

**CALPUFF MODEL VALIDATION IN NEW ZEALAND
METHODOLOGY AND ISSUES**

JUNE 2005

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Foundation for Science and Technology

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Table of Contents

	Page
1. Introduction	1
1.1 FRST Study	1
1.2 Requirements of NES and Regulatory Environment	2
1.3 Why the Concern about Air Dispersion Model Results?	3
1.4 Why use CALPUFF in New Zealand?	3
1.5 Requirements for the CALPUFF Validation Study	4
1.6 Outputs	5
2. Review of Literature	5
3. Methodology of Model Evaluation	6
3.1 Approach	6
3.2 Site Selection and Obtain Raw Data from Industry	7
3.3 Initial CALMET-CALPUFF Model of all Sites all Periods	8
3.4 Case Studies	8
3.5 Reporting and Workshop	8
4. Summary and Conclusions	9
5. References	9

List of Tables

	Page
1.1 National Environmental Standards (NES) for Ambient Air Quality.	2

1. Introduction

1.1 FRST Study

As outlined in the NIWA FRST program proposal (NIWA 2004) The current research program forms part of the FRST program “Protecting New Zealand’s Clean Air” (contract C01X0405). The program aims to provide new information and tools to ensure that the National Environmental Standards for Air Quality are achieved as quickly and efficiently as possible.

As part of the program, Objective 3 aims to “develop and apply modelling methods that can be used to quantify air pollution effects and predict the outcomes of mitigation and management options”.

One of the Milestones in Objective 3 is the “Validation of the CALPUFF model in New Zealand conditions for industrial emissions from tall stacks and domestic-heating emissions”. Note that in referring to the use of CALPUFF, it can be taken as read that this also embodies the use of its association meteorological pre-processing programme “CALMET”, which generate the complex meteorology that is required to run CALPUFF and which critically impacts upon the reliability of predictions by CALPUFF. Therefore the assessment of CALPUFF will by necessity, involve a detailed analysis of CALMET performance and how this effects the reliability of CALPUFF modelling assessments.

A critical success factor identified early in the project formulation phase was the “access to information held by industries on emissions, and site-specific air pollution monitoring data.” This has since proved to be a significant issue. Several large industrial sites which were known to have potentially suitable stack emission and ambient monitoring data were reluctant to join the program for various commercial reasons. One concern appeared to relate to how their data may be used and published. It also became evident that these companies considered their monitoring data as valuable resources for which they would not “give away” unless we could convince them of a direct tangible benefit to their organisation. As a result of this approach, it took close to six months negotiating with five companies to obtain their data and even then, some which initially expressed interest, decided to not be involved in the programme.

The following sites have now been identified and the relevant agreement obtained with the companies to utilise stack emission data and ambient monitoring data from their sites:

- Contact Energy New Plymouth Power Station, Taranaki
- Fonterra Edendale Dairy Processing Plant, Southland
- New Zealand Aluminium Smelter Ltd, Tiwai Point, Southland.

The FRST program would like to acknowledge the important contributions made by the above companies, without whose help the CALPUFF evaluation study could not have proceeded.

1.2 Requirements of NES and Regulatory Environment

The Ministry for the Environment (MfE) has instigated the development of National Environmental Standards (MfE 2004a) and the associated guidelines (MfE 2004b) for various air contaminants in New Zealand.

The National Environmental Standards (NES) are mandatory technical environmental regulations that cover seven activity standards and five ambient air quality standards. The standards also include a design standard for new small-scale domestic wood-burning appliances and for the design and performance of systems for the destruction of landfill gas at large landfills (MfE 2004b).

The primary purpose of the ambient standards is “to provide a guaranteed level of protection for the health of all New Zealanders”. The ambient standards are minimum standards for outdoor air that apply in a region (LAMA) as specified by the Minister and apply to regions where people are likely to be exposed to the specified contaminants. The standards do not apply in outdoor workplace environments where the public are not exposed, as these areas are covered by other health and safety legislation. The ambient air quality standards apply to five contaminants: particulate matter less than ten micrometers (PM₁₀), sulphur dioxide (SO₂), carbon monoxide (CO), nitrogen dioxide (NO₂) and ozone (O₃). The standards are shown in Table 1.1.

Table 1.1: National Environmental Standards (NES) for Ambient Air Quality.

