

# **Generic Guidance and Optimum Model Settings for the CALPUFF Modeling System for Inclusion into the ‘Approved Methods for the Modeling and Assessments of Air Pollutants in NSW, Australia’**

**March 2011**

*Prepared For:*

**NSW Office of Environment and Heritage, Sydney Australia**

*Prepared By:*

**Jennifer Barclay and Joe Scire**

**Atmospheric Studies Group**

**TRC Environmental Corporation**

650 Suffolk Street, Wannalancit Mills

Lowell, MA 01854

USA

**Disclaimer**

This report was prepared by the Atmospheric Studies Group from TRC Environmental Corporation in good faith exercising all due care and attention, but no representation or warranty, express or implied, is made as to the relevance, accuracy, completeness or fitness for purpose of this document in respect of any particular user's circumstances. Users of this document should satisfy themselves concerning its application to, and where necessary seek expert advice in respect of, their situation. The views expressed within are not necessarily the views of the Office of Environment and Heritage (OEH) and may not represent OEH policy.

© Copyright State of NSW and the Office of Environment and Heritage NSW

## Contents

SCOPE OF WORK AND BACKGROUND .....	1
<b>A.1 Introduction .....</b>	<b>1</b>
<b>A.2 Requirements of the NSW OEH .....</b>	<b>1</b>
1. INTRODUCTION .....	3
2. GUIDANCE ON CALMET CONFIGURATIONS .....	4
<b>2.1 Overview .....</b>	<b>4</b>
<b>2.2 General Guidance for CALMET .....</b>	<b>4</b>
<b>2.2.1 CALMET Overview .....</b>	<b>4</b>
<b>2.3 Methodologies for Running CALMET .....</b>	<b>5</b>
<b>2.3.1 No-Observations Approach .....</b>	<b>6</b>
<b>2.3.2 Hybrid Mode .....</b>	<b>7</b>
<b>2.3.3 Observations Only .....</b>	<b>10</b>
<b>2.3.4 Single Station Meteorology .....</b>	<b>11</b>
<b>2.3.5 Screening Model runs .....</b>	<b>11</b>
<b>2.4 Prognostic-Derived Surface (SURF.DAT) and Upper (UP.DAT) files .....</b>	<b>12</b>
<b>2.5 Seven Critical CALMET Parameters When Using Observations .....</b>	<b>12</b>
<b>2.6 Other Important Parameters – Overwater Surface Fluxes and Mixing Heights .....</b>	<b>13</b>
3. RECOMMENDED MODEL OPTION SETTINGS FOR CERTAIN CONDITIONS AND SCENARIOS .....	17
<b>3.1 Introduction .....</b>	<b>17</b>
<b>3.2 Complex terrain .....</b>	<b>17</b>
<b>3.2.1 Terrain Data .....</b>	<b>17</b>
<b>3.2.2 Choosing Grid Resolution and Model Domain Size .....</b>	<b>18</b>
<b>3.2.3 Choosing a value for TERRAD .....</b>	<b>18</b>
<b>3.2.4 Complex Terrain Sub-Grid Scale Terrain Features (CTSG) .....</b>	<b>19</b>
<b>3.3 Shoreline Fumigation .....</b>	<b>20</b>
<b>3.3.1 Sub-grid Scale TIBL .....</b>	<b>20</b>
<b>3.4 Inversion Break-up Fumigation .....</b>	<b>21</b>
<b>3.4.1. Description of how CALMET computes mixing height and its relevance to properly modeling Inversion-breakup fumigation .....</b>	<b>22</b>
<b>3.5 Buoyant line plumes .....</b>	<b>22</b>
<b>3.5.1 Entering Line sources into CALPUFF .....</b>	<b>24</b>
<b>3.5.2 Evaluation Studies .....</b>	<b>27</b>
<b>3.6 Calm winds .....</b>	<b>30</b>
<b>3.6.1 Sub hourly meteorological data and its usage in CALPUFF .....</b>	<b>31</b>
<b>3.6.2 User Options for treating Calms .....</b>	<b>39</b>

4.	DISCUSSION ON THE APPROPRIATE PROCEDURES FOR EVALUATING CALMET AND CALPUFF MODELLING RESULTS .....	41
4.1	<b>Model Output: Uncertainty</b> .....	41
4.2	<b>Procedures for Evaluating Model Output</b> .....	42
	4.2.1 <b>Overview</b> .....	42
4.3	<b>How to Evaluate CALMET</b> .....	42
	4.3.1 <b>Graphical Evaluation</b> .....	43
	4.3.2 <b>Statistical Evaluation</b> .....	46
	4.3.3 <b>Other Meteorological Evaluation Packages</b> .....	47
	4.3.3.1 <b>Key Variable Field Extraction Module</b> .....	47
	4.3.3.2 <b>Gridded Meteorological Extraction and Merging</b> .....	47
	4.3.3.3 <b>Back Trajectory</b> .....	47
	REFERENCES .....	48
	APPENDIX A:.....	50
	MODEL OPTION SWITCHES FOR CALMET AND CALPUFF .....	50

## LIST OF FIGURES

	<b>Page</b>
Figure 2-1. Figure showing examples of how to choose RMAX1, R1, RMAX2 and R2 values. One value of RMAX1, RMAX2, R1 and R2 apply to all surface and upper air stations. RMAX1 and RMAX2 is typically the maximum radius of influence of the surface and upper air station, respectively. The approximate length (km) of RMAX1 and RMAX2 is shown in the figure as black solid lines. The blue circles represent approximate values (km) of R1 values representative of all surface stations. In complex terrain the R1 value is usually smaller than the RMAX value. The pink circle represents the R2 value of the upper air station for level 2 and aloft.....	13
Figure 3-1. Example showing how to estimate TERRAD. Usually, (ridge (km) to ridge (km) ) / 2, plus add 1 or 2 km. A typical value for TERRAD in this example would be 10km.....	19
Figure 3-2. Aerial photograph of a typical aluminum plant showing rows of potrooms. ....	23
Figure 3-3. Shows a cross-section of two adjacent buildings with dimensions defined (Schulman and Scire, 1980). The GUI screen shot below from CALPRO shows the Line Source Input section.....	25
Figure 3-4. CALPRO GUI screenshot showing the CALPUFF user input control screen for entering line source data. ....	25
Figure 3-5 GUI screenshot from CALPRO showing the CALPUFF user input control screen for the average properties for line sources. ....	26
Figure 3-6 Figure shows the difference between point source plume rise and line source plume rise (Scire and Schulman, 1981). If you treat a line source as a set of too few point sources you can seriously under or overpredict the plume rise. ....	27
Figure 3-7 Comparison of AERMOD and CALPUFF predictions of line source impacts from the Arkadelphia Arkansas SF <sub>6</sub> tracer study compared to BLP predictions. This study shows the impacts of the line sources alone.....	28
Figure 3-8. Predictions of 1-hour average SO <sub>2</sub> concentrations at the downwind Alcoa Tennessee monitor for 1977 versus Observations and models, CALPUFF, BLP and AERMOD. The BLP results based on Version 1.1 of the model as well as the current version of BLP on the U.S. EPA web site (with modifications to the meteorological file to allow it to run) are shown. CALPUFF closely matches BLP results while AERMOD significantly overpredicts the observed concentration measurements. ....	29
Figure 3-9 CALPUFF peak, 1-hr average concentration map using 1 hour meteorological data and default calm threshold of 0.5 m/s. Computed turbulence parameters were used assuming the default minimum $\sigma_v$ of 0.5 m/s.....	33
Figure 3-10 CALPUFF peak, 1-hr average concentration map using 10-minute meteorological data and default calm threshold of 0.5 m/s. Real turbulence parameters were used with a minimum $\sigma_v$ of 0.2 m/s, $\sigma_w$ was left unchanged at the model's default values. ....	34
Figure 3-12 CALPUFF computed $\sigma_v$ using model defaults and one hour meteorology. (It is always preferable to use real measured values of real time turbulence wherever possible).....	39
Figure 3-13. Real 10-minute measured $\sigma_v$ . (CALPUFF can read this real time data directly). ....	39

## LIST OF TABLES

---

	<b>Page</b>
Table 2-1. Table shows the difference in effort required by the user to run CALMET in three different modes, (1) the most simple a No-Obs mode, (2) a Hybrid approach which combines observations with prognostic model data, and (3) an Observations only approach – which requires the most decisions and effort by the user.....	8
Table 2-2. Model Option Switches for No-Obs Simulations.....	9
Table 2-3. Tabulated List of Various Methods for Including Meteorological Data into CALMET. The list is detailed in order of decreasing preference. ....	15
Table 3-1. Annual Average SO <sup>2</sup> Concentrations (µg/m <sup>3</sup> ) at Alcoa, TN for 1976 and 1977. Observed and predicted concentrations using the BLP, CALPUFF and AERMOD models. ....	29
Table A-1. An Explanation of the 7 Critical User-Defined, Site Specific Parameters When Using Observational Data in CALMET.....	51
Table A-2. Explanation and Recommendations for the List of Key CALMET Model Options .....	54
Table A-3. Explanation and Recommendations for the Overwater Surface Fluxes Switches.....	58
Table A-4. Explanation and Recommendations for the List of Key CALUFF Model Options .....	61

# SCOPE OF WORK AND BACKGROUND

---

## A.1 Introduction

TRC's Atmospheric Studies Group has been approached by the Office of Environment and Heritage, (OEH), NSW to prepare Generic Guidance and Optimum Model Settings for the CALPUFF Modelling System for inclusion into the *Approved Methods for the Modelling and Assessment of Air Pollutants in NSW*.

To ensure scientific rigueur and consistency in application, the OEH has requested that TRC's Atmospheric Studies Group provide where possible recommended settings for CALMET and CALPUFF in the *Approved Methods for the Modelling and Assessment of Air Pollutants in NSW*. The OEH have in particular asked for generic guidance on determining the site specific model options and guidance for recommended settings for a range of conditions and model scenarios.

## A.2 Requirements of the NSW OEH

1. Generic guidance for setting site specific model options in CALMET and CALPUFF. The guidance is to be suitable for inclusion in the *Approved Methods for the Modelling and Assessment of Air Pollutants in NSW*. Where possible, provide examples to demonstrate the guidance.
2. The recommended model option settings for CALMET and CALPUFF for modelling in the following conditions and scenarios:
  - a. Complex terrain;
  - b. Buoyant line plumes;
  - c. Shoreline fumigation;
  - d. Inversion break-up fumigation; and
  - e. Low wind speed/calm conditions - if the recommended model settings include the use of 10 minute average meteorological data, model option settings are also to be recommended for the use of 1 hour average meteorological data.

The recommended model option settings are to be supported by the results of model evaluation studies. A discussion on the sensitivities to changes in model settings is to be provided.

3. Optimal methodology to incorporate meteorological data in CALMET. In particular, the recommended methodology to incorporate
  - a. Surface and upper air meteorological observations (diagnostic); and
  - b. Surface and upper air meteorological numerical predictions (prognostic).

In recommending the optimal methodology a number of different techniques for incorporating meteorological data should be evaluated. The recommended optimal methodologies are to be supported by the results of model evaluation studies.

4. Discussion on the appropriate procedures for evaluating CALMET and CALPUFF modelling results.

# 1. INTRODUCTION

---

The CALPUFF modeling system provides a non-steady state modeling approach which evaluates the effects of spatial changes in the meteorological and surface characteristics. It offers the ability to treat stagnation, multiple-hour pollutant build-up, recirculation and causality effects which are beyond the capabilities of steady-state models. The CALPUFF modeling system was adopted by the U.S. EPA as a *Guideline Model* for long range transport applications and, on a case-by-case basis, for near-field applications involving complex flows (*Federal Register*, April 15, 2003, Pages 18440-18482). CALPUFF is also recommended by both the Federal Land Managers Air Quality Workgroup (FLAG, 2000, 2008) and the Interagency Workgroup on Air Quality Modeling (IWAQM, 1998). It has been adopted for world-wide use by the United Nations International Atomic Energy Agency (IAEA). CALPUFF is widely used in many countries (over 100 countries) throughout the world. In several countries it has been incorporated as a regulatory model.

CALMET is a diagnostic meteorological model that produces three-dimensional wind fields based on parameterized treatments of terrain effects such as slope flows and terrain blocking effects. Meteorological observations are used to determine the wind field in areas of the domain within which the observations are representative. Fine scale terrain effects are determined by the diagnostic wind module in CALMET. CALPUFF is a non-steady-state puff dispersion model. It accounts for spatial changes in the meteorological fields, variability in surface conditions such as (elevation, surface roughness, vegetation type, etc.), chemical transformation, wet removal due to rain and snow, dry deposition and terrain influences on plume interaction with the surface.

This document is divided into several sections. The first section provides an introduction to the CALMET/CALPUFF modelling system. The second section provides guidance for specific model options in CALMET and CALPUFF and also discusses the optimal methodology to incorporate meteorological data into CALMET. The third and fourth sections provide recommended model settings for complex terrain, buoyant line sources, shoreline fumigation, inversion break-up fumigation and low wind speed and calms. While Section five looks at current best recommended model evaluation procedures for both CALMET and CALPUFF. Appendix A contains the model option tables.

## 2. GUIDANCE ON CALMET CONFIGURATIONS

---

### 2.1 Overview

The aim of this section is to provide model guidance for setting site specific model options in CALMET and CALPUFF and also to provide the optimal preferred methodology for incorporating meteorological data into CALMET. For the sake of brevity, Appendix A, Tables A-1 to A-4 contain the detailed model option switches.

It is important to note that it is impossible to specify a single set of options/user-defined factors for every circumstance as some factors depend entirely on the meteorological and geophysical characteristics of the model domain along with their associated site specific source characterization. The model option switches which are provided in Appendix A for both CALMET and CALPUFF provide the best recommended guidance.

### 2.2 General Guidance for CALMET

#### 2.2.1 CALMET Overview

The CALMET meteorological model consists of a diagnostic wind field module and micrometeorological modules for overwater and overland boundary layers (Scire et al., 2000a). When using large domains, the user has the option to adjust input winds to a Lambert Conformal Projection coordinate system to account for the Earth's curvature. The diagnostic wind field module uses a two-step approach to the computation of the wind fields (Douglas and Kessler, 1988). In the first step, an initial-guess wind field is adjusted for kinematic effects of terrain, slope flows, and terrain blocking effects to produce a Step 1 wind field. The second step consists of an objective analysis procedure to introduce observational data into the Step 1 wind field in order to produce a final wind field. An option is provided to allow gridded prognostic wind fields to be used by CALMET, which may better represent regional flows and certain aspects of sea breeze circulations and slope/valley circulations. The prognostic data as a 3D.DAT file can be introduced into CALMET in three different ways;

- as a replacement for the initial guess wind field
- as a replacement for the Step 1 field
- as observations in the objective analysis procedure

The preferred choice is to use gridded prognostic meteorological data as the initial guess wind field. These options are discussed in detail below.

## 2.3 Methodologies for Running CALMET

The CALPUFF modeling system can be run in several modes requiring different types of meteorological data. The following lists three modes available to run CALMET and a fourth mode using other meteorological processors.

1. CALMET No-Observations (No-Obs) Mode. CALMET using gridded numerical model output (e.g., from the MM5, WRF, RAMS, RUC, Eta or TAPM models). No surface, upper air or buoy observations are used in No-Obs mode.
2. CALMET Hybrid Mode. CALMET run using a combination of gridded numerical meteorological data supplemented by surface and optional overwater buoy data.
3. CALMET Observations-Only (Obs) Mode. – CALMET using observed surface and upper air data, plus optional buoy data.
4. Single meteorological station dataset. CALMET is not used but rather single station meteorological data is passed directly into CALPUFF from a steady-state plume processor. Examples of single station datasets are those used to drive the AERMOD, AUSPLUME, CTDMPPLUS or ISCST3 models. CALPUFF can be driven with any of these meteorological datasets.

**If good quality gridded prognostic meteorological data are available, CALMET No-Obs mode is recommended as the preferred method for regulatory screening modeling.** This recommendation is based on the following factors: (a) No-Obs mode allows the important benefits of the non-steady-state approach in CALPUFF to be included in the dispersion modeling (e.g., spatially varying meteorology and dispersion, causality, recirculation, stagnation, pollutant build-up, fumigation, etc.); (b) No-Obs mode makes use of three-dimensional, hourly prognostic meteorological data often available at high resolution to drive CALMET and CALPUFF; (c) No-Obs mode greatly simplifies the preparation of the CALMET inputs because a large number of input variables dealing with observational data are not required and the difficulties of dealing with potentially incomplete observational datasets are eliminated; (d) No-Obs mode provides a relatively straightforward approach that facilitates agency review and approval of the CALMET/CALPUFF simulations. The level of effort to run CALMET in No-Obs mode is similar to that required to run the AERMOD terrain and meteorological processors (although the output files will be much larger with CALMET). Depending on the results of the initial No-Obs simulations, additional refinements can be made to the meteorological fields by adding meteorological observations to CALMET.

Table 2-1 shows the differences in important CALMET model option switches between the “no-observations” (No-Obs) simulation, vs. the hybrid prognostic observation approach, vs. the observation-only approach. The variables in bold are site specific and care is needed in their choices. All these variables are detailed in Appendix A. Each of the approaches is discussed below.

### 2.3.1 No-Observations Approach

When run this way, CALMET uses gridded wind fields generated by a numerical prognostic model such as MM5, WRF, RUC, RAMS, Eta and TAPM in the form of a three dimensional data file, known as a 3D.DAT file. The procedure permits the prognostic model to be run with a significantly larger horizontal grid spacing and different vertical grid resolution than that used in the diagnostic model. This option allows certain features of the flow field such as the sea breeze circulation with return flow aloft, which may not be captured in the surface observational data, to be introduced into the diagnostic wind field results.

Existing 3D.DAT files are available (see below) or can be obtained by running one of the prognostic models. Existing 3D.DAT files can be used directly in CALMET. If new prognostic modeling is used, the CALMET-compatible 3D.DAT file is created by running independent modules, CALMM5, CALWRF, CALRUC, CALRAMS, CALETA or CALTAPM on the numerical model output in their individual model data format. The 3D.DAT file contains data of horizontal and vertical velocity components, pressure, temperature, relative humidity, vapor, cloud, rain, snow, ice and graupel mixing ratios. Depending on the base model used and also the configuration switch settings within that model, the output may also contain solar and long wave radiation, sea surface temperature, 2m air temperature, precipitation amount and other variables.

There are many important significant advantages in running the model in No-Observations mode using gridded prognostic data. These are listed and described briefly below;

Spatial Variability in the Horizontal and Vertical. The three-dimensional wind field reflects local terrain and mesoscale winds, temperature and stability variations and offer advantages in terms of representing horizontal and vertical spatial variability over point (observation) measurements.

