersions in the Umatilla airshed.**

Both WPUFF and CALPUFF are natural tools for this task. Good, local, real-time meteorological data will continue to be available, and 42 hour mesoscale predictive wind-fields are now routinely computed for Umatilla airshed [and throughout the Pacific Northwest], and are published on web sites by the University of Washington's implementation of "MM5" [ref.4].

To assist this task I shall make WPUFF available to responsible staff at ODEQ and UMCDF, adapted to real-time and predictive wind data, and I shall provide appropriate documentation and training, without cost.

XIV. Summary:

Meteorological data at the Umatilla Chemical Demilitarization Facility near Hermiston, Oregon, show a remarkable 58% of hours with stable air. Dispersion models suggest infrequent but intense plume impacts on the neighboring communities, with short-term concentrations that are several hundred times the annual averages at these sites. Attention should be paid to non-linear effects on the exposed populations and to rapid response to accidental, near-surface emissions.

XV. Acknowledgments

I am grateful to Sue Oliver and Philip Allen of Oregon's Department of Environmental Quality, for supplying me with the meteorological data I have used in this project.

Useful reviews of a draft to this report [Jan 15, 2000] were contributed by Wayne C. Thomas [ODEQ, Manager, Chemical

Detoxification Program", and by E.T. Prater, S.A. Stage, and C. Fosmire, of Innovative Emergency Management, Inc, Baton Rouge, La.

I am further grateful to Drs. L. Brenner and T. Stibolt for helpful correspondence, and for calling my attention to the Umatilla detoxification project.

I am a professor of Atmospheric Sciences at the University of Washington, Seattle, WA 98195. This work was supported by WYNDsoft Inc., a registered corporation of Washington State, that I direct.

Tables:

All concentrations are μg/m^3 per g/s of emissions.

TABLE I-A WPUFF Stack Emissions [60 m]

MetTower	Hermiston	Umatilla	Plymouth	Irrigon	Boardman	Parameter
12.417	7.051	10.694	5.973	5.833	3.426	Percent non-zero
7.609	4.245	3.858	2.382	3.368	2.891	Highest 1-hr
5.988	3.143	2.634	2.182	2.406	1.564	2nd High 1-hr
1.918	0.790	1.093	0.641	0.787	0.483	Highest 8-hr
1.718	0.705	0.910	0.511	0.696	0.413	2nd High 8-hr
0.704	0.306	0.404	0.240	0.343	0.179	Highest 24-hr
0.692	0.269	0.390	0.223	0.313	0.150	2nd High 24-hr
0.075	0.025	0.028	0.014	0.012	0.007	Average [all hrs]
0.375	0.159	0.138	0.094	0.103	0.068	SD
0.004	0.002	0.001	0.001	0.001	0.001	SE
5.064	6.266	4.905	6.715	8.673	9.816	SD/Avg

TABLE I-B WPUFF Stack Emissions [60 m]

MetTower	Hermiston	Umatilla	Plymouth	Irrigon	Boardman	Parameter
102.141	166.480	137.768	170.161	269.480	413.000	Highest 1-hr
80.379	123.245	94.062	155.857	192.500	223.393	2nd High 1-hr
25.742	30.971	39.045	45.750	62.980	68.964	Highest 8-hr
23.064	27.647	32.500	36.500	55.680	59.036	2nd High 8-hr
9.453	11.990	14.420	17.143	27.440	25.536	Highest 24-hr
9.292	10.559	13.920	15.964	25.060	21.500	2nd High 24-hr
1.000	1.000	1.000	1.000	1.000	1.000	Average [all hrs]

TABLE I-C WPUFF Stack Emissions [60 m]

MetTower	Hermiston	Umatilla	Plymouth	Irrigon	Boardman	Parameter
1.000	0.558	0.507	0.313	0.443	0.380	Highest 1-hr
1.000	0.525	0.440	0.364	0.402	0.261	2nd High 1-hr
1.000	0.412	0.570	0.334	0.411	0.252	Highest 8-hr
1.000	0.410	0.530	0.297	0.405	0.241	2nd High 8-hr
1.000	0.434	0.573	0.341	0.487	0.254	Highest 24-hr
1.000	0.389	0.563	0.323	0.453	0.217	2nd High 24-hr
1.000	0.342	0.376	0.188	0.168	0.094	Average [all hrs]

All concentrations are µg/m^3 per g/s of emissions.

TABLE II-A WPUFF Fugitive Emissions [10 m]

MetTower	Hermiston	Umatilla	Plymouth	Irrigon	Boardman	Parameter
13.558	6.826	10.839	5.961	6.626	3.434	Percent non-zero
97.687	23.973	18.573	12.050	26.750	15.492	Highest 1-hr
85.310	18.347	13.310	9.906	18.312	10.470	2nd High 1-hr
31.697	5.290	3.967	2.464	5.341	2.843	Highest 8-hr
30.122	4.594	3.355	2.259	4.899	2.237	2nd High 8-hr
13.942	2.281	1.723	0.949	1.953	1.180	Highest 24-hr
11.990	2.144	1.668	0.900	1.856	1.038	2nd High 24-hr
1.295	0.095	0.129	0.061	0.133	0.058	Average [all hrs]
5.408	0.680	0.667	0.397	0.839	0.480	SD
0.058	0.007	0.007	0.004	0.009	0.005	SE
4.185	7.065	5.310	6.727	6.440	8.939	SD/Avg

TABLE II-B WPUFF Fugitive Emissions [10 m]