Contaminant	Standard ¹	Time average	Allowable Exceedences per year
Particles (PM ₁₀)	50 µg/m ³	24-hour	1
Sulphur dioxide (SO ₂)	350 µg/m ³	1-hour	9
	570 µg/m ³	1-hour	0
Carbon monoxide (CO)	10 mg/m ³	8-hour	1
Nitrogen dioxide (NO ₂)	200 µg/m ³	1-hour	9
Ozone (O ₃)	150 µg/m ³	1-hour	0

Note: The units for CO are in milligrams per cubic metre, whereas all the others are in micrograms.

The definition of LAMAs is subject to ongoing work by other FRST studies (Fisher et al, 2005), as well as regional councils, unitary authorities and the MfE. The Minister will proclaim LAMAs for the whole country on 1 September 2005.

After this date the regional councils and unitary authorities must:

- a) Monitor air quality compliance with the ambient standards in any airshed that will or potentially may exceed the standards;
- b) Give public notice if the standard concentrations are exceeded in an airshed;
- c) Only grant new resource consents in line with requirements outlined in subclauses 17 to 21 of the regulations;

1.3 Why the Concern about Air Dispersion Model Results?

Part (c) above indicates that the granting of new resources consents in any given airshed, has to be assessed in terms of both the individual and cumulative impacts which a new or renewed consent may have on that airshed.

Air dispersion modelling is used as a tool in the assessments of effects on the environment undertaken for many medium to large scale industrial operations. Results from the air dispersion model predictions therefore need to be rigorous and defensible under the Resource Management Act 1991 (RMA) and the new NES. Results from model predictions are used both in assisting design of large facilities (ie stack height and mitigation measures) and also in the scale and location of plants. Air dispersion modelling can therefore be a vital tool for both companies and regulators in ensuring a sustainable and healthy environment.

However both companies and regulators need to have confidence in model results and how these should be interpreted in different situations. This requires a greater understanding of model limitations and their typical bias when predicting either short or long term ground level concentrations. Most commercially available models have gone through extensive model validation, especially those approved through the United States Environmental Protection Agency (USEPA). Models such as ISC3 have had a long history of validation over the last 20 years and have been designated as "Preferred/Recommended" models for regulatory use. In Australasia, the "stalwart" model of use over recent years for industrial applications has been AUSPLUME.

1.4 Why use CALPUFF in New Zealand?

New Zealand is characterised by significant topographic diversity and climate variations over short distances. The presence of the Southern Alps (+2000 m) for example has a major impact on the weather and climate between locations such as Christchurch on the East Coast and the West Coast of the South Island. Mountain-valley features, especially during cold stable winter days can result in significant potential for elevated air pollution levels for towns such as Nelson (South Island) and Tokoroa (North Island).

Complex terrain features that combine relief variation of greater than 200 m in height over length scales of 1-2 km's is fairly common around many New Zealand towns. Furthermore strongly stratified local meteorological circulation under cold stable winter conditions can result in very complex surface and boundary layer meteorology. Calm conditions, surface based upper air inversions and mesoscale thermally driven wind flow such as mountain-valley and sea-land breezes are reasonable frequent.

Steady state plume models such as ISC3 and AUSPLUME cannot adequately model the complex features mentioned above. For this reason (MfE, 2004c) has recommended using CALPUFF and other non-steady state models for complex terrain environments, especially for medium to large industrial sources. The Good Practice Guide for Atmospheric Modelling has recommended the use of complex models (Recommendation No 7, page 18) when:

- Meteorological conditions vary across the modelling domain;
- The modelling domain incorporates complex terrain;
- Pollutants accumulate in calm conditions and re-circulation can occur;
- Frequent low wind speed or calm conditions occur;
- Chemical transformations between pollutants occur; and
- Appropriate meteorological data are available to drive a complex model.

CALPUFF has now been used fairly extensively over the last 5-years in New Zealand for assessments that involve medium to large stack industrial sources. The CALPUFF model has recently gained regulatory approval modelling medium to long-range transport of pollutants (USEPA 2003). CALPUFF can also be used on a case by case basis in environments involving complex flow for near field situations.

Anecdotal evidence from modellers using CALPUFF to model air discharges from medium to large stacks (50 – 200 m in height) in New Zealand have shown that CALPUFF possibly “over predicts” maximum ground level concentrations at 1-hour averaging periods, especially within 1 – 2 km of the stack. This has not been confirmed in any substantive scientific validation study for New Zealand.

With the advent of NES and limits placed on maximum and 99.9th percentile values for 1-hour ambient concentrations such as SO₂, air quality practitioners, industrial companies and regulators want to understand the limitations of the air dispersion modelling, especially at the highest predicted spectrum of model results.