Simplicity of No-Obs Run. It is easy to load a 3D.DAT file into CALMET and execute. The only other input file required is the geophysical (terrain and land use) file and the control file with user switch settings. Three-dimensional MM5 (Fifth Generation NCAR/PENN State Mesoscale Model) data are currently available for all of New South Wales for three years (2006-2008) at 12-km horizontal resolution for 40 vertical levels at the official CALPUFF web site ([www.src.com](http://www.src.com)) or data can be generated with customized runs of any of the readily available prognostic models (MM5, WRF, TAPM, RAMS). Using existing data is generally much easier than running the prognostic models, which depending on the model may require significant effort.

Fast and Efficient – By using an already prepared 3D.DAT file, no additional effort is required to prepare other observational data files or deal with missing data.

No Additional Data Required – A big advantage of No-Obs mode is that no additional data files other than a geophysical data file is required. The 3D.DAT file contains three-dimensional

hourly profiles of wind speed, wind direction, temperature, humidity and pressure, and usually contains precipitation, solar and long wave radiation, sea surface temperature and cloud information (ceiling height and cloud amount are derived variables in CALMET in No-Obs mode). Issues related to the use of observational data such as collecting surface, upper air, precipitation and buoy station data, running the various processor programs and dealing with missing data are all eliminated in No-Obs mode making the CALMET runs straightforward.

Most Decision Making by the User is Eliminated - By using existing 3D.DAT files in No-Obs mode, the number of decisions required of the user when preparing the CALMET control file is substantially reduced. The value of TERRAD and a few other fairly straightforward variables need to be specified by the user. No-Obs mode eliminates the need for decisions on 6 of the 7 'critical variables' because observational data are not used. See Section 3.2.3 for a description on how to compute TERRAD.

No Overwater Data Required – For model domains over coastal regions, meteorological data over the water is very important when considering plume transport across the sea/land interface. Sea surface temperature and air-sea temperature differences over the water will usually be embedded in the 3D.DAT file (depending on the prognostic model).

When good quality prognostic fields are available, the No-Obs simulation should be a reasonable predictor of the results of a refined simulation (e.g., hybrid mode or obs-only mode) where good quality observational data are added to the prognostic data. The quality of the prognostic simulation can be assessed by quantitative and qualitative tools provided as part of the CALPUFF software system.

### **2.3.2 Hybrid Mode**

Running CALMET in Hybrid mode can be considered an 'advanced model simulation', or, 'refined model run' since it combines the numerical prognostic model data in a 3D.DAT file along with surface and overwater observational data. More work is required by the user as preparation is required in the collection and formatting of the surface observational data, upper air data and optional overwater stations and precipitation stations. Plus careful consideration needs to be given with respect to the Seven Critical CALMET parameters discussed in 2.4, below.

Table 2-1. Table shows the difference in effort required by the user to run CALMET in three different modes, (1) the most simple a No-Obs mode, (2) a Hybrid approach which combines observations with prognostic model data, and (3) an Observations only approach – which requires the most decisions and effort by the user.

Description	No-Observations Mode (No-Obs)	Hybrid Mode - Prognostic Model Data + Observations	Observations Only Mode
Data Preparation	Low	Medium	High
Ease of Use	Most Simple	Requires more effort	Requires significantly more effort
CALMET Variables (variables that are in bold require site specific decision making )	NM3D NOOBS ICLLOUD IPROG <b>TERRAD</b>	NOOBS NOWSTA (opt) NSSTA NPSTA (opt) NM3D <b>ICLOUD</b> <b>IEXTRP</b> IPROG <b>RMAX1</b> <b>RMAX2</b> <b>RMAX3</b> <b>TERRAD</b> <b>R1</b> <b>R2</b>	NOOBS NUSTA NOWSTA (opt) NSSTA NPSTA (opt) <b>ICLOUD</b> <b>IEXTRP</b> <b>BIAS</b> IPROG <b>RMAX1</b> <b>RMAX2</b> <b>RMAX3</b> <b>TERRAD</b> <b>R1</b> <b>R2</b>
Input Files	CALMET.INP	CALMET.INP	CALMET.INP
	GEO.DAT	GEO.DAT	GEO.DAT
	3D.DAT	3D.DAT	UP.DAT
		SURF.DAT	SURF.DAT
		PRECIP.DAT (optional)	PRECIP.DAT (optional)
		SEA.DAT (optional)	SEA.DAT (optional)

Table 2-2. Model Option Switches for No-Obs Simulations.

Option	Parameter	Recommend value	Explanation and Justification
<b>Input Group 0. Input and Output Files</b>			
Number of prognostic and IGF CALMET files	NM3D	1 - 52	Number of 3D.DAT files.
<b>Input Group 4. Meteorological Data Options</b>			
Set the control file to reflect NOOBS simulation.	NOOBS	2	For screening model runs option 2 means use prognostic data (MM4/MM5/3D.DAT) file exclusively, i.e., no surface, overwater or upper air stations.
Cloud Data Options – Gridded Cloud Fields	ICLOUD	4	Gridded cloud cover from Prognostic relative humidity at all levels (MM5toGrads algorithm)
Use gridded prognostic wind field model output (3D.DAT) as input to CALMET	I PROG	14	This value can vary depending on the format of the prognostic model data and whether the prognostic data is input as the IGF (14), Step 1 wind field (13) or as observations (15).
Radius of influence of terrain feature	TERRAD*	No Default	There is no default for TERRAD and its value in km requires user input. TERRAD is specific to each model domain.

\* Of these parameters that require changes for a NOOBS model run, the only one that is site specific and requires special attention is TERRAD.

There are two ways to introduce 3-D prognostic wind data into CALMET when using prognostic data combined with observations. The first and preferred option is prognostic data as the initial guess field. In this approach the coarse grid scale prognostic data are interpolated to the CALMET fine-scale grid. The diagnostic module in CALMET will then adjust the initial guess field for kinematic effects for terrain, slope flows and terrain blocking effects using fine-scale CALMET terrain data to produce a Step 1 wind field. Observations are then introduced into the Step 2 wind field. The second approach is to use prognostic wind data directly as the Step 1 wind field. This field is then adjusted using observational data, but additional terrain adjustments at the scale of the CALMET grid resolution are not made. The second approach is not normally recommended.

All the advantages are the same as for the No-Obs run detailed above, but with additional complications such as preparing the observational data, optimizing model input to blend the observations properly with the prognostic data, replacing missing data and making careful site specific choices with respect to several parameters in the CALMET control file. Relevant useful references are; Wu et al (1998), Scire and Robe (1977) and Robe and Scire (1998).

### **2.3.3 Observations Only**

This approach ‘Observations only’ relies on standard hourly surface and twice-daily upper air data and optional hourly precipitation and overwater data to provide the necessary requirements for the computations of the micrometeorological modules for overwater and overland boundary layers.

Computation of the wind field in Obs-only mode is a two-step approach in CALMET which uses the observations twice, once to create the initial guess wind field which is then adjusted for kinematic effects of terrain, slope flows and terrain blocking effects to produce the Step 1 wind field. The second step consists of an objective analysis procedure to introduce observational data, ‘more formally’ into the Step 1 wind field to produce a final wind field.

As a minimum CALMET must be provided surface hourly data from one or many stations as well as radiosonde upper air data at intervals no more than 14 hours apart. Overwater stations and precipitation data are optional. This modeling approach is advantageous in regions where there is good representative surface and upper air data near to the facility and the expected area of impact is nearby, i.e., within a few to several kilometres. However, some complicated choices need to be made, especially with respect to the radiosonde station which may suffer from missing data both in-between levels and missing profiles altogether. Further, unless the upper air station is near to the facility (within 10 – 50km depending on topography) it is not likely to be representative. As a result the user is left with several critical choices to make which can significantly affect the final outcome of the model runs.

### **2.3.4 Single Station Meteorology**

It is recommended to run CALPUFF with a full 3-Dimensional wind field and temperature field, as well as two-dimensional fields of mixing heights and other meteorological variables.

However, in some near-field applications, when spatial variability of the meteorological fields may not be significant (e.g., uniform terrain and land use); the single station data file may be used. CALPUFF supports the following single station file formats; AUSPLUME, ISCST3, CTDMPLUS and AERMOD. CALPUFF assigns the single value of each variable read from the single station file to all grid points, resulting in a spatially uniform field.

Even when using single station meteorological data, some (but not all) benefits of the non-steady-state approach over steady-state models can be realized. For example, the time required for plume material to reach a receptor (the causality effect) is accounted for in the puff transport, and curved trajectories and variable dispersion and stability conditions over multiple hours of transport. . Secondly, the CALPUFF model has ‘memory’, in that each hour’s emissions is retained and may impact concentrations during a subsequent hour. As a result, pollutant build-up during light wind speed and calm conditions can be accounted for in the non-steady-state approach. Also, plume fumigation associated with inversion break-up can be simulated as a result of pollutant memory effect. What is lost when using single station meteorological data is the spatially variability of winds, stability and turbulence fields as may occur due to changes in land use type (especially land vs. water), terrain channeled flow, and mesoscale features such as a land-sea breeze circulation.

This option is only recommended for those near field applications where spatial variability in the winds and dispersion characteristics are not considered significant. Some of the advanced terrain options of CALPUFF cannot be used with this approach. Other options may require additional meteorological parameters be added to the standard single station files as ‘extended data records’. For instance precipitation is needed for wet deposition modeling, and, solar radiation and relative humidity data are needed to use the chemical transformation calculations of SO<sub>2</sub> and NO<sub>x</sub> in CALPUFF.

### **2.3.5 Screening Model runs**

In summary, the No-Obs approach using ready prepared three dimensional data files is recommended for screening runs due to the benefits of using 3-D meteorological fields, ability to perform dispersion calculations within a non-steady-state framework, and ease of use considerations. The results of a No-Obs mode simulation of CALMET/ CALPUFF when used with good quality prognostic data is expected to give a good estimate of a refined run.

## 2.4 Prognostic-Derived Surface (SURF.DAT) and Upper (UP.DAT) files

In light of the other approaches mentioned above and especially the ease and flexibility of using 3-D gridded prognostic data that is readily available either from MM5, WRF, TAPM or other simulations, it is not recommended to use the prognostic models to generate single station surface and upper air meteorological files. In particular in Australasia, TAPM-derived surface and upper air station files are often used to drive CALMET. These ‘pseudo-profiles’ of surface and upper air data are used twice in CALMET (once to setup the initial guess phase and a second time in the Step 2 wind field) and carry the weight of real observations in CALMET. In most instances the TAPM or other prognostic data is best used as a 3-D input field in CALMET as the initial guess field rather than as pseudo-stations. The use of the full 3-D field allows all of the spatial variability in the prognostic model to be carried forward and used by CALMET and using the 3-D data as the initial guess field allows for smaller-scale terrain adjustments to be made by the CALMET diagnostic algorithms. Use of pseudo-stations involves the subjective choice of which “stations” to be selected from the prognostic gridded fields and only partially reproduces the spatially varying winds of the original prognostic fields.

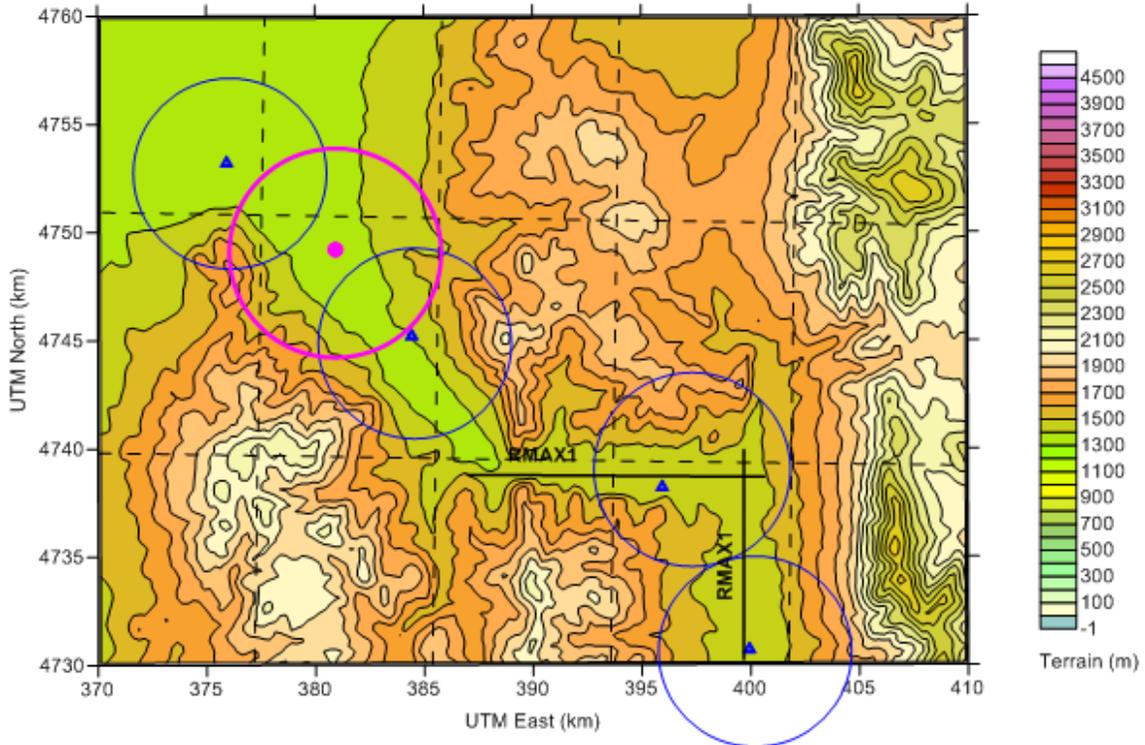
## 2.5 Seven Critical CALMET Parameters When Using Observations

When using CALMET with observational data, seven critical parameters must be carefully assessed and which are unique to every application. These values are; TERRAD, RMAX1, RMAX2, R1, R2, IEXTRP and BIAS. Table A-1 addresses each of these parameters individually.

In developing the Step 1 wind field, CALMET adjusts the initial guess field to reflect the effects of the terrain, including slope flows and blocking effects. At this early stage the model accounts for the surface and upper air data in the initial guess phase and the user has the choice to use BIAS parameters to weight the effects of the wind field from an upper air station that may be located far away and not representative of the facility and site at all. Slope flows are a function of the local slope and altitude of the nearest crest. The crest is defined as the highest peak within a radius TERRAD (km) around each grid point. The value of TERRAD is determined based on an analysis of the characteristic length scale of the surrounding terrain. The Step 1 field produces a flow field consistent with the fine-scale CALMET terrain resolution.

In Step 2, observations are incorporated into the Step 1 wind field to produce a final wind field. Each observation site influences the final wind field within a radius of influence (parameters RMAX1 (km) at the surface and RMAX2 (km) aloft). Observations and the Step 1 wind field are weighted by means of parameters R1 (km) at the surface and R2 (km) aloft. For example, at a distance R1 from an observation site, the Step 1 wind field and the surface observations are weighted equally.

Note that in no-observations (No-Obs) mode only one of the seven parameters is used (TERRAD), which simplifies the setup and operation of CALMET.



**Figure 2-1.** Figure showing examples of how to choose RMAX1, R1, RMAX2 and R2 values. One value of RMAX1, RMAX2, R1 and R2 apply to all surface and upper air stations. RMAX1 and RMAX2 is typically the maximum radius of influence of the surface and upper air station, respectively. The approximate length (km) of RMAX1 and RMAX2 is shown in the figure as black solid lines. The blue circles represent approximate values (km) of R1 values representative of all surface stations. In complex terrain the R1 value is usually smaller than the RMAX value. The pink circle represents the R2 value of the upper air station for level 2 and aloft.

## 2.6 Other Important Parameters – Overwater Surface Fluxes and Mixing Heights

The US Department of the Interior, Minerals Management Service (MMS) is responsible for the managing development of mineral resources including oil and gas on the Outer Continental Shelf (OCS) of the USA. In the early 1980s, the MMS sponsored the development of the Offshore and Coastal Dispersion (OCD) model (Hanna et al., 1985) to evaluate pollutants located over water. More recently MMS has sponsored a three-year study to enhance the capability of CALMET and CALPUFF for overwater transport and coastal interaction effects using the most current knowledge on meteorology and dispersion. An objective of the updated model is for use in both short-range and long-range applications.

As part of the model enhancement program, changes were made to both CALMET and CALPUFF based on the literature review. One of these changes was to include the COARE (Coupled Ocean Atmosphere Response Experiment) overwater flux model. It was found that the original mixing height algorithm in the CALMET model, which consisted of only mechanically-derived mixing over water surfaces, sometimes underestimated the mixing heights in the Gulf of Mexico, especially during light wind conditions over warm water. As a result, convective overwater boundary layer heights are now computed under conditions of positive surface heat flux over water. The mixing height over water is now taken as the maximum of the mechanical and convective mixing heights, as CALMET has always done over land surfaces. Thus in addition to the existing convective mixing height scheme, based on Maul (1980) and Carson (1973), an option for a new land and water parameterization (Batchvarova and Gryning, 1991, 1994) has been incorporated into CALMET. Another change included the explicit adjustment of observed buoy winds to 10m and the application of consistent similarity profile equations used throughout the system.

Model evaluation tests were conducted using five experiments: (1) Cameron, Louisiana – an experiment conducted along the coast of Gulf of Mexico, (2) a tracer study in Carpinteria area along California coast, (3) a tracer dispersion study at Pismo Beach, California, (4) a tracer study in the Ventura area along the CA coast and, (5) the tracer dispersion study over the strait of Oresund, between the coasts of Denmark and Sweden.

The results of the model evaluations indicate that the COARE overwater flux module improves the modeling results over the previous OCD-based model and it should be used as the default in the CALPUFF model. The standard COARE option (no shallow water adjustment or wave model option) appears suitable to these coastal datasets, and there is little performance sensitivity among the COARE options. The Batchvarova-Gryning convective mixing height option in CALMET shows improved performance over the Maul-Carson option. Turbulence advection is an important modeling option to use in coastal applications with the CALMET/CALPUFF system. Table A-3 gives the recommended switches for the Overwater Surface Fluxes.

Table 2-3. Tabulated List of Various Methods for Including Meteorological Data into CALMET. The list is detailed in order of decreasing preference.