MetTower	Hermiston	Umatilla	Plymouth	Irrigon	Boardman	Parameter
75.448	252.353	144.252	195.935	201.130	268.264	Highest 1-hr
65.889	193.126	103.377	161.065	137.682	181.307	2nd High 1-hr
24.481	55.684	30.812	40.061	40.160	49.221	Highest 8-hr
23.265	48.358	26.054	36.732	36.833	38.727	2nd High 8-hr
10.768	24.008	13.381	15.423	14.684	20.429	Highest 24-hr
9.260	22.571	12.959	14.630	13.957	17.978	2nd High 24-hr
1.000	1.000	1.000	1.000	1.000	1.000	Average [all hrs]

TABLE II-C- WPUFF Fugitive Emissions [10 m]

MetTower	Hermiston	Umatilla	Plymouth	Irrigon	Boardman	Parameter
1.000	0.245	0.190	0.123	0.274	0.159	Highest 1-hr
1.000	0.215	0.156	0.116	0.215	0.123	2nd High 1-hr
1.000	0.167	0.125	0.078	0.169	0.090	Highest 8-hr
1.000	0.153	0.111	0.075	0.163	0.074	2nd High 8-hr
1.000	0.164	0.124	0.068	0.140	0.085	Highest 24-hr
1.000	0.179	0.139	0.075	0.155	0.087	2nd High 24-hr
1.000	0.073	0.099	0.047	0.103	0.045	Average [all hrs]

All concentrations are µg/m^3 per g/s of emissions.

TABLE III-A GAUSS Stack Emissions [60 m]

MetTower	Hermiston	Umatilla	Plymouth	Irrigon	Boardman	Parameter
6.016	9.388	17.454	8.461	3.814	6.093	Percent non-zero
14.923	9.061	4.827	5.339	9.687	10.094	Highest 1-hr
7.145	5.033	4.094	3.746	7.697	5.000	2nd High 1-hr
2.066	1.186	0.905	0.707	1.348	1.551	Highest 8-hr
1.831	0.722	0.832	0.641	1.145	1.476	2nd High 8-hr
0.690	0.466	0.414	0.321	0.625	0.625	Highest 24-hr
0.627	0.388	0.382	0.300	0.588	0.606	2nd High 24-hr
0.031	0.032	0.054	0.025	0.019	0.020	Average [all hrs]
0.318	0.221	0.229	0.174	0.255	0.199	SD
0.003	0.002	0.002	0.002	0.003	0.002	SE
10.429	6.891	4.299	6.946	14.194	9.385	SD/Avg

TABLE III-B GAUSS Stack Emissions [60 m]

MetTower	Hermiston	Umatilla	Plymouth	Irrigon	Boardman	Parameter
489.279	283.141	89.814	211.436	503.208	511.076	Highest 1-hr
234.262	157.273	76.158	148.347	399.831	253.190	2nd High 1-hr
67.730	37.070	16.837	28.020	70.013	78.544	Highest 8-hr
60.041	22.555	15.484	25.406	59.481	74.722	2nd High 8-hr
22.615	14.578	7.712	12.723	32.494	31.658	Highest 24-hr
20.541	12.109	7.102	11.901	30.532	30.671	2nd High 24-hr
1.000	1.000	1.000	1.000	1.000	1.000	Average [all hrs]

TABLE III-C GAUSS Stack Emissions [60 m]

MetTower	Hermiston	Umatilla	Plymouth	Irrigon	Boardman	Parameter
1.000	0.607	0.323	0.358	0.649	0.676	Highest 1-hr
1.000	0.704	0.573	0.524	1.077	0.700	2nd High 1-hr
1.000	0.574	0.438	0.342	0.652	0.751	Highest 8-hr
1.000	0.394	0.454	0.350	0.625	0.806	2nd High 8-hr
1.000	0.676	0.601	0.466	0.907	0.906	Highest 24-hr
1.000	0.619	0.609	0.480	0.938	0.967	2nd High 24-hr
1.000	1.049	1.762	0.828	0.631	0.648	Average [all hrs]

All concentrations are µg/m^3 per g/s of emissions.

..TABLE IV-A GAUSS Fugitive Emissions [10 m]

MetTower	Hermiston	Umatilla	Plymouth	Irrigon	Boardman	Parameter
8.275	9.900	18.462	9.195	4.917	6.784	Percent non-zero
289.174	22.705	42.458	43.904	90.127	64.438	Highest 1-hr
150.912	18.261	18.389	29.842	46.515	23.152	2nd High 1-hr
37.391	3.236	6.035	6.300	12.620	8.792	Highest 8-hr
32.104	2.685	5.080	5.738	10.111	8.361	2nd High 8-hr
13.578	1.285	2.814	2.309	4.872	3.212	Highest 24-hr
12.924	1.133	2.463	2.114	4.703	3.139	2nd High 24-hr
0.971	0.092	0.162	0.113	0.203	0.100	Average [all hrs]
7.453	0.735	1.029	1.007	2.082	1.157	SD
0.080	0.008	0.011	0.011	0.023	0.012	SE
7.655	7.981	6.363	9.029	10.421	11.438	SD/Avg

TABLE IV-B- GAUSS Fugitive Emissions [10 m]