1.5 Requirements for the CALPUFF Validation Study

An initial screening of suitable industrial sites through New Zealand with known ambient monitoring data was undertaken. A number of potential companies were approached to establish their possible involvement in the CALPUFF validation study. A few companies declined to become

involved for various commercial reasons. A list of the criteria that was required is described below:

- Study to evaluate 3-4 different industrial sites;
- Site to be of reasonable size and have stack discharges from a minimum of at least 40–50 m above the ground;
- Sites to be located in different coastal, inland and complex terrain environments;
- Hourly ambient monitored data (preferably SO₂);
- Hourly local surface meteorology (wind speed/direction, temperature); and
- Hourly/continuous mass emission rates or fuel use rate, gas volume rates (stack gas velocities) and stack gas temperature.

Once the necessary local site data has been obtained (emission rates and any surface meteorology), then the necessary CALMET (meteorological processor) input files are developed. Input files include data from:

- Surface meteorology (hourly);
- Upper air meteorology from radiosonde data (12-hourly) or meteorological model such as MM5 or TAPM (hourly); and
- Terrain and land-use at CALMET model grid size (ie 250 m by 250 m).

1.6 Outputs

Outputs required for the CALPUFF validation study will include the following:

- 1) Obtain hourly combustion and ambient monitoring data from 3 large industrial sites around New Zealand (by 30 June 2005).
- 2) Prepare report “CALPUFF Model Validation: Methodology and Issues” (by 30 June 2005).
- 3) Prepare report “CALPUFF Model Validation for large stack sources in New Zealand” (by 31 Dec 2005).
- 4) Present workshop on CALPUFF model validation (by 31 Dec 2005).
- 5) Prepare paper for submission to international journal (by 30 June 2006).

2. Review of Literature

A full review of all published papers and reviews on the CALPUFF model will be undertaken in the final report to be completed by December 2005. Some of the relevant studies are provided below.

The beta testing and model evaluation of CALPUFF by various authors for and on behalf of the USEPA was undertaken in the late 1990's and early 2000's (Strimaitis et al 1997, Allwine et al 1998, USEPA 1998a, USEPA 1998b, USEPA 1998c, Earth Tech 2002, USEPA 2003a, USEPA 2003b).

A number of international studies have examined the CALMET/CALPUFF modelling system for meteorological applications (Earth Tech 2003, Chandrasekar et al, 2003) mesoscale transport (Chang et al 2003), regional air quality (Irwin et al. 2001, North Dakota DOH 2002), urban air quality (Elbir 2003, Gimson 2005), power stations (Levy et al 2001, Zhou et al. 2002), model validation (Busillo et al. 2004, Protonotariou et al. 2004, Yau et al 2004, Hurley and Luhar 2005, Hurley et al. 2005). A range of other non-refereed papers are also available on the web.

3. Methodology of Model Evaluation

The model evaluation of CALPUFF in New Zealand involves a range of organisations that include National Institute of Water and Atmospheric Research (NIWA), Kingett Mitchell Ltd (KML), Endpoint Ltd (Endpoint) and the University of Canterbury (UC). The project development, methodology and review are a collaborative effort. NIWA has the primary responsibility of the dispersion modelling. KML's has responsibility for industry liaison, review of emission, ambient and model input data. A detailed methodology is provided below.

Organisation responsible for each activity is given in brackets.

3.1 Approach

- a) Assess likely study sites and approach industrial companies to ascertain their involvement in the FRST study (KML, Endpoint).
- b) Choose 3 sites based on location, relevance to study and partnership agreement with companies (All).
- c) Obtain raw data (emission rates, source, meteorology, ambient monitoring) for each site (KML, Endpoint).
- d) Setup CALMET and CALPUFF models for all sites and run for available data periods (2-4 months) (NIWA) review (KML).
- e) Compare predicted versus monitored values using statistical analysis and other graphical plots (NIWA).
- f) Assess and describe the meteorological conditions, when CALPUFF predictions vary significantly from monitored values (the associated times will become "specific case studies") (NIWA).
- g) Is the model performance sensitive to CALPUFF settings, or is the meteorology the main driver of discrepancy? (NIWA).