Run Type	Description of Run Type	Ease of Use and Representativeness	Data availability	Advantages	Disadvantages
NOOBS	Prognostic model data 3D.DAT file to drive CALMET. No surface or upper air observations at all.	Simple to use Very representative	MM5 TRC ( <a href="http://www.src.com">www.src.com</a> ) 2006, 2007 and 2008 MM5 data as 3D.DAT files at 12km resolution for entire Eastern Australia.  TAPM – (CSIRO DAR – Melbourne) (requires full nested simulation by the user) and CALTAPM to transform data to 3D.DAT format.	<ul style="list-style-type: none"> <li>• Simple</li> <li>• full spatial and temporal variability</li> <li>• no overwater data required</li> <li>• cloud cover has spatial distribution</li> <li>• eliminates need for complicated 7 user-input site-specific variables</li> <li>• ideal as screening run as gives very good estimate of refined run</li> <li>• very inexpensive</li> </ul>	<ul style="list-style-type: none"> <li>• sometimes resolution of prognostic data is too coarse to be representative of local conditions</li> <li>• In case of TAPM a full nested 3D model simulation is required in order to generate the 3D.DAT file</li> </ul>
Partial NOOBS	Prognostic model data 3D.DAT to drive CALMET + one or more surface stations and optional overwater.	Less Simple to use due to: - data preparation, 7 site-specific choices to be made, difficulty in dealing with missing data, disagreement between 3D.DAT file and Surface observations.  Very representative and considered ‘refined modelling’	Same as above + any number of surface stations both on and off the model domain	<ul style="list-style-type: none"> <li>• full spatial and temporal variability</li> <li>• no overwater data required</li> <li>• Can either use real observed cloud cover from observation sites or use 3D.DAT spatially distributed cloud cover.</li> <li>• Refined model run as using combined approach of numerical model and observations.</li> <li>• Ability to incorporate surface representative</li> </ul>	<ul style="list-style-type: none"> <li>• Surface data, especially winds may be different to that in the 3D.DAT file.</li> <li>• User must include 7 site-specific variables</li> <li>• Data preparation and missing data</li> </ul>

<b>Run Type</b>	<b>Description of Run Type</b>	<b>Ease of Use and Representativeness</b>	<b>Data availability</b>	<b>Advantages</b>	<b>Disadvantages</b>
				Observation data when 3D data is too coarse to fully pick up local effects.	
Observations Only	CALMET driven solely by surface, upper air and optional overwater and precipitation stations	<p>Complicated due to: - data preparation, 7 site-specific variable choices to be made, difficulty in dealing with missing data.</p> <p>Considered representative if sufficient observation stations and site specific choice of parameters by the modeller.</p>	Any number of Surface stations + upper air stations (usually 12 hourly) + precipitation stations (optional) + overwater data (optional)	Very good if upper air and surface stations are located close to the facility and if upper air data are recorded at sunrise and sunset.	<ul style="list-style-type: none"> <li>• Surface data, especially winds may be different to that in the 3D.DAT file.</li> <li>• Upper air data typically 12 hourly, poor spatial and temporal resolution</li> <li>• Model has to interpolate between 12 hour soundings</li> <li>• Soundings at incorrect time of the day.</li> <li>• User has to deal with missing surface and upper air data</li> </ul>

## **3 RECOMMENDED MODEL OPTION SETTINGS FOR CERTAIN CONDITIONS AND SCENARIOS**

---

### **3.1 Introduction**

TRC have been requested to recommend model option settings for CALMET and CALPUFF for modelling in the following conditions and scenarios:

- Complex terrain;
- Buoyant line plumes;
- Shoreline fumigation;
- Inversion break-up fumigation; and
- Low wind speed/calm conditions

The OEH have requested that model option settings are to be supported by the results of model evaluation studies along with a discussion on the sensitivities to changes in model settings.

### **3.2 Complex terrain**

CALPUFF is a Lagrangian Gaussian Puff model and is well suited for modeling complex terrain when used in conjunction with CALMET which includes a diagnostic wind field model which contains treatment of slope flows, valley flows, terrain blocking effects and kinematic effects – the speed up over hills.

Meteorological observation stations are usually sparsely located and in moderate terrain are often limited in their spatial extent as they are often only representative of the immediate local area surrounding them. Numerical models which include sophisticated physics and produce 3D gridded meteorological fields are often preferable for ‘infilling’ in these situations, even if the data is coarse. The combined numerical-diagnostic model approach, where coarse spatial resolution gridded numerical model output is used as an initial guess field for fine spatial resolution diagnostic model such as CALMET is recommended for capturing terrain effects. Further, the diagnostic model applies dynamically consistent diagnostic algorithms in concert with available observed data to develop terrain effects.

Resolving the grid resolution adequately is a key decision in order to accurately represent terrain features. Users should examine the data to ensure that the grid spacing used in creating the data is adequate for their application and the winds appropriately characterize the mesoscale flows within the modeling domain.

#### **3.2.1 Terrain Data**

High resolution terrain data < 90m can be purchased from providers of terrain data within New South Wales. The Atmospheric Studies Group of TRC Environmental Corporation

([www.src.com](http://www.src.com)) offers direct links to the USGS website for the global resolution terrain data set at ~900m resolution and the Shuttle Radar Topography Data (SRTM), 90m resolution for the entire world. The SRTM data is recommended for all applications conducted in NSW, Australia. Both the 900m global USGS data and the SRTM data are free of charge.

### **3.2.2 Choosing Grid Resolution and Model Domain Size**

It is important to find the optimum balance between the desire to make the grid size as large as feasible in order to reduce the run times and file sizes, and the desire to make the grid size small enough to optimize the terrain effects on the wind field. The best grid spacing for any application will depend on the size of the model domain and the complexity of the terrain within it.

Graphical analysis is the most useful way to decide whether terrain is properly resolved or not, a poorly resolved model domain will show significant loss of peak terrain heights, or an isolated hill may be smoothed out, plus, unique terrain features and characteristics will not be preserved, and, valleys will be in-filled such that they do not appear as valleys.

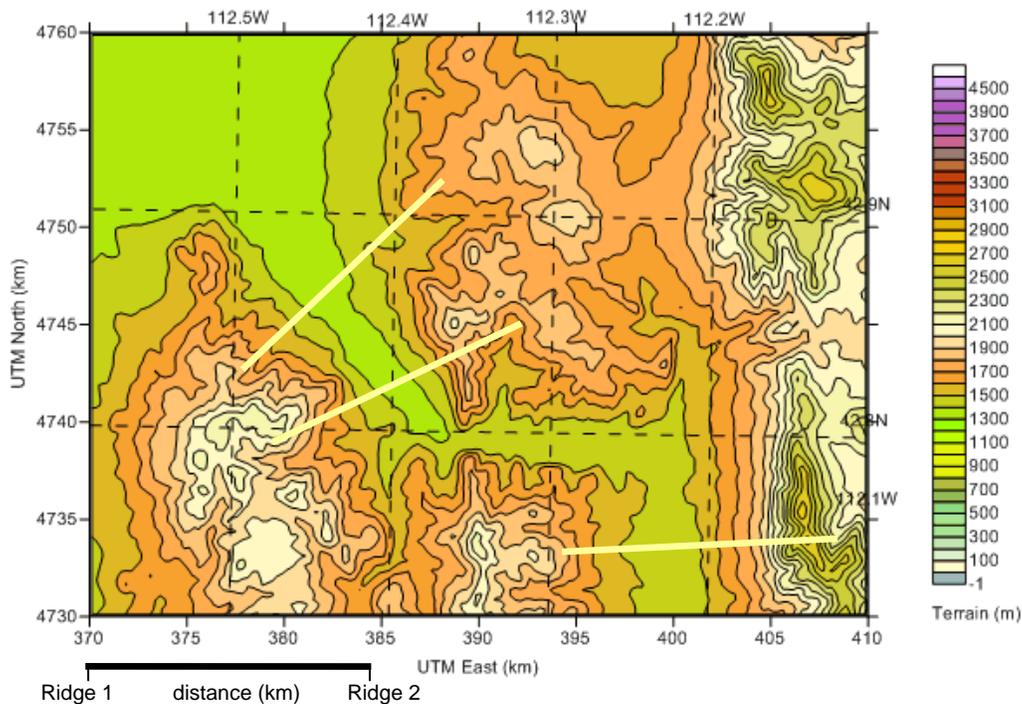
One method for evaluating whether the grid spacing is adequate for a particular application is to select a light wind case where terrain induced flows will dominate and compare the resulting wind field using the selected grid spacing with a simulation using twice the resolution (half the grid spacing). If the wind field patterns are similar, then it is likely that the selected grid spacing is adequate. Typical applications of CALMET on a PC will include between 100 to 300 grid cells in both the x- and y- directions. Therefore, for a domain that is about 200 kilometers on each side, a grid spacing of about 1 to 2 kilometers should be adequate. Smaller domains for near-field applications may require a grid spacing of about 250 meters. Use of 20 to 30 grid cells in each direction is generally not adequate, regardless of the size of the domain.

Most CALMET/CALPUFF applications are run with a relatively small grid resolution of around 250m, this should allow for at least 10 or more grid points to resolve each terrain feature. If the dominant terrain features are not resolved it is recommended to go to an even smaller grid resolution of say 150m.

### **3.2.3 Choosing a value for TERRAD**

The value of TERRAD is given in km as a radius of influence of terrain features and is a function of the dominant scale of the terrain. The value of TERRAD must be greater than 0 and can only be used if diagnostic winds are computed as it is used in computing the kinematic effects (IKINE), the slope flow effects (ISLOPE), and the blocking effects (IFRADJ) on the wind field. If TERRAD is too small, then the nearby valley wall will not be seen by the model, if it is too large, then the hill several valleys away is seen, instead of the one nearby. A simple rule of thumb is 'ridge-to-ridge divide by 2, rounded up'. Typical values of TERRAD are 5-15 km and rarely larger than 20 km (except for very large grid spacing simulations).

UTM Zone: 12  
 Hemisphere: N  
 Datum: WGS-84



**Figure 3-1.** Example showing how to estimate TERRAD. Usually, (ridge (km) to ridge (km)) / 2, plus add 1 or 2 km. A typical value for TERRAD in this example would be 10km.

### 3.2.4 Complex Terrain Sub-Grid Scale Terrain Features (CTSG)

The complex terrain sub-grid scale (CTSG) module is based on that used in CTDMPPLUS (Perry et al 1989). Plume impingement on sub-grid scale hills is evaluated using a dividing streamline to determine how much pollutant material is deflected around the sides of the hill, below  $H_d$  and how much is deflected over the hill, above the dividing streamline height ( $H_d$ ) individual puffs are split into three sections for these calculations.

The sub-grid scale terrain feature of CALMET is offered for those applications where individual 'regular shaped' terrain features such as mine dumps which are not easily resolved by the chosen grid resolution becomes an obstacle to the general flow in that grid cell. Usually the CTSG option is not commonly employed due to the significant amount of work that is required to explicitly detail the hill. Frequently the easiest solution is to resolve the grid resolution in order to include the terrain feature.

For long range transport applications > 50km, the CTSG option is not usually considered as impacts on far-field receptors is of the most interest. In near-field applications involving complex flows, the grid spacing should usually be sufficiently small enough to resolve both the dominant and small terrain features adequately.

However, on both near and far field applications, if a terrain feature, such as a mine dump that is too small to be resolved by the chosen grid cell resolution is expected to directly influence the plume then the CTSG scheme may be invoked to explicitly detail the flow of plume material around that terrain obstacle.

### **3.3 Shoreline Fumigation**

Fumigation is classified into two types depending on whether it is a temporal or spatial phenomenon. The former process, termed “nocturnal inversion breakup fumigation,” occurs when pollutants from an elevated stack are entrained into the growing convective boundary layer as it breaks up the nocturnal inversion in the morning. The spatial phenomenon, termed “shoreline fumigation,” occurs when a thermal internal boundary layer growing with downstream distance entrains pollutants from an elevated stack near a shoreline. Both phenomena are discussed.

#### **3.3.1 Sub-grid Scale TIBL**

The majority of cities in New South Wales are located within a few kilometers of the coastline such that many sources are affected by complex 3-D flow patterns typical of coastal regions. As well as sea and land breeze circulation systems, the significant differences between the boundary layers of marine and overland means distinct changes occur to a dispersing plume moving from land to sea and vice versa. The CALPUFF modeling system is well suited to handling these complex phenomena and will do so on a grid by grid cell basis without any invocation by the modeler as long as CALMET supplies the meteorology to CALPUFF.

Briefly, there are important differences in the structure of the marine and continental boundary layers which can have significant effects on plume dispersion in the overwater and coastal environments. The sensible heat flux over the open water is typically more than an order of magnitude less than that over land. The reasons for this are; water has a higher heat capacity and is partially transparent to solar radiation resulting in a small diurnal temperature difference; the sea is more uniform, and, there is a constant supply of moisture in the marine boundary layer. As a result of these differences the mixing heights overwater are much lower. At the land sea interface, rapid changes in the dispersion characteristics occur which can significantly affect the ground-level concentrations from coastal sources. For stacks emitting into the stable zone above the shallow marine boundary layer, narrow plumes are intercepted by a growing Thermal Internal

Boundary Layer (TIBL) over the land, the deeper vertical mixing over the land caused by rapid heating of the ground causes the elevated plume to be brought to the ground quickly.

The land-sea interface in CALPUFF is resolved on the scale of the computational grid. The model computes turbulence and dispersion characteristics that are consistent with the land use properties of each cell in the grid, whether the cell is classified as land or water, from the gridded meteorological fields provided by CALMET. Once a puff within a marine layer enters the mixed layer over land, the puff growth is changed to that appropriate for the overland boundary layer.

CALPUFF will compute TIBL effects as resolved by the CALMET grid automatically. However, CALPUFF also contains a sub-grid-scale TIBL option (MSGTIBL), a module that allows parameterization of the thermal internal boundary layer at scales smaller than the grid spacing. The MSGTIBL should be used where the issue of coastal fumigation is thought to be important such as cases involving tall stacks located close to the shoreline and the CALMET grid resolution is not fine enough to resolve the land-water border sufficiently in the vicinity of the source. For example, the sub-grid-scale TIBL option might be used with grid resolution of 1-2 km or greater, but it is unlikely to be necessary for very fine resolution such as 100-200m.

CALPUFF will compute interactions with a sub-grid-scale resolved Thermal Internal Boundary Layer (TIBL) when the MSGTIBL option is selected. The TIBL calculations are computed when certain criteria are met:

- Sensible heat flux over land exceeds  $5 \text{ W/m}^2$
- TIBL height is less than overland mixing height
- Winds must be onshore
- Puff is influenced by TIBL in current time step or previous time step

The user must input the X, Y coordinates of one or more coastlines in an optional file called COASTLN.DAT. The purpose of this file is to better resolve the relationship between the coastline and source locations during periods conducive to onshore fumigation events. The more general effects of land/sea breeze circulations on transport of the plume should be addressed through use of mesoscale prognostic meteorological data, such as MM5, WRF or other numerical models, in the CALMET processing.

### **3.4 Inversion Break-up Fumigation**

Inversion breakup fumigation is the phenomenon in which pollutants lying above the growing convective boundary layer are entrained into the boundary layer by penetrating thermal plumes. This process can increase the ground-level concentrations of pollutants significantly during daytime (e.g., Deardorff and Willis 1982, Kim et al 2005).

Inversion break up fumigation is really an issue for tall point sources which are typically located in moderate terrain where calm conditions frequent in the valleys in which the sources occupy.

Usually the top of the inversion is approximately at the height of the top of the valley, so any plumes emitted into the stable layer aloft will not mix down to the ground until the inversion breaks down, either through mechanical mixing or convective mixing.

The CALPUFF modeling system will compute inversion breakup fumigation without any user intervention as long as it is supplied certain key information which includes the following;

- Sufficiently fine enough model resolution (150-250m) so that the nearby terrain is adequately resolved
- CALMET must be used in order to get a varying spatial distribution of mixing height across the model domain
- Sufficiently good meteorological data, preferably from a combined approach of gridded 3-Dimensional data from a prognostic model such as MM5 and observational data.

Realistic computation of inversion break up fumigation is a function of each of these interdependent criteria above which are all required in order for the model to have enough information with respect to the height of the terrain, terrain slopes, temperature profiles, local flows etc.

#### **3.4.1. Description of how CALMET computes mixing height and its relevance to properly modeling Inversion-breakup fumigation**

In CALMET the daytime mixing height is taken to be the maximum of the convective and mechanical mixing heights. An upwind looking mixing depth averaging scheme is employed by the model to avoid an x-y field of mixing heights having unreasonably large cell-to-cell variations, as each grid cell's mixing heights are computed independently. In an inversion break up situation or inland mixing depths during a sea breeze, the upwind looking mixing depth averaging scheme is able to handle the advective effects of these phenomena. Because CALMET is explicitly marched in time a simple scheme has been incorporated which approximates the back trajectory method. For any given grid cell (i,j), the most upwind grid cell would have a direct impact. An upwind-looking cone originating at (i,j) is then generated to allow smoothing between cells.

A fine resolution CALMET domain along with good Landuse data and the upwind looking averaging mixing depth means that the temporal and spatial aspect of inversion breakup can be captured.

### **3.5 Buoyant line plumes**

CALPUFF contains algorithms to specifically model buoyant line sources

- algorithms were designed to treat plume rise and dispersion from buoyant line sources such as roof top vents from smelters
- uses special line source plume rise equations
- dispersion component divides lines into many segments
- not meant to be used on roadways

An aerial view of a typical aluminum plant with long potrooms ideally suited to line sources



**Figure 3-2. Aerial photograph of a typical aluminum plant showing rows of potrooms.**

Calpuff's Line source algorithm is a specialized algorithm to simulate concentrations from buoyant line sources using techniques from the Buoyant Line and Point (BLP) source dispersion model (Schulman and Scire, 1980). The model is able to describe buoyant line source plume rise as well as account for the low-level release of both the point and line source plumes. The algorithm can handle multiple finite line source plume rise enhancement, wind direction dependence of line source plume rise and building downwash and vertical wind shear effects on both the point and line source plumes.

The difference between the old outdated BLP model and CALPUFF, is that CALPUFF will treat this complex source configuration within a modern state-of-the-science framework that includes interfaces to currently available meteorological datasets.

Aluminum reduction plants are a complex arrangement of emission sources, composed of parallel, low-level buoyant line sources called potrooms interspersed, typically, by short point sources or, scrubber stacks. Alumina is reduced through electrolysis to aluminum in the potrooms. A typical reduction facility usually consists of 2 to 20 potroom buildings about 500m

long. Some of the buoyant emissions from the reduction process escape through a continuous ridge ventilator, which is a few meters wide, running the length of the potroom. Most of the emissions, however, are collected by hooding above the reduction cells and are treated and exhausted through nearby stacks. There are typically 2 to 20 point sources, usually low-level, for each potroom primary control system.

Since a buoyant line source has one less degree of freedom than an isolated point source in entraining air, the plume rise will be enhanced. In addition, the line source rise will be dependent on wind direction, line length, the number of parallel lines, and their spacing. Both the line source and the short point sources are subject to building downwash effects.

### 3.5.1 Entering Line sources into CALPUFF

The coordinates of the beginning and ending locations of each line are used to determine the points of release, and the orientation of the lines. In addition, for a group of such buildings, the average source attributes are needed:

- L the average building (line) length (m)
- Hb the average building height (m),
- Wm the average line source width (m)
- Dx the average spacing between buildings (m) and
- F| the average line source buoyancy parameter ( $m^4/s^3$ )

Where

$$F| = \frac{g L W_M w (T_s - T_a)}{T_s}$$

And,

- g is the gravitational acceleration ( $m/s^2$ )
- w is the exit velocity (m/s)
- $T_s$  is the exit temperature (K), and
- $T_a$  is the ambient air temperature (K)

The buoyancy parameter is computed for each line and then averaged.