MetTower	Hermiston	Umatilla	Plymouth	Irrigon	Boardman	Parameter
297.734	246.799	261.280	387.671	444.522	644.385	Highest 1-hr
155.379	198.486	113.165	263.506	229.423	231.523	2nd High 1-hr
38.498	35.177	37.142	55.625	62.242	87.922	Highest 8-hr
33.055	29.185	31.260	50.664	49.872	83.612	2nd High 8-hr
13.980	13.962	17.315	20.389	24.028	32.120	Highest 24-hr
13.307	12.321	15.154	18.667	23.196	31.392	2nd High 24-hr
1.000	1.000	1.000	1.000	1.000	1.000	Average [all hrs]

..TABLE IV-C GAUSS Fugitive Emissions [10 m]

MetTower	Hermiston	Umatilla	Plymouth	Irrigon	Boardman	Parameter
1.000	0.079	0.147	0.152	0.312	0.223	Highest 1-hr
1.000	0.121	0.122	0.198	0.308	0.153	2nd High 1-hr
1.000	0.087	0.161	0.168	0.337	0.235	Highest 8-hr
1.000	0.084	0.158	0.179	0.315	0.260	2nd High 8-hr
1.000	0.095	0.207	0.170	0.359	0.237	Highest 24-hr
1.000	0.088	0.191	0.164	0.364	0.243	2nd High 24-hr
1.000	0.095	0.167	0.117	0.209	0.103	Average [all hrs]

All concentrations are µg/m^3 per g/s of emissions.

TABLE V-A WPUFF/GAUSS Stack Emissions [60 m]

MetTower	Hermiston	Umatilla	Plymouth	Irrigon	Boardman	Parameter
0.510	0.469	0.799	0.446	0.348	0.286	Highest 1-hr
0.838	0.624	0.643	0.583	0.313	0.313	2nd High 1-hr
0.928	0.666	1.208	0.905	0.584	0.311	Highest 8-hr
0.938	0.977	1.093	0.797	0.608	0.280	2nd High 8-hr
1.021	0.655	0.974	0.747	0.548	0.286	Highest 24-hr
1.105	0.695	1.021	0.744	0.533	0.248	2nd High 24-hr
2.443	0.797	0.521	0.554	0.649	0.354	Average [all hrs]

TABLE V-B-WPUFF/GAUSS Fugitive Emissions [10 m]

MetTower	Hermiston	Umatilla	Plymouth	Irrigon	Boardman	Parameter
0.338	1.056	0.437	0.274	0.297	0.240	Highest 1-hr
0.565	1.005	0.724	0.332	0.394	0.452	2nd High 1-hr
0.848	1.635	0.657	0.391	0.423	0.323	Highest 8-hr
0.938	1.711	0.660	0.394	0.484	0.267	2nd High 8-hr
1.027	1.776	0.612	0.411	0.401	0.367	Highest 24-hr
0.928	1.892	0.678	0.426	0.395	0.331	2nd High 24-hr
1.333	1.033	0.792	0.543	0.656	0.577	Average [all hrs]

TABLE VI-A Fugitive/Stack WPUFF

MetTower	Hermiston	Umatilla	Plymouth	Irrigon	Boardman	Parameter
12.837	5.647	4.815	5.058	7.941	5.359	Highest 1-hr
14.246	5.838	5.054	4.540	7.610	6.696	2nd High 1-hr
16.528	6.698	3.629	3.847	6.785	5.888	Highest 8-hr
17.530	6.516	3.686	4.421	7.038	5.412	2nd High 8-hr
19.797	7.460	4.267	3.952	5.694	6.600	Highest 24-hr
17.320	7.964	4.281	4.026	5.926	6.899	2nd High 24-hr
17.379	3.725	4.598	4.393	10.640	8.250	Average [all hrs]

TABLE VI-B Fugitive/Stack GAUSS

MetTower	Hermiston	Umatilla	Plymouth	Irrigon	Boardman	Parameter
19.378	2.506	8.795	8.224	9.304	6.384	Highest 1-hr
21.121	3.628	4.492	7.967	6.044	4.630	2nd High 1-hr
18.101	2.728	6.669	8.904	9.363	5.668	Highest 8-hr
17.531	3.720	6.104	8.944	8.831	5.666	2nd High 8-hr
19.685	2.753	6.788	7.188	7.789	5.137	Highest 24-hr
20.630	2.925	6.451	7.035	8.002	5.182	2nd High 24-hr
31.844	2.875	3.023	4.485	10.532	5.063	Average [all hrs]

Appendix A. WPUFF

Introduction:

WPUFF is a "non-guideline" air-quality dispersion model copyrighted by WYNDsoft, Inc., 1999, with all rights reserved. In contrast with Gaussian plume models, WPUFF is a simulation, not a computation. It accepts tabular input data specifying sources, receptors, and the evolving meteorology. At specified intervals [one minute in the present case] symmetric tracer puffs are emitted at specified heights [10 and 60 meters in the present case]. These puffs then advect and grow, and their concentrations at the surface below are summed, averaged, and displayed.

All dynamic air-quality models have problems with numerical diffusion. Puff models minimize these problems during the transport phases of simulations, but at some point displays must be generated to show isopleths of concentrations averaged over some finite spatial scale, dX. If that scale is too small, some cells will contain few or no puffs, and the concentration fields will appear granular. Too large a scale sacrifices resolution.