- h) Are the types of meteorological conditions where predicted values versus observed values consistent/inconsistent across all the study sites? (NIWA).
- i) Review the predicted vertical meteorological profiles associated with poor model predictions against expectations based on current theory, knowledge and empirical knowledge – do the predicted profiles seem realistic or not? (NIWA – All).
- j) If meteorological conditions appear unrealistic then consider adjustments to the setup of CALMET for these “non-performing” periods and remodel with CALPUFF. Do the problematic meteorological conditions remain? Is the overall performance model improved? Do we create new problems when solving the current one? (NIWA, KML).
- k) Use prognostic meteorological data (MM5 + TAPM) data in CALMET for case studies. Does this fix the problems with unrealistic meteorology? Does all the extra effort result in useful improvements or help confirm what the limitations of using CALMET with limited raw data inputs? (NIWA, KML, UC).
- l) Run TAPM dispersion for case studies. Compare with CALPUFF/CALMET performance. Undertake a similar analysis as for CALMET and CALPUFF (NIWA).
- m) Prepare a final report on study results by December 2005 (NIWA, All).
- n) Present results to a workshop by December 2005 (NIWA, All).
- o) Prepare a paper for publication by June 2006 (NIWA, All).

3.2 Site Selection and Obtain Raw Data from Industry

- a) Assess likely study sites and approach industrial companies to ascertain their involvement in the FRST study. (KML, Endpoint).
- b) Identify 3 preferred sites based on location, relevance to study and partnership agreement with companies. (KML, Endpoint).
- c) Selection of 3 sites identified are New Plymouth power station (Contact Energy), Edendale milk processing plant (Fonterra) and Bluff aluminium smelter (NZAS).
- d) Obtain 2 – 4 months of continuous data (emission, meteorology and ambient monitoring data) for evaluation purposes (KML, Endpoint) for each site.
- e) Review and confirm reliability of hourly emission data for modelling (KML, Endpoint).
- f) Review hourly ambient monitoring data (KML, Endpoint, NIWA), identify times of highest impact and associated meteorology and plant operating conditions.
- g) Review hourly meteorology data and confirm use for modelling (KML, NIWA, Endpoint).

- h) Obtain agreement on modelling periods to be evaluated (NIWA, All).

3.3 Initial CALMET-CALPUFF Model of all Sites all Periods

- a) Setup CALMET and CALPUFF model input files based on “best practise” (NIWA, KML).
- b) CALMET 5.53A and CALPUFF 5.711A (Prime – Beta version) to be used.
- c) Initial CALMET setup to only use monitored upper air and surface data.
- d) Define domain size and grid resolution (NIWA, KML, UC).
- e) Prepare geo.dat/surf.dat/up.dat for CALMET (NIWA) review (KML).
- f) Prepare input file for CALPUFF (NIWA), review (KML).
- g) Run CALMET and CALPUFF Models for evaluation period for each site (2-4 months) (NIWA).
- h) Undertake CALMET/CALPUFF model performance evaluation (NIWA). Review results (KML, Endpoint, UC).
- i) Identify “non-performing” case studies (NIWA) review (KML, Endpoint, UC).
- j) Check for consistency of results over the different sites (NIWA), review (KML, Endpoint, UC).
- k) Conference call discussion on initial results (NIWA, All).
- l) Case studies identified for further evaluation (All).

3.4 Case Studies

- a) Run MM5 and TAPM for case studies (UC, NIWA).
- b) CALMET rerun with prognostic meteorology (NIWA) review (KML).
- c) CALPUFF rerun with new CALMET (NIWA) review (KML).
- d) Results collated (NIWA).
- e) Conference call review of study progress (NIWA, All).

3.5 Reporting and Workshop

- a) Drafting of final report by December 2005 (NIWA, KML) review (All).
- b) Preparation for December 2005 workshop (NIWA) to assist (Endpoint, KML).
- c) Organise and run workshop (NIWA, Endpoint) to assist (KML).
- d) Drafting of paper (by June 2006) (NIWA) to assist (All).

4. Summary and Conclusions

The CALPUFF/CALMET validation study will need to provide clear guidance on the use and limitations of CALPUFF for the modelling of medium to large industrial stacks in New Zealand. Recommendations for New Zealand conditions on the following are required:

- a) “Best practise” options for the development of 3D meteorological data sets.
- b) “Best practise” options for CALMET model setup.
- c) “Best practise” options for CALPUFF model setup.
- d) Suitability and use of TAPM and MM5.
- e) Appropriate interpretation and treatment of near and far-field CALPUFF predicted model values and the highest model values (maximum, 99.9th percentile etc.) at the hourly averaging period. This has significant implications for achieving regulatory compliance and particularly the NES.
- f) Identification of any particular meteorological conditions for which the model predictions are consistently under or overstated and the typical level of model bias.
- g) Recommended approaches for conducting site specific assessments of modelling performance for New Zealand industrial sites.

Results need to be presented in suitable form for dissemination to regulatory authorities for the implementation of NES.

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