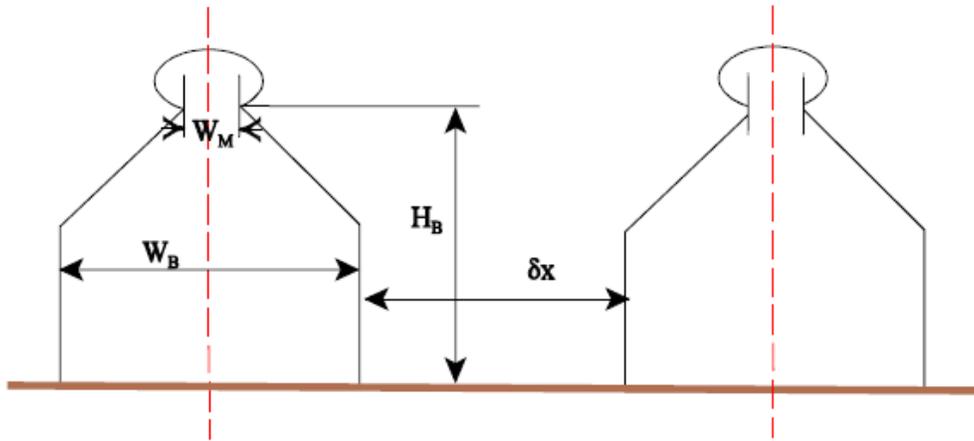


Figure 3-3. Shows a cross-section of two adjacent buildings with dimensions defined (Schulman and Scire, 1980). The GUI screen shot below from CALPRO shows the Line Source Input section.

Line Sources: e:\data\new-ep-1\task2\LINESO-1.INP

Number of Line Sources in Control File: 4 Edit Emission Data

Source Name	Beginning X (km)	Beginning Y (km)	Ending X (km)	Ending Y (km)	Release Height (m)	Base Elevation (m)
L01	231.418	3963.390	231.444	3962.933	19.0	271.1
L02	231.470	3963.393	231.496	3962.935	19.0	271.1
L03	231.519	3963.396	231.546	3962.939	19.0	271.1
L04	231.570	3963.398	231.596	3962.940	19.0	271.1

Add Row   Insert Row   Delete Row   Row Up   Row Down

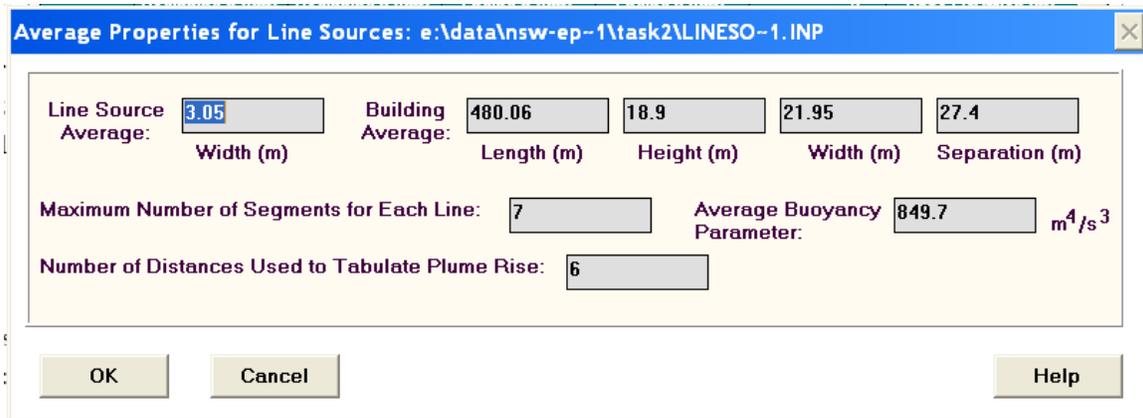
Number of Lines in External File:  Browse...   Default

File Name:

Edit Average Properties

Terminate Sequential   Previous   Next   Help

Figure 3-4. CALPRO GUI screenshot showing the CALPUFF user input control screen for entering line source data.



**Figure 3-5** GUI screenshot from CALPRO showing the CALPUFF user input control screen for the average properties for line sources.

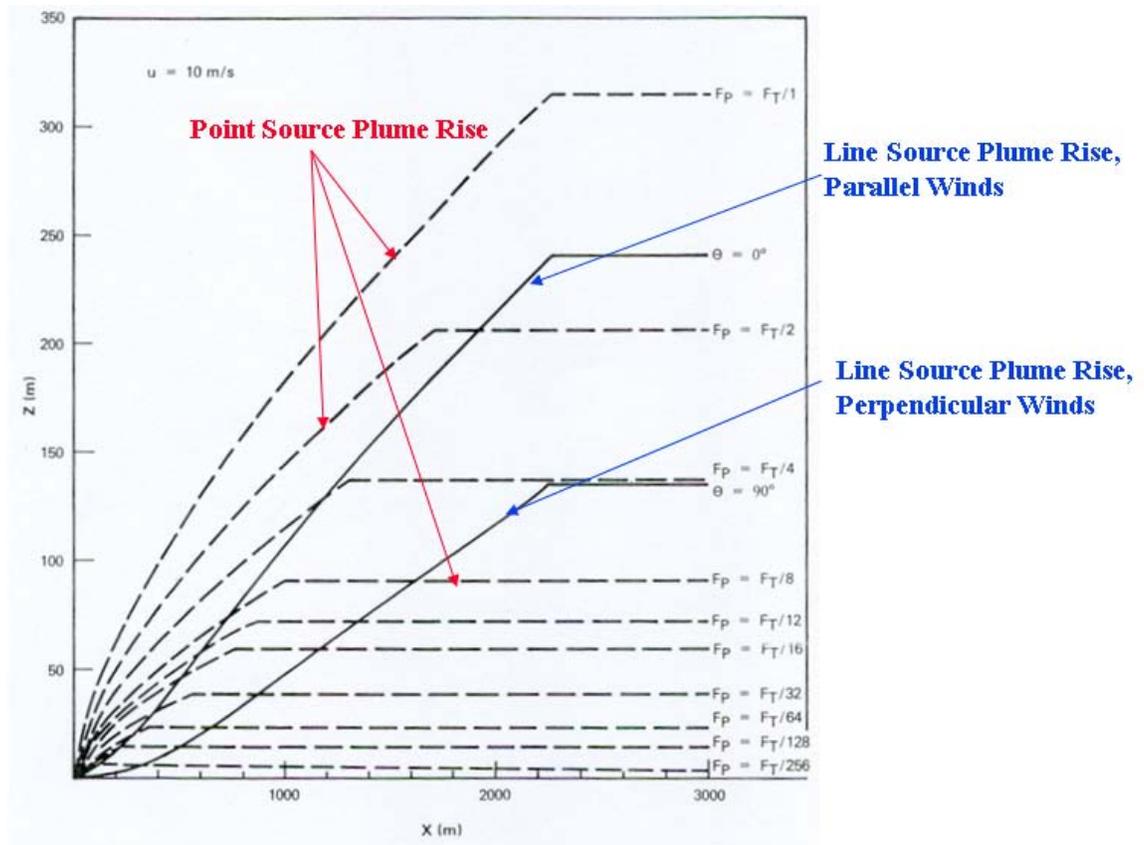
The average buoyancy parameter is used in the plume rise equations. For multiple line sources of comparable buoyancy flux, the buoyancy parameter is calculated for each line source and then averaged.

If using the slug model, the maximum number of segments for each line is the maximum number of line segments into which each line can be divided. The default is 7. If using the puff model this parameter is the actual number of virtual point sources used to represent each line.

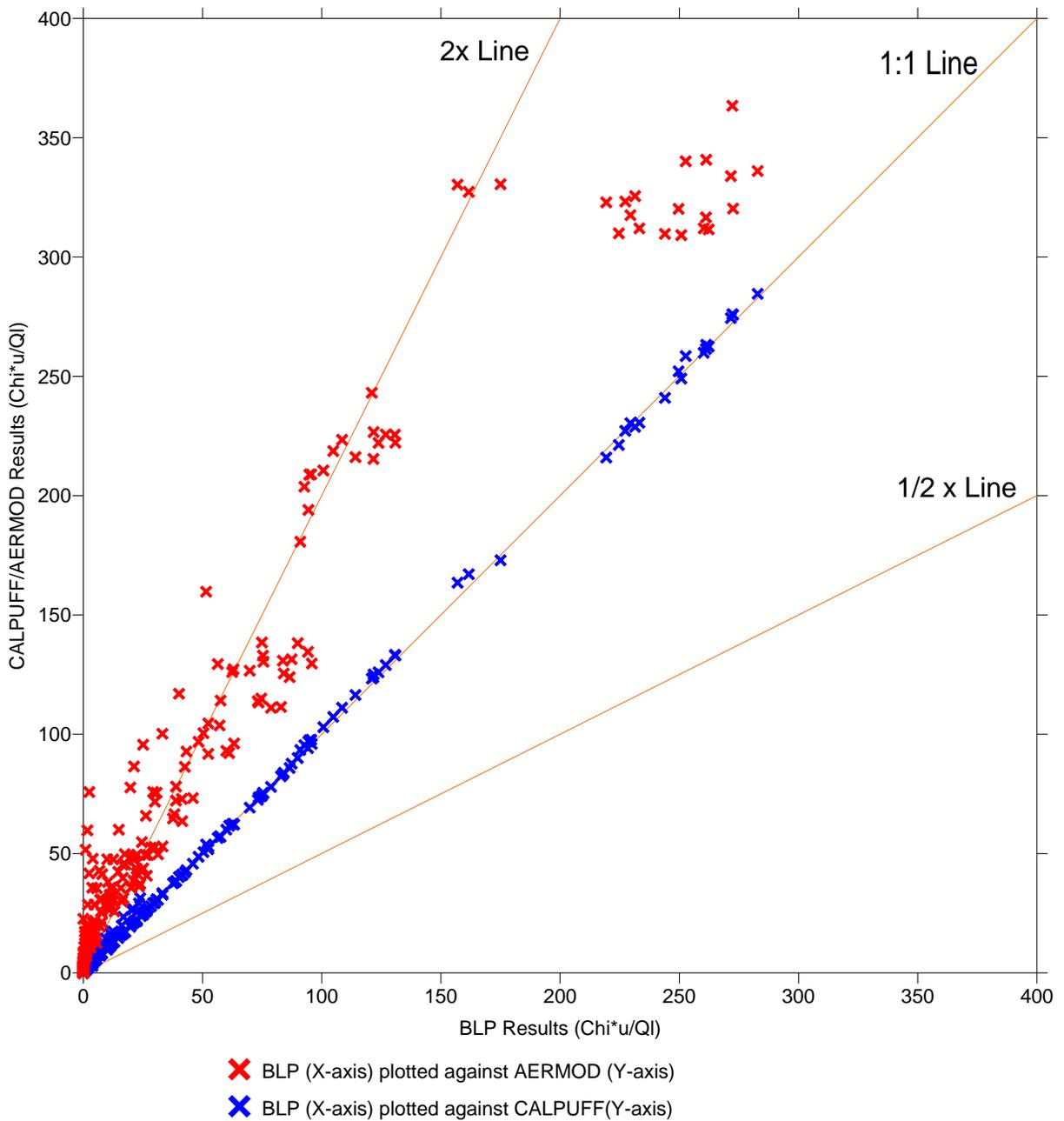
#### Buoyant Line Source Modeling Summary

- Line source plume rise has a different functional relationship with buoyancy and distance than point source plume rise
- Other effects include directionality and multiple source enhancement effects
- Cannot reproduce proper line source buoyant rise with point source plume rise model (potentially large under or over estimation of impacts)
- Treatment of buoyant line sources such as potrooms as non-buoyant volume sources significantly underestimates plume heights and overestimates concentrations.
- Non-buoyant lines can be represented by a series of volume or point sources, but buoyant lines cannot be properly represented in this way

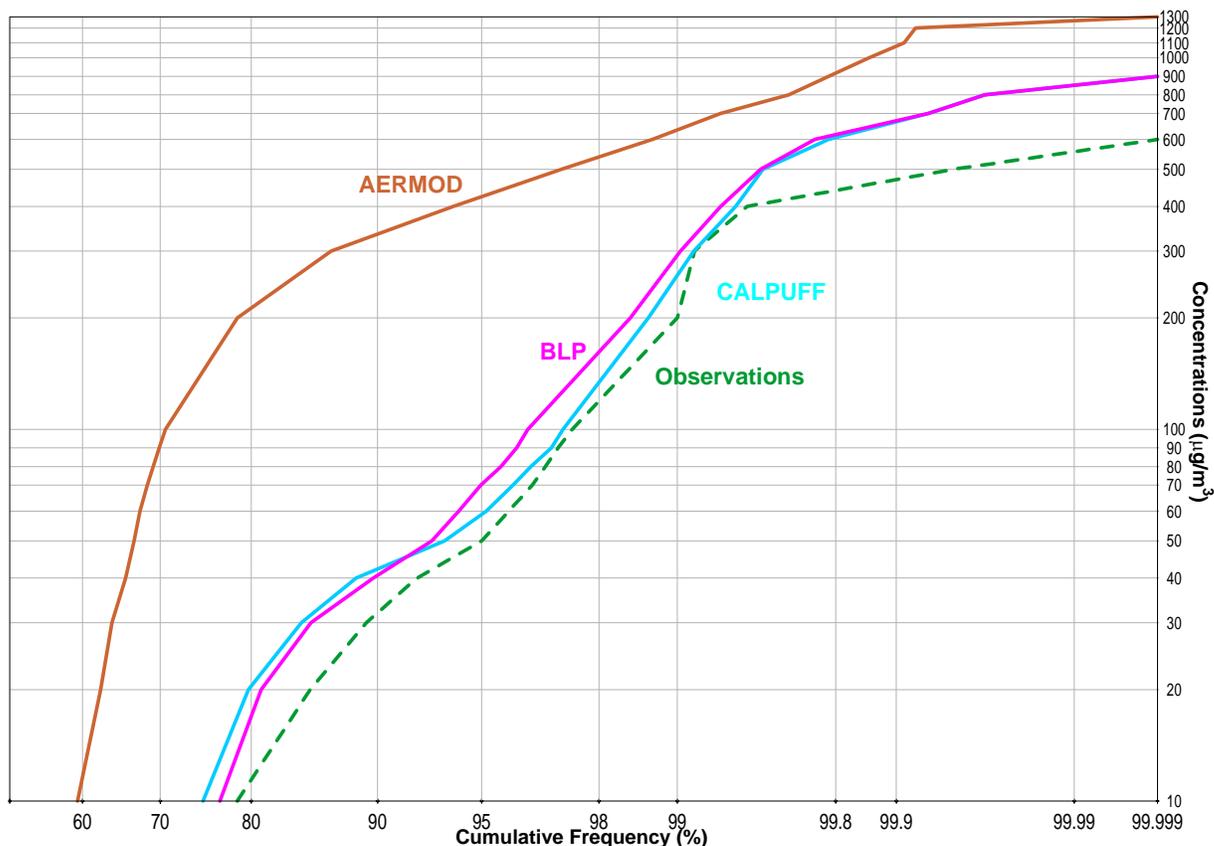
### 3.5.2 Evaluation Studies



**Figure 3-6** Figure shows the difference between point source plume rise and line source plume rise (Scire and Schulman, 1981). If you treat a line source as a set of too few point sources you can seriously under or overpredict the plume rise.



**Figure 3-7 Comparison of AERMOD and CALPUFF predictions of line source impacts from the Arkadelphia Arkansas SF<sub>6</sub> tracer study compared to BLP predictions. This study shows the impacts of the line sources alone.**



**Figure 3-8. Predictions of 1-hour average SO<sub>2</sub> concentrations at the downwind Alcoa Tennessee monitor for 1977 versus Observations and models, CALPUFF, BLP and AERMOD. The BLP results based on Version 1.1 of the model as well as the current version of BLP on the U.S. EPA web site (with modifications to the meteorological file to allow it to run) are shown. CALPUFF closely matches BLP results while AERMOD significantly overpredicts the observed concentration measurements.**

Table 3-1. Annual Average SO<sub>2</sub> Concentrations (µg/m<sup>3</sup>) at Alcoa, TN for 1976 and 1977. Observed and predicted concentrations using the BLP, CALPUFF and AERMOD models.

	1976	1977
Observed	8	13
CALPUFF	15.8	18.5
BLP	17.1	19.6
AERMOD	116.2	114.2

### 3.6 Calm winds

Calm and stagnant conditions are characterized by synoptic pressure gradients so weak that they have little or no effect on air flow near the ground. This flow and the turbulence accompanying it are driven mostly by surface heat flux inducing buoyancy, which interacts with terrain slopes. The resulting flows and diffusion patterns created by these flows are as varied as are topographies. Short term diffusion is also strongly affected by uneven surface heating or cooling induced by various sun azimuth and elevations, uneven surface cover, soil type and moisture, even by cloud shadowing.

Steady state Gaussian plume models such as AUSPLUME, ISCST3, and AERMOD are unable to treat true calm wind and stagnation events due to the inverse wind speed dependency as shown in the equation below.

$$C \sim \frac{Q}{u_* x \sigma_y} \quad \sigma_y = \frac{\sigma_v x}{u}$$

$$\sigma_v, u_* \sim u \text{ in AUSPLUME, AERMOD and ISCST3}$$

ISCST3 and AERMOD use the same routines for processing calm hours, namely hourly predicted concentrations for zero winds are not considered valid and treated as missing. As well as the above treatment, ISCST3 also had a NOCALM option which modeled the calm hours' by setting the wind speed to 1.0 m/s. AUSPLUME modifies the wind speed data so that an hour with a wind speed of less than 0.5 m in the meteorological file are assumed to have a wind speed of 0.5 m/s. Neither of these treatments is realistic, these steady state models either underpredict the effect of calms since the calm hours are effectively thrown out, or they allow a plume released in these conditions to travel a minimum of 1-2 km an hour. A calm hour in either an AUSPLUME or AERMOD meteorological file is identified by a reference wind speed of 0.0 m/s in the meteorological file and left as such so their input files may be used by other models.

CALPUFF on the other hand does not have any limitations to a minimum permissible wind speed and will allow a puff to grow and diffuse with time without advecting the puff anywhere. This is very important for stagnation events – extended periods of true calm events where puffs are allowed to accumulate with time. Comparison of CALPUFF (15-minute time step) to the STAGMAP data set, (Stagnation Model Analysis, Medford, Oregon 1991) showed very good agreement with SF6 Tracer releases under multiple hours of true calm conditions (Barclay 2008).