WPUFF attempts to optimize dX by considering series of expanding puffs located with centers at the horizontal points, X, Y, within a cell of dimensions dX•dY [dX = dY in most cases], and with a vertical height Z. Each puff advects in X, Y, Z, and may grow diffusively and anisotropically in three dimensions, σx, σy, σz. We wish to know the incremental contribution of the puff to the tracer concentrations at the surface, dC, expressed within a small two-dimensional increment of surface area, dx^2. [Note: dx << dX]

To do this we must integrate the dC's [that is, average them] over some larger, *finite*, unit cell on the surface, of area dX^2. Because many puffs exist over the field at all times, and all of them [at least in the Gaussian approximation] contribute to all the [small, dx by dy] increments in every modeled cell, and because this integration must be repeated at every time step, it becomes computationally expensive. All puff models that I know of make approximations to simplify and accelerate this essential task.

WPUFF approaches this problem by assuming that Z, σx, σy, and σz are all << dX. [That is, dX must be chosen to meet this criterion: more about this later in the paragraphs that follow.]

With this approximation:

1. The tracer concentrations of each puff at the surface, <dC>,averaged over dX^2, become proportional to their concentrations at the surface below each puff's center, Co(X,Y,Z=0,time);

2. Increments to <dC> from puffs outside each unit cell contribute only in 2nd order, and may be neglected.

Thus: $\langle dC \rangle \approx \kappa\ Co(X=0,Y=0,Z)$

With these approximations, the proportionality coefficient, κ, can be evaluated through a Monte-Carlo integration over distributions of puff radii, altitude, and lateral positions. The resulting value is insensitive to those distributions, as expected, provided that dX > Z, σx, σy, σz.

In the present special case dX was 460 meters. σz is constrained by WPUFF to be less than or equal to H/2, where H is the height of a well mixed boundary layer. In the simulations of the Umatilla airshed H varied with time of day between 100 and 700 meters. . Thus σz was <= H/2 < dX at all times, though with aging, larger puffs the excess was not great; these cases, however, contribute little to the surface concentrations.

Some of the aging puffs, however, do grow laterally [σx and σy] to dimensions that are comparable to dX = 460 meters, and some of these puffs wander near to the ground, where they may significantly affect the concentrations there. One sensible choice to minimize this problem might simply be to expand dX. This would proportionally degrade the spatial resolution of the tracer's concentration field at the surface. Another sensible choice, adopted with WPUFF, is to split the horizontal diffusivities into two scales, by the following algorithm.

Where σx and σy are less than ½ dX, WPUFF assumes Gaussian diffusion in the ordinary way. Additionally, however, an inner scale of σx and σy is constrained not to exceed ½ dX, and an outer-scale diffusion is simulated with increments of a random "zitterbewegung",δx and δy, added to the mean advective motions.

Specifically, WPUFF assumes:

$$\delta x = \delta y = \xi\ [2\ \varepsilon h\ U\ dt\ \sigma]^{1/2}$$

In this equation

δx & δy are increments of horizontal displacements added to every puff's mean advective motions, at every time step.

ξ is a random variable with zero mean and unit standard deviation.

εh is an efficiency factor for horizontal diffusivities

U is the mean scalar wind velocity.

dt is an increment of time-step [60 seconds, in the present example.

σh is a characteristic scale for the horizontal diffusion, computed for every puff at every time step as

$$\sigma h(t) = \sigma h(t-dt) + \varepsilon h\ U\ dt.$$

This recipe generates an effective outer-scale diffusivity

$$K = ½\ d(\sigma^2)/dt = \varepsilon h\ U\ \sigma$$

Further discussion of diffusivities may be found in a following section.

Winds:

The governing winds for WPUFF are assumed to be measured within the domain by one or more near-surface observing meteorological [Met] sites. Initial approximations [Uo, Vo] of the components of the winds at varying distances from these Met sites are interpolated, in both time and space, for every puff. [If only one site is available, as at Umatilla, no spatial interpolation is possible.]

An innovation of WPUFF is to adjust wind directions and intensities for effects of local terrain by minimizing, for every puff and at every time, the function:

$$F(U,V,\lambda) = (U - Uo)^2 + (V - Vo)^2 + \lambda * W^2 \qquad [eqn.3]$$

In equation 3:

Uo, Vo are the uncorrected x- and y- components of the measured winds.

U, V are the corrected components that are used by WPUFF

λ is an empirical, non-negative, biasing parameter

W is the vertical component of the winds, which, near the surface, is approximated by U*Hx + V*Hy, where

Hx, Hy are the x- and y- gradients of the terrain, dH/dx , dH/dy.

The solution of equation 3 that minimizes F(U,V,L) is:

$$U = a11\ Uo + a12\ Vo \qquad [eqn.4a]$$
$$V = a21\ Uo + a22\ Vo \qquad [eqn.4b]$$

with:

$$a11 = (1 + \lambda\ Hy * Hy) / D$$
$$a22 = (1 + \lambda\ Hx * Hx) / D$$
$$a12 = a21 = -\lambda\ Hx * Hy / D$$

and: $D = 1 + \lambda\ (Hx * Hx + Hy * Hy)$

The limiting U,V when $\lambda \rightarrow 0$ are just Uo, Vo. The limits when $\lambda \rightarrow$infinity are the cosine projections of Uo, Vo onto the topographic iso-contours. With increasing λ this simple, *local*, algorithm increasingly biases the winds to divert around the hills. Those puffs that perversely still try to burrow through terrain are reflected upwards.

The parameter λ is empirical and equal to 1000 in the present case, an *ad hoc* value that produces "sensible" wind fields.

In later versions of WPUFF λ will be parameterized in terms of local stabilities and Froude numbers. In my judgment, however, this step should wait for model-validation studies, assisted by good measurements.