In CALPUFF, by default, a calm period is defined as that when the puff transport speed is less than the user-supplied threshold speed which has a current default value of 0.5 m/s. The default calm threshold speed is used to identify periods when the transport distances are minimal, but not zero.

In CALPUFF, several adjustments are automatically made to the normal algorithms to simulate calm periods. These adjustments affect the way the slugs are released, the way gradual plume rise is addressed, the way near-source effects are simulated and the way the puff size changes during each sampling step. Conceptually, under calm conditions it is expected that a fresh release will rise virtually straight up from the source and disperse as a function of time due to wind fluctuations about a mean of zero.

The following adjustments are made to puffs released into a calm period

- Slugs are released as puffs, the length of the slug is zero
- All mass for the period (typically one hour) is placed into one puff
- The distance to final rise is set to zero (therefore no gradual plume rise)
- Building downwash effects are not included
- The growth of  $\sigma_y$  and  $\sigma_z$  is based on time, rather than distance traveled during the sampling step, regardless of the dispersion option chosen by the user in the control file
- Minimum values of turbulence velocities for  $\sigma_v$  and  $\sigma_w$  are imposed.

When CALMET has been used,  $u_*$  and  $w_*$  may be available even when the puff transport speed is less than the threshold, so that turbulence can be estimated. However, it is recognized that this may not be a robust procedure if the wind data used by CALMET includes true calms, since under these conditions estimates of turbulence velocities  $\sigma_v$  and  $\sigma_w$  can be indeterminate. CALPUFF relies on these velocities to grow the puffs using time dependent dispersion formulas during periods that are calms which can occur under both stable and convective conditions.

There are two ways to improve CALPUFF's behaviour in calm conditions, the first is to use sub-hourly meteorological data and the second is to use sub hourly meteorological data combined with true measured turbulence parameters,  $\sigma_v$  and  $\sigma_w$ . This is discussed below;

### **3.6.1 Sub hourly meteorological data and its usage in CALPUFF**

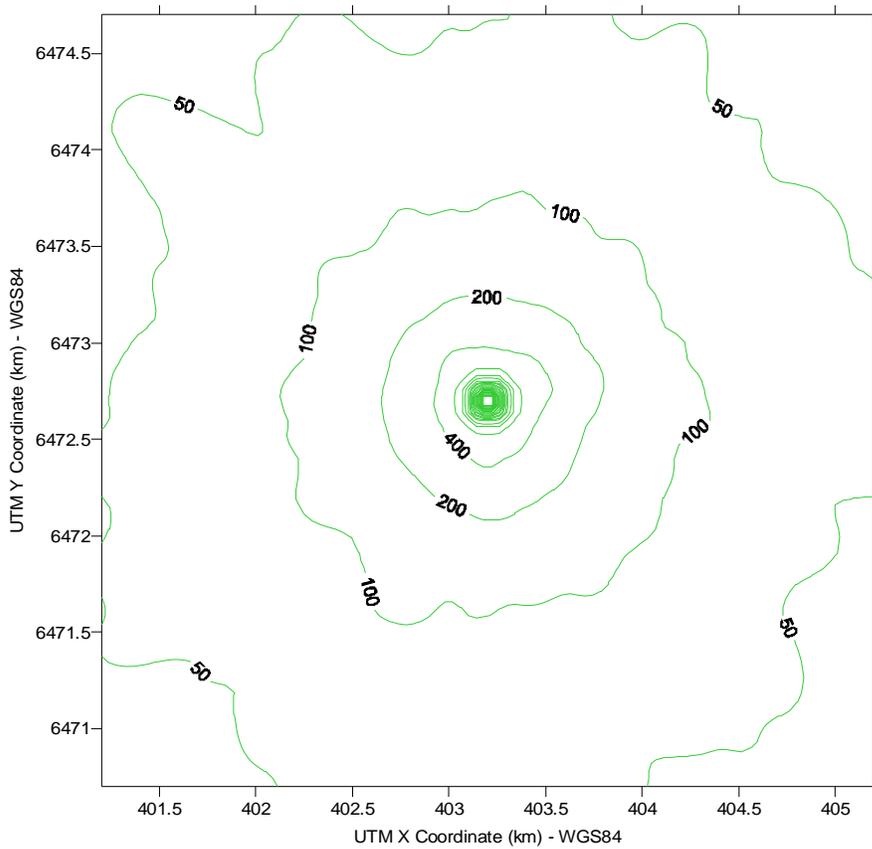
Steady state Gaussian regulatory models are traditionally limited to a one hour time step and one hour meteorological data even though sub-hourly meteorological data is typically recorded and stored at most Automatic weather stations around the world. Of the currently available regulatory models CALPUFF is the only regulatory model that is able to use sub hourly meteorological and emissions data. The consequences of this for realistically modelling calm conditions are significant.

True calm/stagnation events seldom last longer than several consecutive hours at a time before some instability, mechanical or convective destroys' the event. Traditional models with their

limitation of hourly meteorology mean that just several hours of light winds can be simulated at any one time, this is not sufficient temporal resolution to resolve the subtle fluctuations and variations that typically occur under these conditions as a result CALPUFF will produce a ‘bull’s-eye’ of predicted concentrations when using the model default options and hourly meteorology. It is worth noting that AUSPLUME and AERMOD will have transported the plume in the direction of the wind by ~ 1.8km as they will have assumed a minimum wind speed of 0.5m/s.

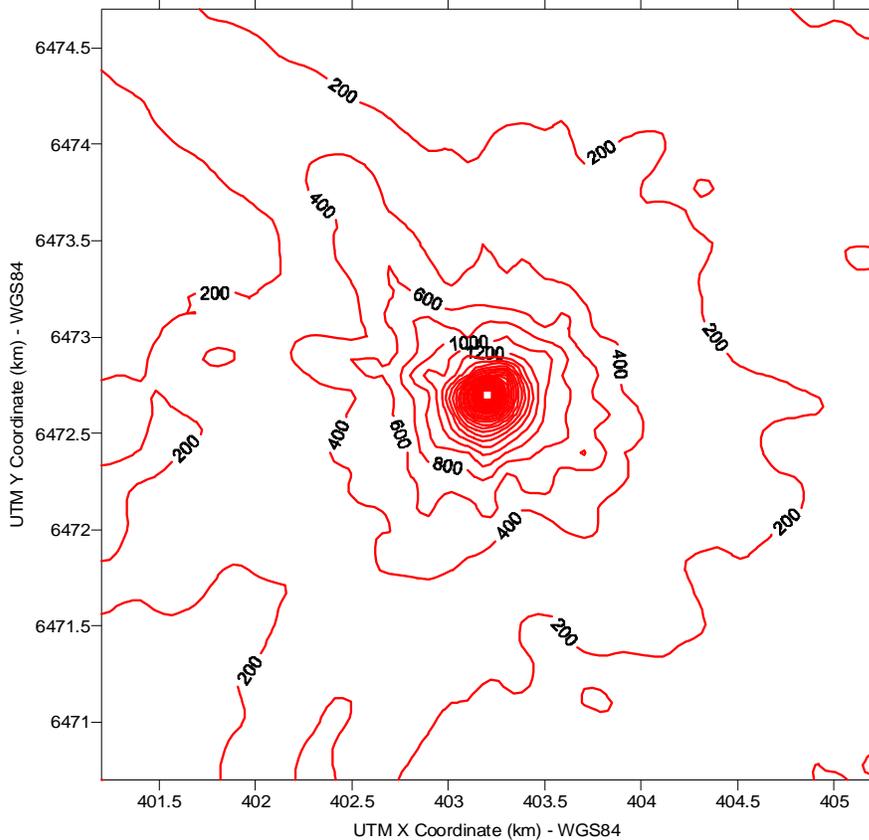
Analysis of Caversham 1 hour and 10-minute meteorological data from Western Australia is used to examine various user options when modeling calm conditions. The user has the choice to set (1) the minimum low wind speed threshold, which is currently defaulted at 0.5 m/s, (2) use either real or computed turbulence parameters, (3) use either hourly or sub hourly meteorology and (4) alter the minimum sigma v and w thresholds. In most instances users are limited to hourly meteorology and in most cases will have to rely on computed turbulence parameters. For most calm applications the user will be limited in what options to choose for calm conditions. Figures 3-9 to 3-11 shows the resulting concentration contour plots for a single volume source when various ‘calm’ options (1-4) are chosen.

Figure 3-9 shows a typical peak ground level concentration contour plot for a single volume source after a prolonged period of calm to very light winds. In this plot the model uses the default values for calm conditions which include a  $\sigma_v$  value of 0.5 m/s and a minimum low wind speed threshold of 0.5 m/s. Since the puffs are not being advected anywhere they diffuse and grow slowly and can create unrealistically high concentrations at the point of release. However, by substituting hourly meteorology for 10 minute meteorology, lowering the minimum overland  $\sigma_v$  value of 0.5 m/s to 0.2 m/s and using real time turbulence parameters a completely different more realistic concentration contour pattern can be achieved, see Figure 3-10, where the combination of higher frequency winds and real turbulence parameters account for variation and advection of puff material from the centre previously missed. The peak concentration between the two plots (Figures 3-9 and 3-10) are similar but the spatial distribution of concentration contours are completely different on each plot. Although there is no monitoring data on which to properly evaluate these concentration plots the use of sub-hourly data, along with a lowering of the minimum  $\sigma_v$  value over land to 0.2 m/s and the inclusion of measured turbulence provides a more realistic spatial footprint of ground level concentration in these instances.



**Figure 3-9 CALPUFF peak, 1-hr average concentration map using 1 hour meteorological data and default calm threshold of 0.5 m/s. Computed turbulence parameters were used assuming the default minimum  $\sigma_v$  of 0.5 m/s.**

In comparison 10-minute meteorology and using real time 10 minute  $\sigma_v$  turbulence data produced the following completely different ground level footprint, see Figure 3-10.



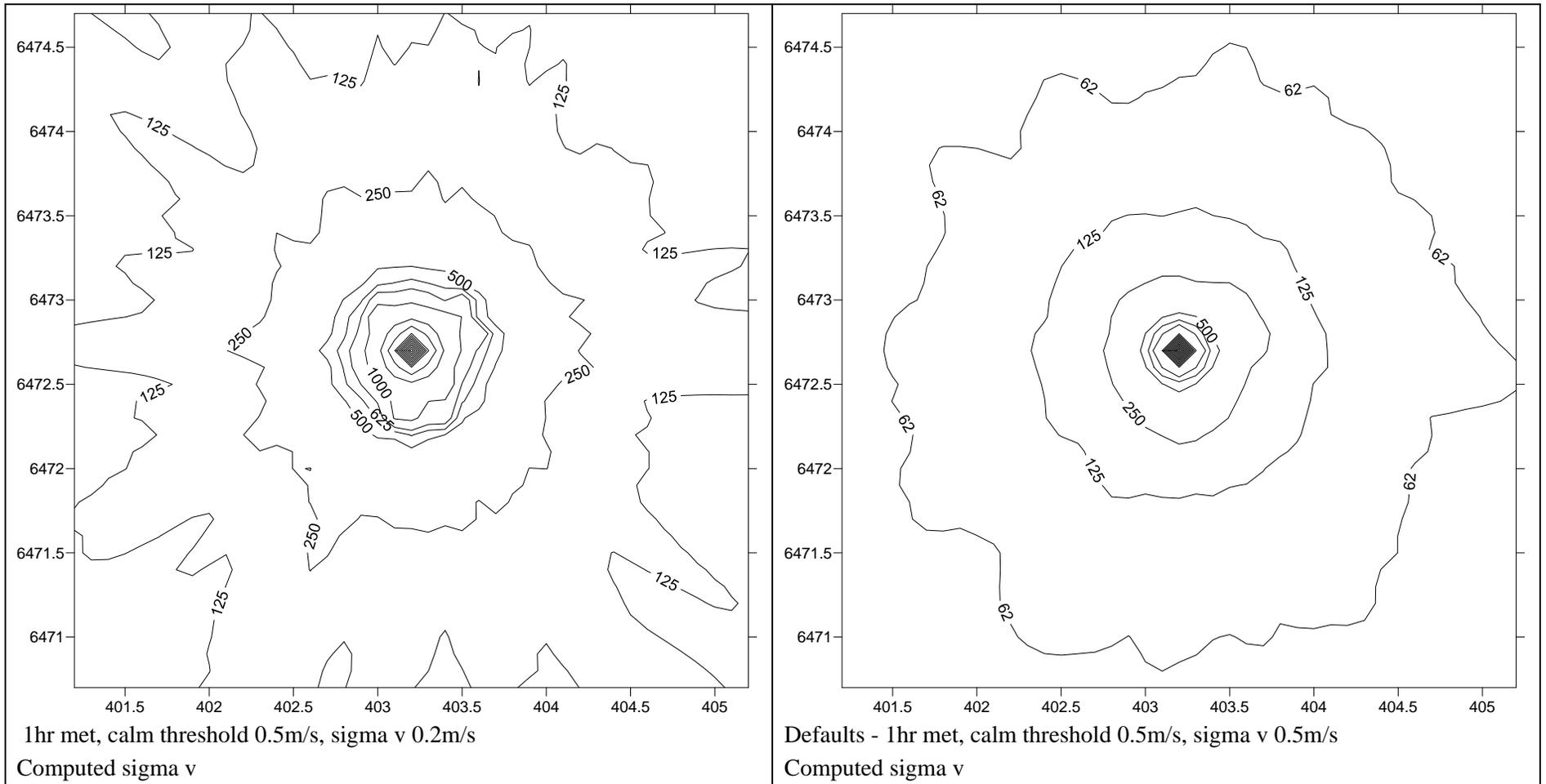
**Figure 3-10 CALPUFF peak, 1-hr average concentration map using 10-minute meteorological data and default calm threshold of 0.5 m/s. Real turbulence parameters were used with a minimum  $\sigma_v$  of 0.2 m/s,  $\sigma_w$  was left unchanged at the model's default values.**

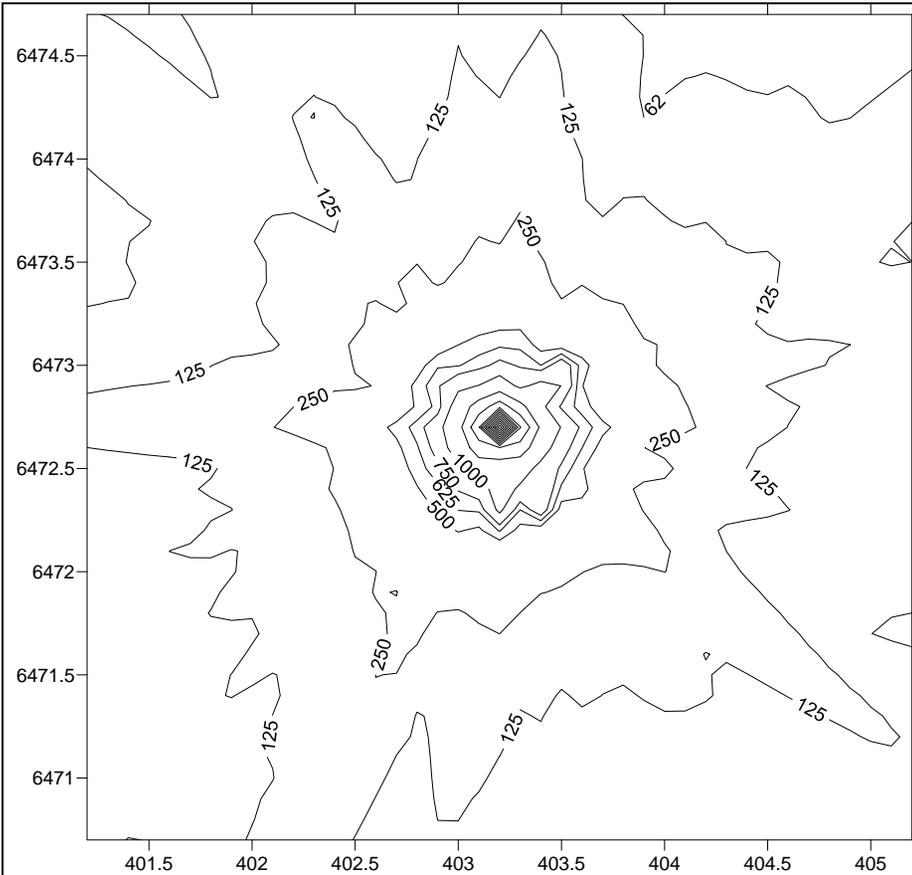
Various calm user options were evaluated for a single volume source and using either the 10-minute or 1-hour Caversham, WA meteorological data sets. The results are presented in Figure 3-11. Both Figures 3-9 and 3-10 are shown a second time in Figure 3-11 for brevity. There is little difference detected when lowering the minimum calm threshold  $< 0.5$  m/s which forces the model to step from distance to time based dispersion. In many instances 0.5 m/s is also the threshold of the instrument. There is also little difference when using 1-hour meteorology and real turbulence parameters when compared to the case using 1-hour meteorology and computed  $\sigma_v$  or, the case using 10-minute meteorology and computed  $\sigma_v$ .

These results show that the single biggest difference is not the inclusion of the real time turbulence data or the sub-hourly data but using a  $\sigma_v$  threshold of 0.2 m/s. Clearly the combined effect of  $\sigma_v$  of 0.2 m/s, real turbulence parameters and sub-hourly meteorological data is the preferred and most realistic option to treat calm and light wind periods, but in the event of not having sub-hourly meteorological data, or real turbulence data there is still strong evidence to use a  $\sigma_v$  value of 0.2 m/s overland (Barclay 2007).