It should be remarked that the real physics governing near-surface winds are *not* local, as mass must also be conserved by accounting for convergences, in three dimensions. A higher approximation for the non-local, three-dimensional problem in complex terrain is described by J-C Barnard et al, in ref.7.

A solution to this next-higher approximation by Barnard's algorithm requires solving Laplace's equation in three dimensions [roughly 6000 grid points in the present case] at every time step. The computational requirements for this would put the model beyond the capabilities of inexpensive, desktop hardware. It remains to be tested whether WPUFF's present neglect of higher approximations to equations [eqns.3-4] are of similar order with other approximations in WPUFF [and other models], and with the quality of the data.

More about diffusivities:

For a puff of radius σ, a spherically symmetric radial eddy diffusivity coefficient may be defined as

$$K = 1/2\, d[\sigma^2]/dt \quad m^2/s \qquad \text{[eqn.5]}$$

With puff radii on the order of 10-100 meters experiments [ref. 2] confirm a semi-empirical relationship of the form

$$K \sim \varepsilon\, [\underline{U}\, \sigma] \quad m^2/s \qquad \text{[eqn.6]}$$

In equation 6, ε is a dimensionless scaling factor that is related to the stability, and $\underline{U}$ is the horizontal wind velocity, $\sqrt{[U^2 + V^2]}$.

Substituting equation 6 into equation 5 and differentiating,

$$d\sigma/dt = \varepsilon\, \underline{U} \qquad \text{[eqn.7a]}$$

$$\sigma(t+dt) = \sigma(t) + \varepsilon\, \underline{U}\, dt \qquad \text{[eqn.7b]}$$

$0 <= \sigma <= Z \sim 100$ m , for vertical diffusion

The solutions of equations 7 are observed to hold when Z <~ 100 meters, roughly the upper limit where equation 6 is valid, for vertical eddy diffusivities [ref.2].

It should be remarked here that we are speaking of "eddy-diffusivities", for which puff growth is observed to be nearly linear at these intermediate scales [10 - 100 meters in the vertical, 0.01 - 10 km in the horizontal]. Were the diffusivities scale independent, as is indeed so at much smaller scales, we would [and do] observe puff radii to grow with the square root of time. At larger scales [>~ 10 km] we observe exponential growth in horizontal radii, with characteristic times on the order of 10^5 sec.

In the real atmosphere, the vertical and transverse eddies are not isotropic near the surface, and separate diffusivity coefficients must be defined for horizontal [Kh, εh] and vertical [Kv, εv] dispersions. In Turner's classical workbook [ref. 2] dispersion curves are presented, in terms of empirical "stability classes" [A, B, ...] that are empirically related to wind speeds, time of day, and cloud cover.

From these curves and Monin-Obhukhov similarity theory can be derived a useful but approximate conversion table:

Table VII

Turner's Stability Class	εh	εv	dΘ/dZ
A	0.215	0.215	-0.04
B	0.155	0.110	-0.02
C	0.105	0.060	0.00
D	0.070	0.034	0.02
E	0.050	0.023	0.04
F	0.035	0.015	0.06

At Umatilla, however, good data are available of both horizontal variances and vertical gradients of the wind directions and velocities. I therefore prefer to assume:

$$\varepsilon h = 1/2 \langle\theta\rangle \quad \text{[eqn.8a]}$$

where <θ> is the standard deviation of horizontal wind directions, in radians,

and

$$\varepsilon v = k^2 [dLnU/dLnZ] / \Phi m . \quad \text{[eqn.8b]}$$

In equation 8b:

k = 0.40 , von Karman's constant

[dLnU/dLnZ] = is the observed logarithmic derivative of wind speeds with height, and

Φm = an empirical relationship based on Monin-Obhukhov similarity theory, as described by Arya [ref. 8] and many others.

With these approximations the increments of surface concentrations contributed in each grid cell by every puff were computed as:

$$dC = 1.71 * M / [dx^2 *(\sigma+Z)] * \exp\{-1/2(Z/\sigma)^2\} \quad \text{[eqn.9]}$$

[micrograms/m^3]

In equation 9:

dC = the increment of concentration from puffs at altitude Z, above the surface, [micrograms/m^3].

dx = the horizontal grid dimension, [460 meters in the present case].

M = the puff mass emitted during dt, [micrograms].

σ = current puff radius, [meters].

Z = puff-center height above the surface, [meters].

The leading coefficient [1.71] in equation 9 derives from an integration over the projected puff concentrations at the surface, averaged over the surface grid cells.

Accuracy:

WPUFF is not yet validated by comparison with observations.

Failing this, and far less usefully, I have intercompared WPUFF with the Gaussian model, for a single plume at 60 meters, over flat terrain as follows:

The "simple Gaussian model" referred to throughout this report is from Turner's workbook, with

$$C(X,Y,0)/Q = [\pi\ U\ Sy\ Sz]^{-1} \exp\{-1/2[(y/\sigma y)^2+(H/\sigma z)^2]\}$$

In one of many tests I assumed

$Q = 1$ gm / sec

$U = 1$ m/s

$H = 60$ meters, and

$\sigma y \cong \varepsilon h\ X^{\alpha} \qquad \sigma z \cong \varepsilon v\ X^{\beta}$

These last two equations approximate Turner's famous graphs, where $\alpha \cong \beta \cong 0.92$. These exponents are approximate and are known both theoretically and by observations to vary with X, with α increasing from 0.5 at small scales [X < 1 m] to 2.00 [X > 10 km]. At X = 1 km [roughly two grid cells in the Umatilla exercise] both α and β do not significantly differ from unity. I have for simplicity and consistency adopted this value in both WPUFF and Turner's "simple model".

In the comparison I am now describing the coefficients εh and εv were respectively 0.070 and 0.034, values roughly equivalent to the Pasquill-Turner stability class "D". For this comparison, only, simulations with both models assumed infinite mixing depths, H. The WPUFF model was run time increments of one minute, for 17 hours, after an initial "warm up" of 7 hours to allow an approximate steady state. With these conditions about 200 puffs were contained in the modeled field at all times.

With these parameters, figure 11 illustrates the steady-state isopleths of surface concentrations by the Gaussian model, and the following figure 12 similarly shows isopleths from WPUFF.

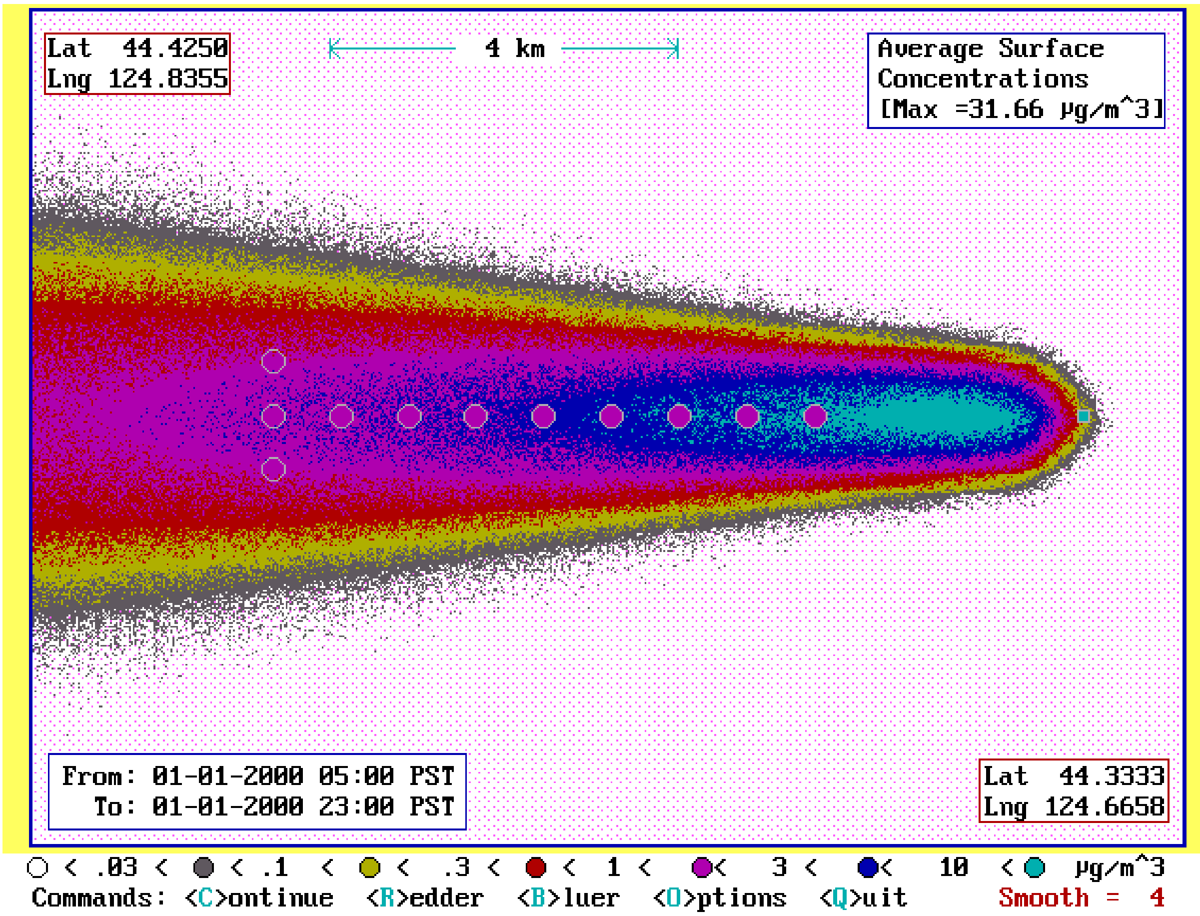

Figure 11:

Concentration Isopleths from a steady-state Gaussian Model. The source is at the right [small green box] and the wind is easterly. The purple circles locate fictitious "receptors sites".