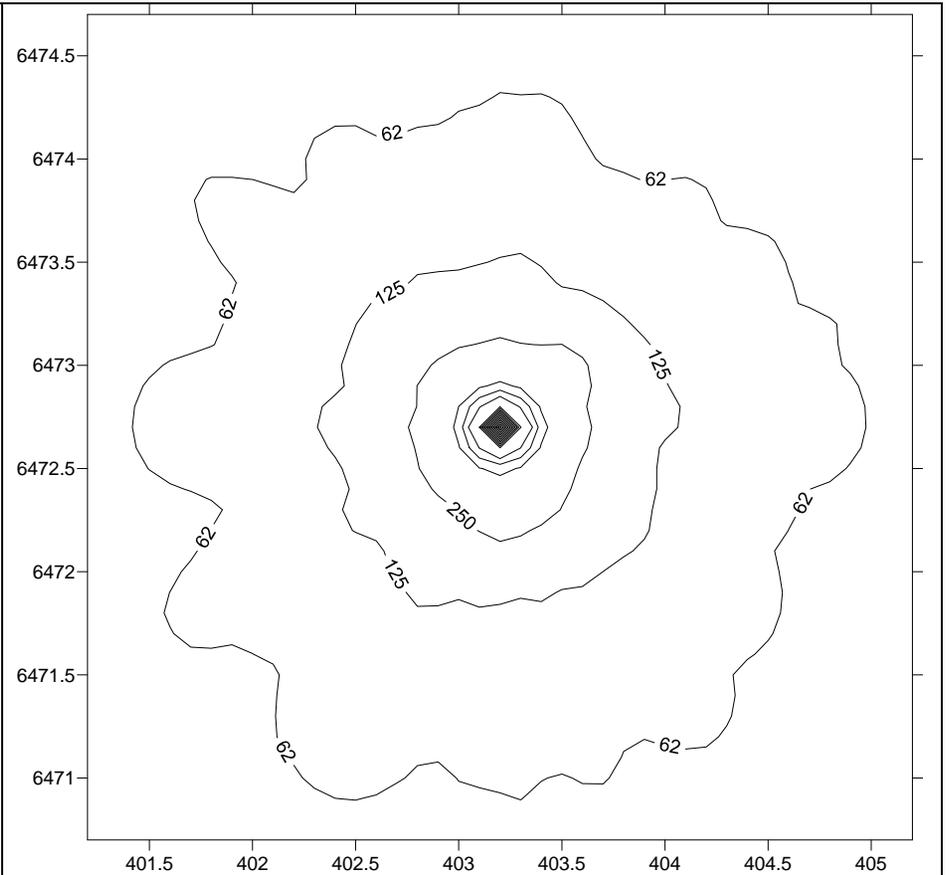
It is important to note that no evaluation of the concentration results with monitoring data has occurred. However, the 10-minute meteorological data which includes measured turbulence values have been evaluated and the concentration plots are a direct reflection of the meteorology.

Figure 3-11 Concentration contour plots for a single volume source using 1 hour and 10-minute meteorological data from Caversham,WA. The following plots show the different results when various calm options are chosen using either 1 hour or 10-minute meteorological data. The range of concentrations on each plot as well as the peak concentrations measured are similar for all plots.

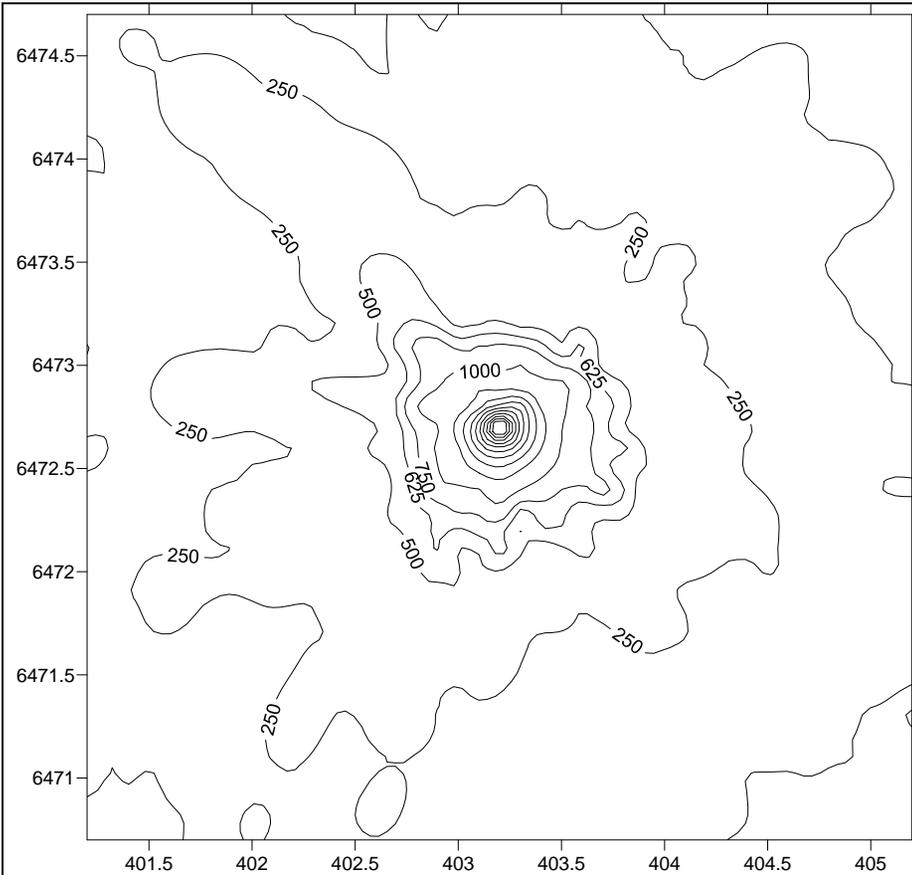




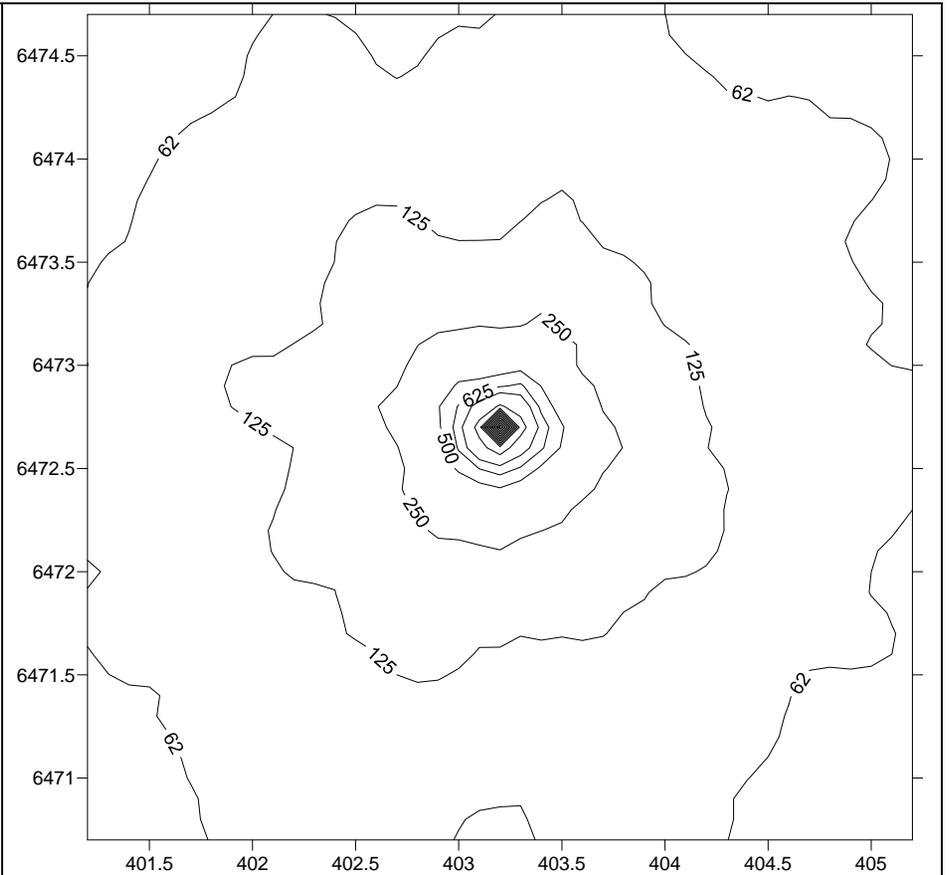
1hr met, calm threshold 0.5m/s, sigma v 0.2m/s  
Real turbulence parameters



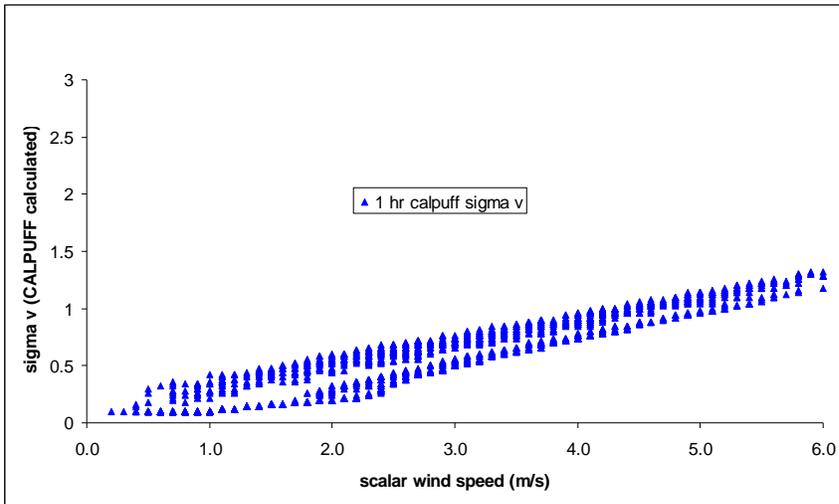
Defaults - 1hr met, calm threshold 0.5m/s, sigma v 0.5m/  
Real turbulence parameters



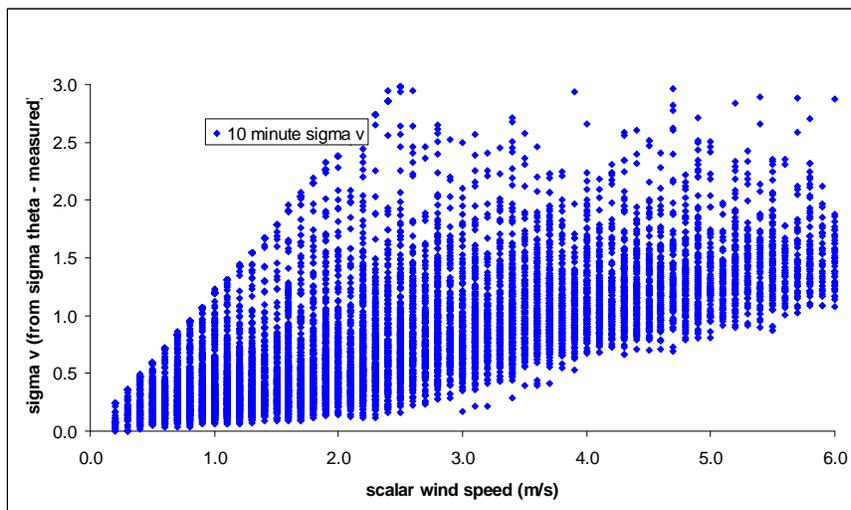
10min met, calm threshold 0.5m/s, sigma v 0.2m/  
Real turbulence parameters



10min met, calm threshold 0.5m/s, sigma v 0.5m/  
Real turbulence parameters



**Figure 3-12** CALPUFF computed  $\sigma_v$  using model defaults and one hour meteorology. (It is always preferable to use real measured values of real time turbulence wherever possible).



**Figure 3-13.** Real 10-minute measured  $\sigma_v$ . (CALPUFF can read this real time data directly).

### 3.6.2 User Options for treating Calms

- Sub-hourly meteorological and emissions data
- Model has a default minimum calm wind speed threshold, of 0.5 m/s, below which model switches from distance dependent to time dependent sigmas.

- User can define minimum sigma v and sigma w values. (It is recommended to lower the minimum  $\sigma_v$  from 0.5 to 0.2).

----- LAND -----      ----- WATER -----

Stab Class : A B C D E F      A B C D E F

Default SVMIN : .50, .50, .50, .50, .50, .50,      .37, .37, .37, .37, .37, .37

Default SWMIN : .20, .12, .08, .06, .03, .016,      .20, .12, .08, .06, .03, .016

- Model can read real turbulence parameters and can use this in replacement of computed turbulence parameters, or PG curves.

## **4. DISCUSSION ON THE APPROPRIATE PROCEDURES FOR EVALUATING CALMET AND CALPUFF MODELLING RESULTS**

---

### **4.1 Model Output: Uncertainty**

Accuracy of model predictions is often a source of debate. Measurements and model predictions can be compared in a variety of ways, each providing a different perspective on model performance. A model may show good competency in certain predictions (e.g., maximum concentrations) but poor in others (e.g. the frequency of concentrations above a certain threshold). Usually the reasons for poor model performance is due to uncertainties in the input values for example, poor quality or unrepresentative meteorological, geophysical and source emission data, or, lack of modeling expertise, or, incorrect and unsuitable model depending on the application.

The sources of uncertainty in model predictions can be significantly reduced by collecting the proper input data, preparing the input files correctly, checking and re-checking for errors, correcting for 'odd' model behaviour, insuring that errors in the measured data are minimized and applying the correct model to suit each application. As well as user 'error' inputs there is some 'inherent uncertainty' in model predictions which occurs in all dispersion models' due to the uncertainty of atmospheric behaviour.

Consider the following general statements on model performance which have been derived from the EPA 2003 and are to be considered in their totality, i.e., altogether.

- Models are more reliable for estimating longer time averaged concentrations than for estimating short-term concentrations at specific locations
- Estimates of concentrations that occur at a specific time and site are poorly correlated with actual observed concentrations (paired in space and time) and are less reliable (mostly due to reducible uncertainty such as error in plume location due to a wind direction error).
- Models are reasonably reliable in estimating the highest concentrations occurring sometime, somewhere in an area. Model certainty is expected to be in the range of a factor of 2.

Further it is important to note that model performance will vary depending on the application. For example, in some cases models will overpredict and in other cases underpredict. Further, under some conditions CALPUFF will produce higher concentrations than AUSPLUME and in other applications it may do the opposite. It is important to note that there are many differences that can occur between AUSPLUME and CALPUFF especially under complex meteorological and terrain conditions. But, generally under near field flat terrain and over a full year, the results of AUSPLUME are likely to be similar to that of CALPUFF.

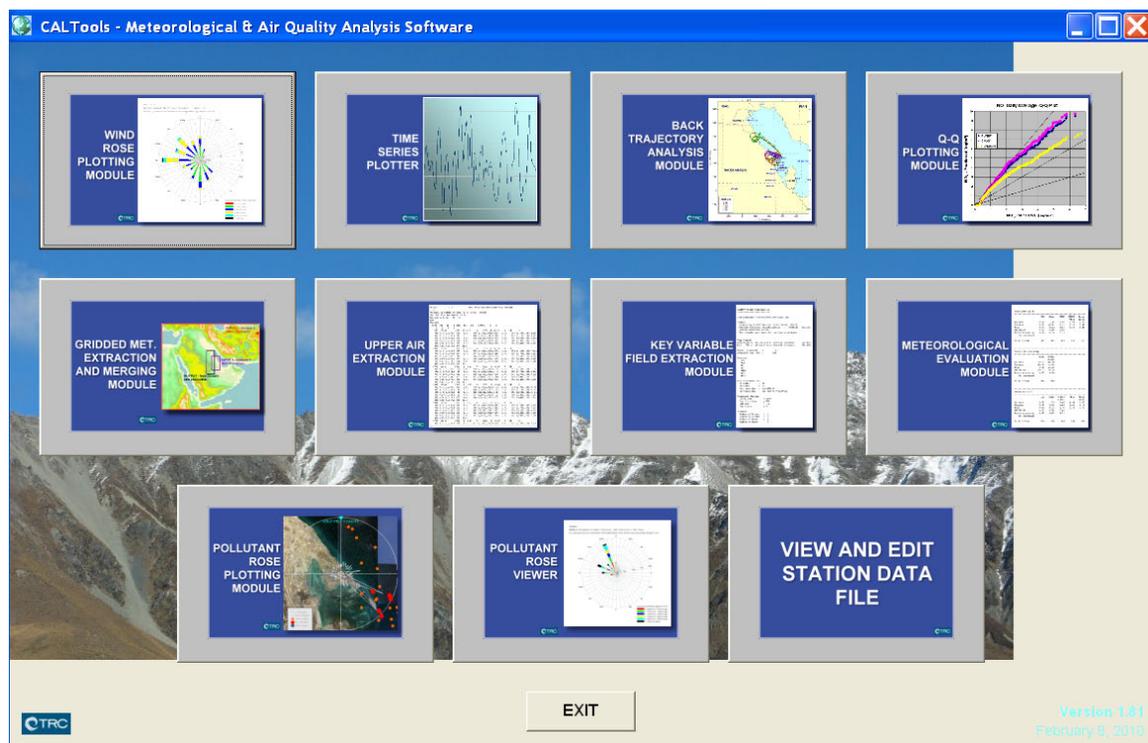
## 4.2 Procedures for Evaluating Model Output

### 4.2.1 Overview

In this section a range of procedures has been provided to assist the user in the evaluation of CALMET and CALPUFF modeling results. Of the two models evaluation of CALMET is significantly more difficult and complicated than the dispersion component of CALPUFF. The CALMET module requires careful consideration which includes, the input meteorological data, choosing the size of the model domain, grid resolution and several critical switches. CALPUFF on the other hand is more straightforward with significantly fewer choices for the user to make.

### 4.3 How to Evaluate CALMET

Evaluation of the model data inputs and outputs includes statistical procedures and graphical display methods. The preparation of input files involves the manipulation of many pieces of different information. For all levels of assessment, careful evaluation and quality control procedures are required to confirm the accuracy of the input source, receptor and meteorological data and the proper behaviour of models. The CALPRO model suite comes with a range of graphical and statistical procedures that are recommended to be used for evaluating the model information. Below is a screenshot of TRC's Meteorological and Air Quality Analysis Software.



### 4.3.1 Graphical Evaluation

Graphical display methods are easily accessed through TRC's CALPRO Graphical User Interface which has its own graphical display capability called CALVIEW. CALVIEW displays plots of terrain, land use, concentrations, wind vectors, mixing heights, precipitation and other meteorological fields. CALVIEW also has options to display animations.

Evaluation by the user has to occur at every stage of the model process

#### Calview –

Step 1. Whilst setting up your CALMET model domain, use CALVIEW to display the model domain, terrain contours, Land use data, and, allow surface and upper air stations to be plotted onto the map. This step is important to make sure;

- (a) Your model domain is sufficiently large enough to encompass any terrain features that may be near or alongside the model boundary which may affect the local flow conditions over the domain.
- (b) the location of the surface and upper air stations are in the locations you expect them to be
- (c) Check the Landuse data and make sure no missing data, incorrect Land Use categories.

Step 2. Once CALMET and its postprocessor package PRTMET have been executed use CALVIEW to plot the hourly wind fields, mixing heights, stability fields etc. Make sure;

- (d) The wind fields look as you would expect them to be. Terrain effects should be noticeable in calm stable conditions during the nighttime.
- (e) Look at the upper level winds and consider whether they are realistic with respect to the underlying terrain, above the terrain height wind flow is expected to reflect dominant southwesterly and westerly winds.
- (f) Check the mixing height to make sure it is consistent with what you would expect especially where large water bodies over land are involved

#### Wind Roses –

The Wind Rose Module computes and then generates wind rose plots which indicate the direction from which wind speed events are coming. The percentage of a range of wind speed for each wind direction is displayed using a concentric scale of frequencies (i.e., each circular ring corresponds to a particular frequency, in percent). The wind rose plotter module processes various formats of meteorological data including a CALMET binary data file, surface and upper air data file as well as a 3D.DAT file.