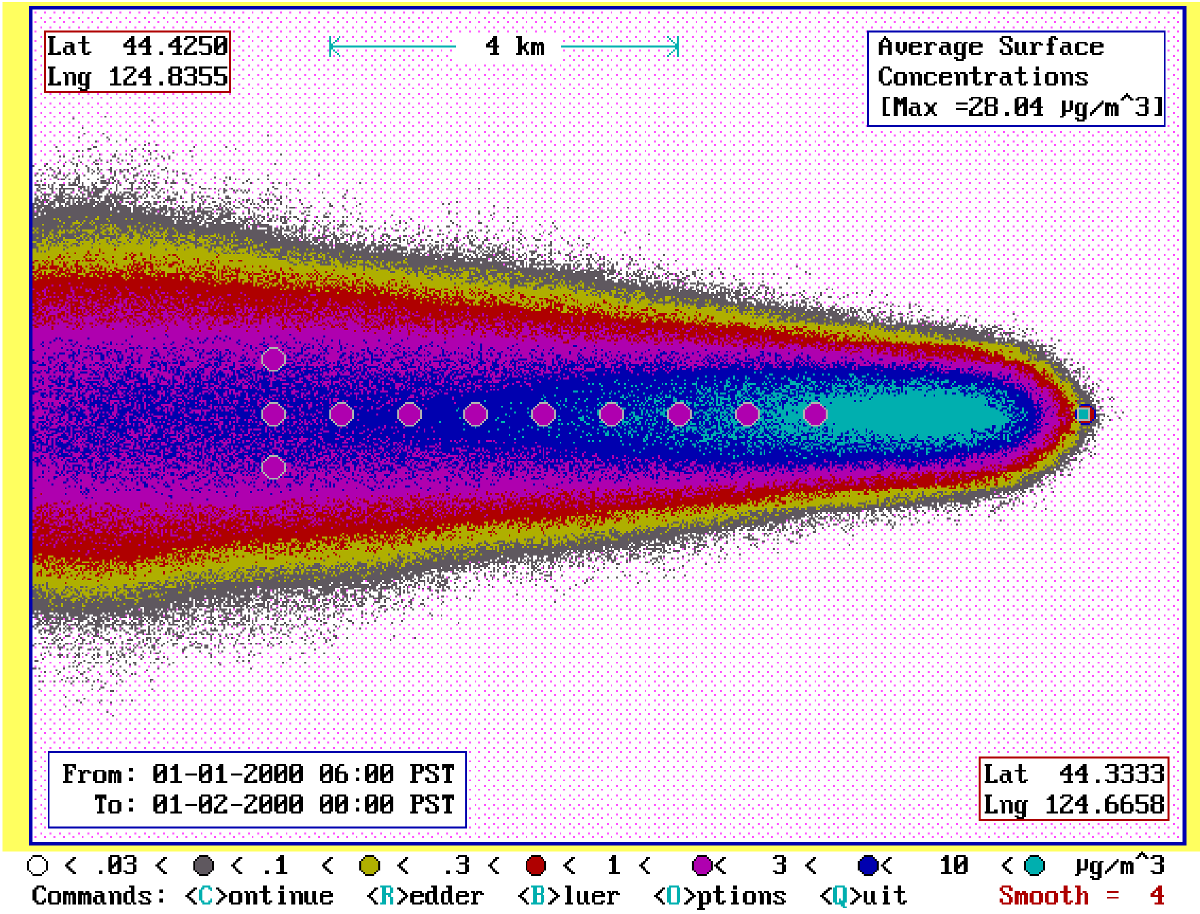

Figure 12

Similar concentration isopleths from WPUFF.