Wind roses provide one of the most powerful graphical evaluation procedures of evaluating wind speed and direction at specific site locations of both model input data and model output data. Wind roses give an information laden view of how wind speed and direction are typically

distributed at a particular location and they provide an excellent way to graphically present wind speed data and wind direction data that has been collected over a long record of time.

Wind roses should be used to;

- Compare observation stations vs. winds at similar location from the 3D.DAT file, to evaluate how well the prognostic model is doing.
- Evaluate the winds at upper air levels from the 3D.DAT file.
- Consider the flow at locations where no observations are present.

### **Time Series Plotter –**

The time series plotter is a graphical method for depicting the time variability of meteorological variables over an event, a day, a week, a month, season or a year. A time series is a sequence of data points measured typically at successive times spaced at uniform time intervals. Time series data have a natural temporal ordering, this makes time series analysis distinct from other common data analysis problems in which there is no natural ordering of the observation. A time series model will generally reflect the fact that observations close together in time will be more closely related than observations further apart. In addition, time series make use of the natural one-way ordering of time so that values for a given period will be expressed as deriving from some past values rather than from future values.

TRC's time series package allows the user to export, analyze and plot time series data into Excel spreadsheets for easy viewing. The time series plotter module will extract meteorological time series files from any of the following; CALPUFF.CON, 3D.DAT, CALMET.DAT, UP.DAT, SURF.DAT. Access is also available to the following pollutants, SO<sub>2</sub>, CO, O<sub>3</sub>, H<sub>2</sub>S, NO, NO<sub>2</sub>, NO<sub>x</sub>, NO<sub>3</sub>, PM<sub>10</sub>, PM<sub>2.5</sub>

Use Time Series plotter to show;

- (a) Transgression of various meteorological parameters through time, by season, month, and time of day
- (b) Comparisons of long term mean vs. standard deviation vs. shorter period

### **Scatter Plots –**

An option of TRC's Time Series Package is Scatter Plots which is a tool for displaying two variables for a set of data. The data is typically displayed as a collection of points, each having the value of one variable determining the position on the horizontal axis and the value of the other variable determining the position on the vertical axis.

The aim of a scatter plot is to suggest various kinds of correlations between variables with a certain confidence interval. Correlations may be positive (rising), negative (falling), or null

(uncorrelated). A line of best fit, 'a trend line' can be drawn in order to study the correlation between variables being studied. One of the more powerful aspects of a scatter plot is that it can show nonlinear relationships between variables. The scatter diagram is one of the basic tools of quality control.

### **Quantile Quantile Plots –**

In statistics a Q-Q plot is a probability plot which is a graphical method for comparing two probability distributions by plotting their quantiles against each other. If the two distributions being compared are similar, the points in the Q-Q plot will lie approximately on the line  $y = x$ .

A Q-Q plot is used to compare the shapes of distributions, providing a graphical view of how properties such as location, scale, and skewness are similar or different in the two distributions. Q-Q plots can be used to compare collections of data or theoretical distributions. The use of Q-Q plots to compare two samples of data can be viewed as a non-parametric approach to comparing their underlying distributions. Unlike scatter plots where the values are observed as pairs, the Q-Q plot compares distributions.

TRC's Q-Q Plotting Module allows the user to do either, quantile-quantile plot (either in a linear scale or in a logarithmic scale) or a probability scale plot in a Logarithmic scale.

When 'probability scale plot' is selected, the program opens Surfer and displays a distribution of concentration for the pollutant chosen. On the Y-axis are the concentration values on a base 10 logarithmic scale. On the x-axis, the cumulative frequency in percentage is plotted.

The Q-Q plotter module can either read a time series formatted file, \*.TSF or a CALPOST time series, \*.DAT format. If the user does not already have a \*.TSF formatted data ready for analysis thus can be created by extracting from CALPUFF.CON, 3D.DAT, CALMET.DAT, UP.DAT, SURF.DAT, AERMET.SRF.

Use the Q-Q Plotter especially for plotting probability plots of concentration.

### **Pollutant Rose Plotter**

TRC's Pollutant Rose Module computes and then generates pollutant rose plots which indicate the direction from which high pollution concentration events are coming. Three types of pollutant rose plots are available. In the first plot, the percentage of a range of concentration for each wind direction is displayed using a concentric scale of frequencies (i.e., each circular ring corresponds to a particular frequency in percent). In the second plot, instead of frequencies of a range of concentrations, maximum or average concentration for each wind direction is displayed using a concentric scale of pollutant concentration levels (i.e., each circular ring corresponds to a particular concentration such as  $50 \mu\text{g}/\text{m}^3$ ,  $100 \mu\text{g}/\text{m}^3$ ,  $150 \mu\text{g}/\text{m}^3$ , etc.). The third type of plot is a

scatter type plot containing a color coded symbol reflecting the concentration for a particular pollutant and the scale consists of concentric rings of distance, where the distance is the travel time during one hour for the wind speed measured for the same time period as the concentration, and the direction of the data point relative to north is plotted based on the simultaneous measured wind direction.

TRC's pollutant rose module supports the following meteorological data sets, 3D.DAT, SURF.DAT, CALMET.DAT and, it supports all pollutant species captured in the CALPUFF.DAT binary file.

The pollution wind rose plot gives very detailed information about the direction from which high pollution events are coming.

Use the Pollutant rose plotter along with a terrain map to show multiple pollution wind roses at specific locations which will show the overall spatial distribution and high pollution events.

### **4.3.2 Statistical Evaluation**

TRC's Meteorological Evaluation Module performs quantitative statistical comparisons of two meteorological datasets comprised of time series of meteorological parameters at a number of locations.

This package performs analysis of various types of modeled meteorological data such as CALMET, MM5 and WRF and observed data. It is especially useful for model-to-model comparisons, model to observation comparisons and observation to observation comparisons. An example of observation to observation comparisons is the 'evaluation of co-located instruments or different types of instrumentation (e.g. a tower and SODAR/RASS system).

Examples of the suite of statistical performance measures include scalar and vector mean wind speeds, standard deviations in measured and observed winds, RMSE errors (total plus systematic and unsystematic components), two model skill measures, the Index of Agreement, as well as the mean and standard deviations in modeled and observed wind speeds.

The Statistical measures include

- mean value (e.g. mean observation and mean prediction)
- bias error (average difference e.g. Predicted – Observation)
- Gross or Absolute error (average of the absolute value of the |P-O| values)
- Root-mean square error (RMSE), including its systematic (RMSEs) and unsystematic (RMSEu) components
- Index of Agreement (IOA)

The bias and gross errors for wind speed and wind direction are computed from the wind speed and wind direction values, not the U, V components of the winds.

### **4.3.3 Other Meteorological Evaluation Packages**

#### **4.3.3.1 Key Variable Field Extraction Module**

The Key Variable Field Extraction Module analyzes a CALMET or CALPUFF binary file or an Ascii MM5 2D and 3D.DAT file and extracts and presents key variable fields and their values for QA review.

The output of the ‘Key Variable Field Extraction Module’ is presented in two formats: an ASCII-format text file and a comma-delimited CSV-format file which may be viewed in Excel.

#### **4.3.3.2 Gridded Meteorological Extraction and Merging**

The Gridded Meteorological Extraction and Merging GUI module allow users to generate CALMET-ready 3D.DAT files from MM5, WRF or ETA data already in a 3D.DAT format by either extracting smaller domains from larger domains or merging together smaller domains to create larger domains.

For the latter option of merging together smaller domains, if there are gaps between the smaller domains being merged these can be treated by using coarser resolution data if such coverage exists.

#### **4.3.3.3 Back Trajectory**

The Back Trajectory Analysis Module creates plots of back trajectories corresponding to user-specified air quality events and locations. Each trajectory is initiated for a particular starting time and location, and the path of an air parcel that impacts that location at that time is mapped back in time to identify potential transport patterns and source regions associated with an air quality event

## REFERENCES

---

Federal Register. Part III. Environmental Protection Agency, 40 CFR Part 51. Revision to the Guideline on Air Quality Models: Adoption of a preferred Long Range Transport Model and Other Revisions; Final Rule. Vol 68, No. 72/Tuesday, April 15, 2003.

Federal Land Managers' Air Quality Related Values Workgroup (FLAG). Phase I report, December 2000. US Forest Service – Air Quality Program National Park Service – Air Resources Division U.S. Fish and Wildlife Service – Air Quality Branch.

Interagency Workgroup on Air Quality Modeling (IWAQM). Phase 2 Summary Report and Recommendations for Modeling Long Range Transport Impacts. United States Environmental Protection Agency, Office of Air Quality Planning and Standards, Research Triangle Park, NC 27711, EPA-454/R-98-019.

Douglas, S. and R. Kessler, 1988: User's Guide to the Diagnostic wind Model. California Air Resources Board, Sacramento, CA.

Hanna, S.R., L.L. Schulman, R.J. Paine and M. Baer, 1985: Development and Evaluation of the Offshore and Coastal Dispersion Model. JAPCA, 35, 1039-1047.

Maul, P.R., 1980: Atmospheric transport of sulfur compound pollutants. Central Electricity Generating Bureau MID/SSD/80/0026/R. Nottingham, England

Carson, D.J., 1973: The development of a dry, inversion-capped, convectively unstable boundary layer. Quart. J. Roy. Meteor. Soc., 99, 450-467

Batchvarova and Gryning, 1991: Applied Model for the Growth of the Daytime Mixed Layer. Boundary Layer Meteorology., 56, 261-274.

Batchvarova and Gryning, 1994: A Model for the Height of the Internal Boundary Layer over an Area with an Irregular Coastline. Boundary Layer Meteorology., 78, 1573-1472.

Perry, S.G., D.J. Burns, L.H. Adams, R.J. Paine, M.G. Dennis, M.T. Mills, D.G. Strimaitis, R.J. Yamartino, E.M. Insley, 1989: User's Guide to the Complex Terrain Dispersion Model Plus Algorithms for Unstable Situations (CTDMPLUS) Volume 1: Model Description and User Instructions. EPA/600/8-89/041, U.S. Environmental Protection Agency, Research Triangle Park, NC.

Deardorff, J.W. and G.E. Willis, 1982: Ground-level concentrations due to fumigation into an entraining mixed-layer. Atmospheric Environ., 16, 1159-1170

Schulman, L.L. and J.S. Scire, 1980: Buoyant Line and Point Source (BLP) dispersion model user's guide. Document P-7304-B, Environmental Research & Technology, Inc., Concord, MA.

Wu, Z, J.Scire, R O'Neal, 1998. Comparison of One Year of MM5 and Calmet Meteorological Fields with Observations in the Western United States. Preprints Eighth PSU/NCAR Mesoscale Model User's Workshop, 15-16 June, Boulder, CO, pp 131-137.

Scire, J.S. and F.R. Robe, 1997. Fine Scale Application of the CALMET Meteorological Model to a Complex Terrain Site. Air and Waste Management Association's 90<sup>th</sup> Annual Meeting and Exhibition, Toronto, Ontario, Canada.

Robe, F.R and J S Scire, 1998. Combining Mesoscale Prognostic and Diagnostic Wind Models: A Practical Approach for Air Quality Applications in Complex Terrain. Preprints 10<sup>th</sup> Joint Conference on the Applications of Air Pollution Meteorology, 11-16 January, Phoenix Arizona.

Barclay, J.J. Low wind speeds and Calms, Part II. *MODSIG Workshop*, November 2008, Sydney, Australia.

Barclay, J.J. Low wind speeds and Calms, Part I. *MODSIG Workshop, IUAPPA Conference*, September 2007, Brisbane, Australia.

## **APPENDIX A: MODEL OPTION SWITCHES FOR CALMET AND CALPUFF**

---

A full description of key model variables for both CALMET and CALPUFF are detailed in Tables A-2 and A-5. Table A-1 lists in detail the 7 Critical User-Defined Parameters that are required when running CALMET with observational data and Table A-3 includes the recommended model settings for overwater fluxes.

Although the tables below are intended to be as specific as possible, it is impossible to specify any single set of options/user-defined factors for every circumstance as some factors depend entirely on the meteorological and geophysical characteristics of the model domain.

**Table A-1. An Explanation of the 7 Critical User-Defined, Site Specific Parameters When Using Observational Data in CALMET**

Option	Parameter	Recommended Value	Explanation and Justification
Terrain radius of influence (km)	TERRAD	<p>No Default</p> <p>Requires user input. Value in km specific to each model domain</p> <p><u>Used in both No-Obs and Obs modes</u></p>	<p>TERRAD a terrain scale used in computing slope flow effects (ISLOPE) and terrain blocking effects (IFRADJ) on the wind field. Consider TERRAD as the distance (km) that CALMET 'looks' at in computing each of these effects. For instance the distance of the slope of the nearby terrain is needed to compute the slope flow. TERRAD should not be too small otherwise nearby valley walls which contribute to the slope flow will not be seen. On the other hand TERRAD must not be so large that hills more than one valley away is seen. TERRAD can be estimated as the typical ridge-to-ridge distance divided by two, and usually rounded up. Typical values of TERRAD are between 5-15 km with an upper limit of about 20 km, however this does depend on grid resolution (see discussion on terrain resolution)</p>
Vertical extrapolation of surface wind observations	IEXTRP <sup>*1</sup>	<p>Default is 'to extrapolate using similarity theory' and to exclude upper air observations from Layer 1</p> <p><u>Not used in No-Obs mode</u></p>	<p>This switch affects whether the model allows vertical extrapolation of surface data or not. This switch was developed since upper air observations are typically only taken every 12 hours. The vertical extrapolation of surface wind observations allows for the hourly surface data to impact layers above the surface layer.</p> <p>The default of this value is set to -4, which means similarity theory is used to extrapolate the surface winds into the layers aloft, which provides more information on the observed local effects to the upper layers.</p> <p>A value of IEXTRP &lt; 0 means that upper-air observations will not be considered in the Layer 1.</p>

Table A-1 An Explanation of the 7 Critical User-Defined, Site Specific Parameters When Using Observational Data in CALMET/ Cont.....			
Option	Parameter	Recommended Value	Explanation and Justification
Layer dependent weighting factor of surface vs. upper air wind observations in defining the Initial Guess Field (IGF) winds. Observations are always weighted by inverse distance squared ( $1/R^2$ ) from the station to the grid point. The BIAS parameter changes that weight.	BIAS (NZ)	<p>Default (NZ * 0) is to not change the <math>1/R^2</math> weighting given equally to surface and upper air data</p> <p><u>Not used in No-Obs mode</u></p> <p>Requires user input, depending on validity of surface and upper air stations</p>	<p>The BIAS parameter is most often used in complex terrain situations. The BIAS value ranges from -1 to +1, and a value is input by the user for each vertical layer. A value of -1 means the surface station has 100% weight, while a value of +1 means the upper air station has 100% weight. In simple terrain situation, BIAS is often set to zero (0) for each vertical layer which means the upper air and surface wind and temperature observations are given equal weight in the <math>1/r^2</math> interpolations used to initialize the computational domain.</p> <p>The BIAS affects how the initial Step 1 winds will be interpolated to each grid cell in each vertical layer based on upper air and surface observations. By setting BIAS to -1, we eliminate upper-air observations in the interpolations for this layer. Conversely by setting BIAS to +1, we eliminate the surface observations in the interpolations for this layer.</p> <p>An example where non-default settings for BIAS may be used is for a narrow, twisting valley, where the only upper-air observations were 100 km to the west, and the only local surface wind observations were in one location in the valley. For this example, we might set BIAS to -1 within the valley forcing surface data only to be used for the lowest layers, and BIAS to +1 above the valley forcing upper air data only to be used aloft, and BIAS might go from -1 to +1 in the transitional layers at the top of the valley.</p>
Weighting parameter for Step 1 wind field vs. observations in Layer 1 (R1) and Layer 2 and above (R2)	R1 and R2	No Default	The value of R1 and R2 are used in the construction of the Step 2 wind field, where the observed winds are 'blended' in with the Step 1 winds and observations. R1 represents the distance from a surface observation station at which the surface observation and the Step 1 wind field are weighted equally.

Table A-1 An Explanation of the 7 Critical User-Defined, Site Specific Parameters When Using Observational Data in CALMET/ Cont.....			
Option	Parameter	Recommended Value	Explanation and Justification
		Requires user input. Value in km specific to each model domain 1 value represents all stations  <u>Not used in No-Obs model</u>	R2 represents the comparable distance for winds in layers 2 and above. It is important to note that all the results of the diagnostic wind model (kinematics, slope and blocking effects) are contained in the Step 1 wind field, thus if too much weight is given to the observations, then you will essentially erase all the information generated in creating the Step 1 winds. Rule of thumb is to start with small R1 and R2 values and slowly increase these values if you do not believe the surface stations are showing enough weight. Typically for observation sites in flat terrain values of R1 and R2 are larger than in mountainous terrain where a station's flow is limited by the valley segment.
Maximum radius of influence for meteorological stations in layer 1 (Step 2) and layers aloft (Step2)	RMAX1 and RMAX2	No Default  Requires user input. Value in km specific to each model domain 1 value represents all stations  <u>Not used in No-Obs model</u>	The values of RMAX are also used in the construction of the Step 2 wind field, where the observed winds are 'blended' in with the Step 1 winds. Any observation for which $R_k$ (the distance from the grid cell to the k-the observation location) is greater than RMAX1 in the surface layer, or RMAX2 aloft is excluded from the above 'blending' formula. We can use RMAX1 and RMAX2 to exclude observations from being inappropriately included (as they are in the next valley, on the other side of a mountain, etc.). Note, if you are using RMAX1 and RMAX2 to exclude observations, then you do not want to set LVARY to T, as then CALMET will increase the values of RMAX1 and RMAX2 to at least capture the nearest observation, regardless of whether this makes sense.  Typically values of RMAX1 and RMAX2 are smaller than R1 and R2, this way 'sharp' boundaries between the Step 1 wind field and the weighted observation station are prevented.

\*1 **IEXTRP** - affects vertical extrapolation of surface winds, and whether layer 1 data from upper air stations are ignored, and is normally is set to -4. Setting IEXTRP < 0, means that the lowest layer of the upper-air observation will not be considered in any interpolations. Since upper-air observations are only taken every 12-hours, the time-interpolated surface wind values from the upper-air observations are usually of no use. When IEXTRP is set to -4, similarity theory is used to extrapolate the surface winds into the layers aloft, which provides more information on observed local effects to the upper layers. Setting IEXTRP to 0 means that no vertical extrapolation from the surface wind data is used.

**Table A-2. Explanation and Recommendations for the List of Key CALMET Model Options**

Option	Parameter	Recommend value	Explanation and Justification
<b>Meteorological data Options (In. group 4)</b>			
This switch determines whether you use just observational data, or, a combination of surface and prognostic data, or, prognostic data only	NOOBS	0,1,2	NOOBS can be any of 0, 1 or 2, depending on whether CALMET is run with observation data only (0), a combination of prognostic and surface data (1) or, just prognostic model data (2).
Cloud data options; 0, 1, 2, 3, 4	ICLOUD	4	Compute the gridded cloud cover from relative humidity profile using all levels of data (MM5toGrads algorithm).
<b>Wind field Model Options (In. group 5)</b>			
Wind field model selection variable	IWFCOD	1	Use of the diagnostic wind module is recommended
Compute Froude number adjustment effects	IFRADJ	1	Used to evaluate thermodynamic blocking effects of the terrain on the wind flow and are described using the critical Froude number (see CRITFN to define)
Compute kinematic effects	IKINE	0	Do not calculate a terrain-forced vertical velocity in the initial guess wind field. (This option is normally turned off, especially at when using fine resolution due to occasional non-convergence of algorithm producing anomalous wind speeds in Layer 2.)
O'Brien procedure for adjustment of the vertical velocity	IOBR	0	No adjustment required to the vertical velocity profile at the top of the model domain.
Compute slope flows	ISLOPE	1	Yes, compute upslope and downslope flows which are calculated as a function of sensible heat flux, distance to the crest or valley bottom and slope angle
Extrapolate surface wind observations to upper layers	IEXTRP	-4	Extrapolate surface station information using similarity theory. Ignore layer 1 of upper air station data if surface station is nearby, it is likely to be more representative.
Extrapolate calm winds aloft (0=no, 1=yes)	ICALM	0 or 1	Selection depends on whether adequate upper air data are available to determine winds in Layer 2 and above. Normally ICALM=0 when using gridded prognostic data. Extrapolating calms in a steep valley may be appropriate. A (1) for ICALM will extend calm conditions to the top of the boundary layer.

<b>Table A-2 Explanation and Recommendations for the List of Key CALMET Model Options/Continued</b>			
<b>Option</b>	<b>Parameter</b>	<b>Recommend value</b>	<b>Explanation and Justification</b>
Minimum distance between upper air station and surface station for which extrapolation of surface winds will be allowed	RMIN2	-1	This option is designed to avoid extrapolated surface data “competing” with actual upper air measurements when both surface and upper air measurements are co-located. However, the better time resolution of the surface data (hourly) suggests extrapolating may be appropriate. RMIN2 defined the distance between measurements defining “co-located”. Using -1 when IEXTRP = +/- 4 will ensure extrapolation of all surface stations
Gridded prognostic wind field model output fields as initial guess wind field	IPROG	14	This option uses gridded prognostic meteorological model output as the initial guess wind field in CALMET.
Time step (hours) of the prognostic model input data	ISTEPPG	1	Usually this is an hourly time step. Some gridded prognostic data may be available only every 3 hours (ISTEPPG=3).
Use coarse CALMET fields as initial guess fields	IGFMET	0	Default is off (0), but useful option if you do not have prognostic model data. When switch is on (1) the coarse CALMET fields from an earlier run will be used to define the IGF.
<b>Radius of Influence Parameters</b>			
Use varying radius of influence	LVARY	F	The recommended value is F which turns off the varying radius of influence option. LVARY=T may be used when using objective analysis rather than the diagnostic wind module (IWFCOD=0). LVARY=T results in the radius of influence being expanded when no stations are within the fixed radius of influence value. Caution is warranted because when LVARY=T, the model effectively enlarges RMAX to incorporate the ‘nearest’ station regardless of whether it is suitable or not.
Critical parameters and are discussed in the above table	RMAX1 RMAX2 RMAX3	-	See Table 1-1 above
<b>Other Wind Field Input Parameters</b>			
Minimum radius of influence used in the wind field interpolation	RMIIN	0.1	Recommendation is a very small value (0.1 km). Used to prevent a divide by zero error when a grid point and station are co-located.
Critical parameter and are discussed in the above table	TERRAD	-	See Table 1-1 above
Critical parameters and are discussed in the above table	R1, R2	-	See Table 1-1 above
Relative weighting of the prognostic wind field	RPROG	0	Only change this value if CSUMM winds are used in the Step 1 wind field. CSUMM model data is very rarely used and outdated format of entering prognostic wind speeds and direction into the model.

<b>Table A-2 Explanation and Recommendations for the List of Key CALMET Model Options/Continued</b>			
<b>Option</b>	<b>Parameter</b>	<b>Recommend value</b>	<b>Explanation and Justification</b>
Maximum acceptable divergence in the divergence minimization procedure	DIVLIM	5 x 10 <sup>-6</sup>	No need to change this default value which has been rigorously tested.
Maximum number of iterations in the divergence minimization procedure	NITER	50	Recommended default value (50) is normally used.
Number of passes in the smoothing procedure	NSMTH (NZ)	2, 4,4,4,...	Recommended values are 2 passes in the lowest layer, 4 passes in the higher layers. More passes will result in more smoothing of the final wind field. But rarely altered
Maximum number of stations used in each layer for the interpolation of data to a grid point	NINTR2	99	Normally, recommended default value (99) is used.
Critical Froude Number	CRITFN	1	Terrain blocking occurs when Froude number < CRITFN. Default value should be used except when justified by data.
Empirical factor controlling the influence of kinematic effects	ALPHA	0.1	Use default
Multiplicative scaling factor for extrapolation of surface observations to upper layers	FEXTR2 (NZ)	NZ x 0.0	Seldom used and not used when IEXTRP = +/- 4
<b>Barrier Information</b>			
Number of barriers to interpolation of the wind fields	NBAR	0	Usually not used. Use barriers to block out a certain station effects. Barriers can extend from the surface layer to user-defined upper layer limit
X and Y coordinates of barriers	XBBAR, YBBAR, XEBAR, YEBAR	(varies)	Used only if NBAR > 0 to define the coordinates of the barrier.
Level (1 to NZ) up to which barriers apply	KBAR	(varies)	Used only if NBAR > 0. User defined switch to control vertical extent of barriers. This requires careful examination of the resulting wind field at each level.
<b>Diagnostic Module Data Input Options</b>			
Surface temperature	IDIOPT1	0	Compute the surface temperature internally from hourly surface observations or prognostic model data. DIAG.DAT file is no longer used.
Surface station to use for the surface temperature	ISURFT	-1	Use 2-D spatially varying surface temperatures

<b>Table A-2 Explanation and Recommendations for the List of Key CALMET Model Options/Continued</b>			
<b>Option</b>	<b>Parameter</b>	<b>Recommend value</b>	<b>Explanation and Justification</b>
Diagnostic module domain-averaged lapse rate option	IDIOPT2	0	Computed internally using twice daily upper air data or, prognostic fields. DIAG.DAT file is no longer used.
Upper air station to use for domain scale lapse rate	IUPT	-1	Use spatially varying potential temperature lapse rate
Depth through which the domain scale lapse rate is computed	ZUPT	200m	Only used when temperature lapse rate is computed internally from available upper air or gridded prognostic data. Recommended ZUPT value is based on model testing and should not be changed without supporting data.
Initial Guess Wind Field	IDIOPT3	0	Computed internally from observations and or prognostic winds
Upper air station to use for initial guess field (IGF).	IUPWND	-1	Use 3-D varying initial guess field. Only used if when using observational data to define the IGF (i.e., NOOBS=0). Default means use the 3-D initial guess field.
Bottom and top of layer through which the domain-scale winds are computed	ZUPWND	1 – 1000m	Option not used with 3-D IGF.
Observed surface wind components for wind field module	IDIOPT4	0	Keep at recommended value. DIAG.DAT file is no longer used.
Observed upper air wind components	IDIOPT5	0	Keep at recommended value. DIAG.DAT file is no longer used.

**Table A-3. Explanation and Recommendations for the Overwater Surface Fluxes Switches**

Option	Parameter	Recommended value in typical conditions	Explanation and Justification
<b>Overwater Surface Fluxes Method and Parameters</b>			
COARE (Coupled Ocean Atmosphere Response Experiment) with no wave parameterization (JWAVE=0), Charnock	ICOARE	10	Recent COARE overwater flux module improves model performance over the previous Overwater Coastal Dispersion (OCD) model algorithm. The US EPA default of ICOARE = 0, which is to use the original deltaT method of OCD model is not recommended because MMS-sponsored model evaluations have demonstrated better performance with the COARE algorithm.
Coastal/Shallow water length scale	DSHELF	0 km	Used for COARE fluxes. Default value is 0 km assumes deep water. User can enter a different value in km, to represent the length scale of the shallow water which is then modified for roughness (zo). However, MMS-sponsored model evaluations have demonstrated similar performance with the
COARE warm layer computation	IWARM	0	Used for COARE fluxes. Default value is 0 assuming deep water and well mixed ocean layer. Warm layer computation must be off (IWARM=0) if sea surface temperature is measured with an IR radiometer.
COARE cool skin layer computation	ICOOL	0	Used for COARE fluxes. Default value is 0 assuming deep water and well mixed ocean layer. Cool skin layer computation off (ICOOL=0) if sea surface temperature is measured with an IR radiometer.
<b>Mixing height – Input Group 6</b>			
<b>Empirical Mixing height constants</b>			
Neutral mechanical equation	CONSTB	1.41	Value based on empirical data - no need to change
Convective mixing height equation	CONSTE	0.15	Value based on empirical data - no need to change
Stable mixing height equation	CONSTN	2400	Value based on empirical data - no need to change
Overwater mixing height equation	CONSTW	0.16	Value based on empirical data in Gulf of Mexico. May be a function of locations.
Absolute value of Coriolis	FCORIOL	1.0E-04 s <sup>-1</sup>	Suitable default for mid-latitudes, will need to be changed if in higher or lower latitudes accordingly

<b>Table A-3 Explanation and Recommendations for the Overwater Surface Fluxes Switches/Continued</b>			
<b>Option</b>	<b>Parameter</b>	<b>Recommended value in typical conditions</b>	<b>Explanation and Justification</b>
Spatial Averaging of Mixing Heights	IAVEZI	1	Conduct spatial averaging which is recommended to smooth mixing heights between grid cells
Maximum search radius in averaging process (in grid cells)	MNMDAV	1 grid cell	Typical value is several (1-10) km, but must be expressed in terms of number of grid cells (MNMDAV = X km/DGRIDKM). Note, default value of 1 cell is not the recommended value. MNMDAV must be computed (in grid cell units) from the search radius in km divided by the grid cell size (km)
Half-angle of upwind looking cone for averaging	HAFANG	30 deg	Default value based on model testing
Layer of winds used in upwind averaging	ILEVZI	1	Default value based on model testing.
<b>Convective Mixing Height Options</b>			
Method to compute the convective mixing height	IMIXH	1	Maul-Carson for land and water cells. The recommendation reflects the recent research findings of the study sponsored by the MMS. The US EPA default of IMIXH=-1 (Maul-Carson mixing height for over land only and the OCD mixing height overwater) is not recommended because it does not reflect the findings of the MMS-sponsored model evaluation work.
Threshold buoyancy flux required to sustain convective mixing height growth overland	THRESHL	0.0 W/m <sup>3</sup>	
Threshold buoyancy flux required to sustain convective mixing height growth overwater	THRESHW	0.05 W/m <sup>3</sup>	Recommended value based on testing sponsored by MMS over the Gulf of Mexico.
<b>Other Mixing Height Variables</b>			
Minimum potential temperature lapse rate in stable layer above the current convective mixing height	DPTMIN	0.001 deg K/m	Based on empirical testing, do not change unless have data to prove otherwise

<b>Option</b>	<b>Parameter</b>	<b>Recommended value in typical conditions</b>	<b>Explanation and Justification</b>
Depth of layer above current convective mixing height (ZI) through which potential temperature lapse rate is computed	DZZI	200m	Based on empirical testing, do not change unless have data to justify alternative setting
Minimum overland mixing height	ZIMIN	50m	Reflects presence of typical surface roughness elements, such as vegetation, structures, trees and shear-induced mixing near the ground. User can modify ZIMIN, but do so with caution
Maximum overland mixing height	ZIMAX	3000m	In Australia ZIMAX should typically be 3000m or more.
Minimum overwater mixing height	ZIMINW	50m	Based on testing, modify only with supporting data
Maximum overwater mixing height	ZIMAXW	3000m	Based on testing, modify only with supporting data

**Table A-4. Explanation and Recommendations for the List of Key CALUFF Model Options**

Option	Parameter	Recommended value	Explanation and Justification
<b>Technical Options - Input Grp 2</b>			
Vertical distribution used in the near field	MGAUSS	1	Always use
Terrain adjustment method	MCTADJ	3	Partial plume path adjustment
Sub grid-scale complex terrain	MCTSG	0	Usually 0, but does allow for CTDM-like treatment of sub grid scale hills (See input Group 6)
Near-field puffs modeled as slugs	MSLUG	0	Default is not to use slug model. But it is the recommended approach for area sources with receptors in the very near field or for time-varying emissions such as accidental releases are modeled.
Transitional plume rise	MTRANS	1	Yes, always allow transitional rise
Stack tip downwash	MTIP	1	Yes, always allow stack tip downwash. It becomes important if ratio of stack gas exit velocity to wind speed is $< 1.5$
Method to compute plume rise for point sources not subject to downwash	MRISE	1	Yes, to Briggs plume rise (1). The other option (2) is meant for very hot sources such as flares where the Bousinesq equation is no longer valid and plume rise needs to be treated numerically
Method to simulate building downwash	MBDW	2	PRIME Method unless long such as aluminum smelters with aspect ratios of L/W over 5-10. For these situations use MBDW=1 (ISC/BLP downwash method)
Vertical wind shear modeled above stack top	MSHEAR	0	The default is for no vertical wind shear. The model inherently includes variable flow in the vertical from the upper air data. If this option is used the model applies a power law wind speed profile above stack top.
Puff Splitting allowed	MSPLIT	0	No puff splitting. In long range transport, puff splitting may be necessary. In short-range modeling, MSPLIT=0 is recommended.
Chemical transformation	MCHEM	1	Chemistry to be modeled and transformation rates are computed internally using MESOPUFF II scheme (recommended when dealing with SO <sub>2</sub> , SO <sub>4</sub> , NO <sub>x</sub> , HNO <sub>3</sub> and NO <sub>3</sub> concentration predictions over 10-20 km or more.
Aqueous phase chemistry	MACHEM	0	Aqueous phase chemistry (option is not currently active)
Wet removal modeled	MWET	1	Wet deposition is often important long range transport. May be used in near-field in certain circumstances. Depends on the pollutant characteristics.

<b>Table A-4 Explanation and Recommendations for the List of Key CALPUFF Model Options/Continued</b>			
<b>Option</b>	<b>Parameter</b>	<b>Recommended value</b>	<b>Explanation and Justification</b>
Dry deposition modeled	MDRY	1	Dry deposition is often important long range transport. May be used in near-field in certain circumstances. Depends on the pollutant characteristics.
Gravitational settling (plume tilt)	MTILT	0	Default is for plume tilt switch to be turned off. Usually unimportant for small (combustion size particles less than 10 um). May be needed for very large particles with substantial gravitational settling effects.
Dispersion coefficients	MDISP	2	Use of turbulence based dispersion coefficients is recommended for the same reasons ISCST PG-based dispersion has been replaced by turbulence-based AERMOD dispersion in US plume regulatory modeling. The US EPA default is still to use PG dispersion in CALPUFF, but best science practice and model evaluation studies indicate MDISP=2 performs better.  MDISP=1, which is to compute dispersion coefficients from measured $\sigma_v$ and $\sigma_w$ is preferred when good quality, representative turbulence observations are available.
$\sigma_v / \sigma_\theta$ and $\sigma_w$ measurements from PROFILE.DAT to compute $\sigma_y$ and $\sigma_z$	MTURBVW	3	Only used if MDISP = 1 or 5 which means that when measured sigmas are available. The default is to use observed measured $\sigma_v / \sigma_\theta$ and $\sigma_w$ from the PROFILE.DAT file to compute $\sigma_y$ and $\sigma_z$ .
Backup method used to compute dispersion when measured turbulence data are missing	MDISP2	3	Used only if MDISP=1 or 5. Backup method is PG dispersion coefficients for RURAL areas when turbulence data is missing.
Method used for Lagrangian time scale for $\sigma_y$	MTAULY	0	Default Lagrangian time scale (Draxler) is 617.284s. No need to modify. Only used when MDISP = 1,2
Method used to compute turbulence $\sigma_v$ and $\sigma_w$ profiles	MCTURB	1	Use standard CALPUFF subroutines. MCTURB=2 will use turbulence profiles based on AERMOD algorithms. Model evaluations have shown both options have similar performance.
PG $\sigma_y$ , $\sigma_z$ adjusted for roughness	MROUGH	0	Not needed for CALPUFF. If trying to simulate an AUSPLUME run using single station PLMMET.DAT file then user has choice to adjust for $z_o$ as is done in AUSPLUME.
Partial plume penetration into elevated inversions	MPARTL	1	Recommend setting is to evaluate partial plume penetration into elevated inversions applied to point sources.

<b>Table A-4 Explanation and Recommendations for the List of Key CALPUFF Model Options/Continued</b>			
<b>Option</b>	<b>Parameter</b>	<b>Recommended value</b>	<b>Explanation and Justification</b>
Partial plume penetration from buoyant area sources	MPARTLBA	1	Recommended setting is to model partial plume penetration into elevated inversions. An important option for very hot buoyant area sources such as forest fires.
Strength of temperature inversion as provided in PROFILE.DAT file	MTINV	0	In most cases users do not have detailed temperature profiles which need to be placed into the PROFILE.DAT file; therefore the default is to compute the strength of the inversion from default gradients and upper air data.
Probability Density Function (PDF) used for dispersion under convective conditions	MPDF	1	If using computed turbulence-based dispersion coefficients (MDISP=2), the PDF should be invoked.
Sub-grid TIBL module used for shore line	MSGTIBL	0, 1	Default is not to use the sub grid scale TIBL option (MSGTIBL=0), but this option may often be beneficial for applications located along a coastline. Decision to use it is application specific. If invoked the user must prepare a coastline file (COASTLN.DAT) to specify the location of the land-water boundary.
Boundary conditions modeled	MBCON	0	The default is to not use boundary conditions. When boundary conditions may be important, this option should be used.
Fog Module	MFOG	0	The default is to not invoke CALPUFF's FOG module, which is a specialty module designed for visible plume length calculations and plume-induced frequency calculations from cooling tower sources and other sources with visible water vapor plumes.
Minimum turbulence velocities, sigma v and sigma w for each stability class over land and water	SVMIN SWMIN	$\sigma_v = 0.2$ for A, B, C, D, E, F $\sigma_w = \text{default}$	For applications where calm wind and stagnation events are significant, turn SVMIN to 0.2 to better represent lateral spread of the plume material. Leave SWMIN as default values

\*Note. The default switches in CALPUFF are recommended for all applications, although in Australia neither chemistry nor wet and dry deposition may always be required.