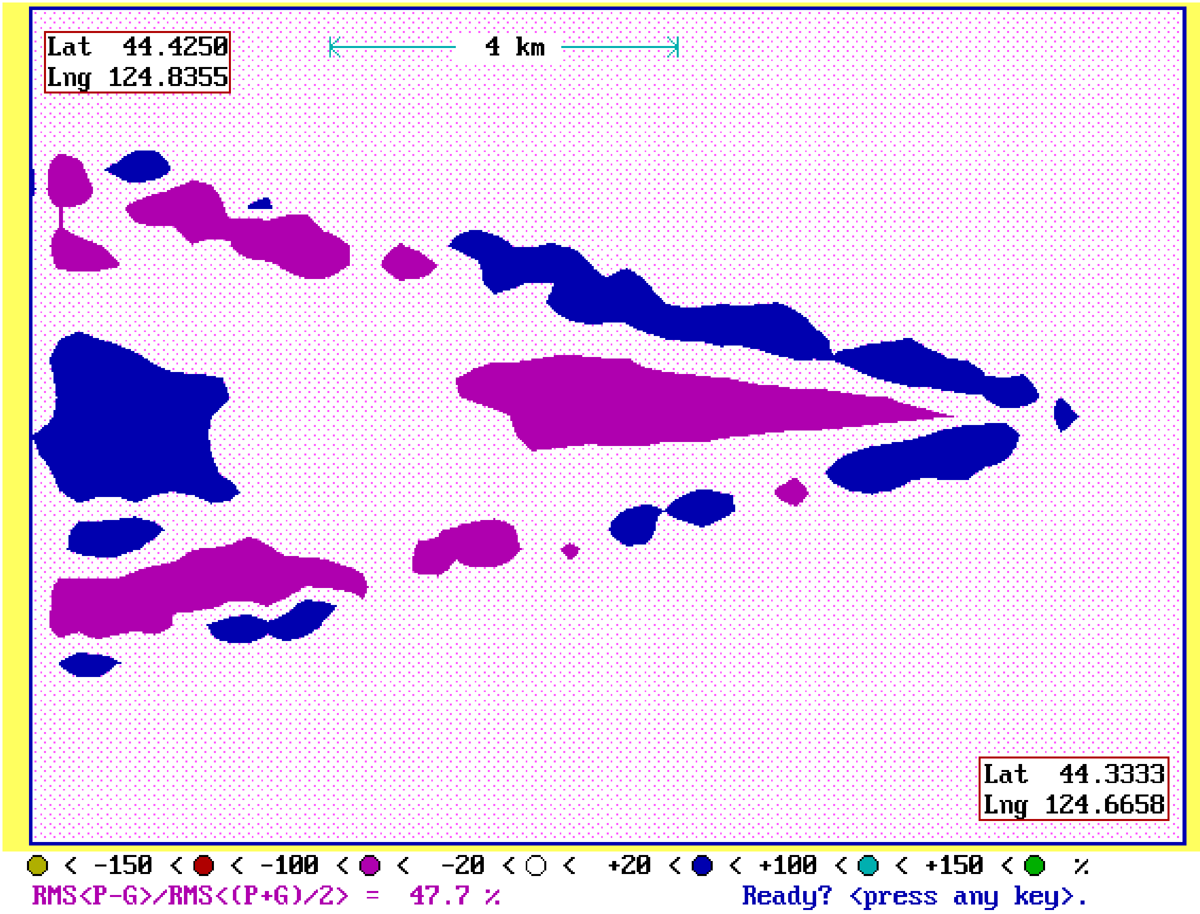

Figure 13

Relative Differences between the two models.
Plotted are isopleths of 2[P-G] / [P+G] where "P" are concentrations from the Puff model [figure 3] and "G" are concentrations from the Gaussian Model [figure 2].

In the blue areas P exceeds G by ratios between 0.2 and 1.0. In the purple areas G similarly exceeds P. In the blank areas the differences are less than 20%

The granularity in this figure results from sampling fluctuations that are proportional to the square-root of the puff numbers that are sampled by each cell. Caution should be exercised in comparisons at the edges of this figure, where both P and G are very small.

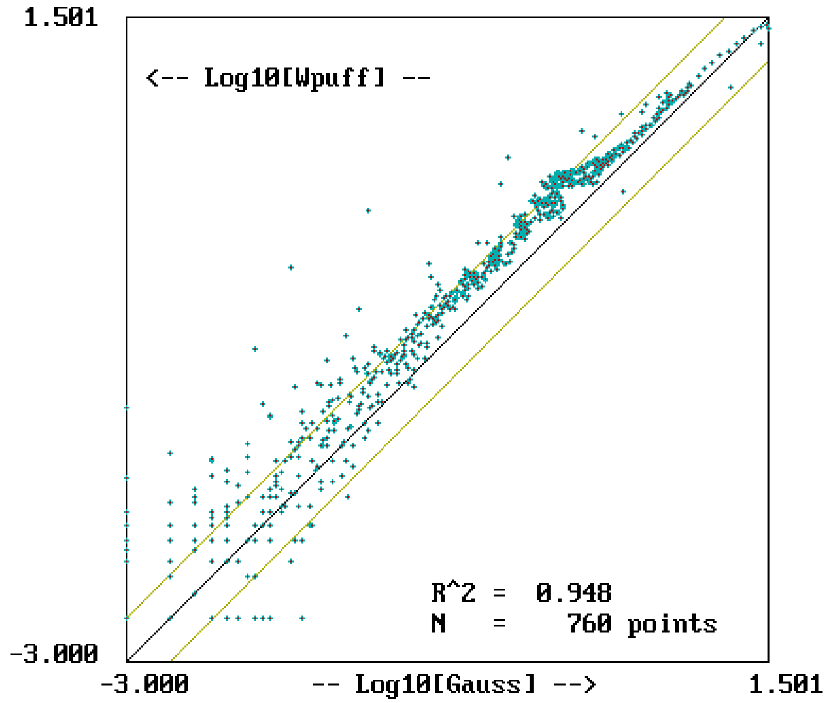

Figure 14

Log-Log scattergram of surface concentrations predicted by the two models. The central diagonal line shows the 1:1 slope. The two bracketing diagonals are displaced above and below the 1:1 slope by factors of 2.

In presenting the comparisons of figures 11-14, I emphasize that neither model is “correct”. Both are approximate, and comparisons with real data are strongly to be preferred. I wish also to emphasize that the “factors of two” brackets shown in figure 14 are comparable to model comparisons with real data, where they exist [Olesen, 1994-1997].

Speed:

WPUFF is a floating-point intensive program that makes high demands on desktop microprocessing. With my 450 Mhz AMD K6-II, running in WINDOWS 95, the Umatilla simulations run about 5000 times faster than the world, or about 2 hours to simulate one calendar year. The Gaussian model used here is in turn about 6 times faster than WPUFF.

Depositions:

WPUFF does not explicitly compute either wet or dry depositions. The SAIC study with ISCST-3 [ref.1] concluded that dry depositions of tracer gases and aerosols at Umatilla exceed those from rain and snow. Simple models for dry deposition assume fluxes to the surface to be proportional to the near-surface concentrations, C, as in:

$$\text{Flux}[g/m^2/sec] = \nu[m/s] \bullet C[g/m^3] \qquad \text{[eqn.10]}$$

In equation 10 the coefficient ν is called a "deposition velocity", and is of order 0.01 meters/sec for CO_2 and SO_2, and 0.003 meters/sec for aerosols. The larger of these numbers corresponds to about 3 kg of deposition per hectare per yr, per μg/m^3 of near-surface tracer concentrations. Thus at Hermiston, for example, where WPUFF estimates the annually averaged near-surface concentrations to be 0.025 μg/m^3 per g/sec of emissions, the corresponding dry deposition there is expected to approximate 80 grams/hectare/yr per g/sec of emissions from the incinerator stack at the UMCDF facility. [One hectare is 10,000 square meters.]

Enough:

WPUFF is a work in progress. I have probably written more of it here than all but a few of you may wish to know. I welcome questions and discussion.

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