Newfoundland Labrador

Government of Newfoundland and Labrador

Department of Environment & Conservation

Pollution Prevention Division
(Environment)

Guidance Document

Title: Guideline for Plume Dispersion Modelling

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Plume Dispersion Modelling
GD-PPD-019.2

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SUBJECT

The plume dispersion modelling methods approved by the Department for the purpose of determining compliance with the ambient air quality standards in the *Air Pollution Control Regulations, 2004*.

OBJECTIVE

To define the terms and conditions that proponents are to follow when conducting an air quality assessment of a facility in Newfoundland and Labrador. In so doing, the Department ensures that the quality of all results obtained and submitted to the Department are complete and consistent across all facilities and employ the latest advances in modelling technology.

BACKGROUND

Under the *Air Pollution Control Regulations, 2004*, the ambient air quality standards are defined for a series of contaminants. These standards define levels that the Minister deems to be acceptable for the protection of the environment, including human life, wildlife and vegetation.

By their very nature, the ambient air quality standards are based on the emissions from all potential sources within an air zone. For some pollutants, such as sulphur dioxide, the number of potential sources in an air zone contributing to the concentrations in ambient air would be limited due to the chemistry involved in the formation of sulphur dioxide. For other pollutants, such as particulate matter, the number of potential sources in an air zone can be quite large, and difficult to assign to any particular source.

To determine the ambient levels of a particular pollutant, typically a series of monitors are located within the air zone. If the level of a pollutant exceeds the corresponding ambient air quality standard, then by Section 3 of the *Air Pollution Control Regulations, 2004*, the Minister can specify conditions in a Certificate of Approval or develop an air quality management plan for the air zone. However, it may be the case that in an air zone which includes major industrial operations, the series of monitors do not record an ambient concentration in excess of the associated standard, yet an exceedance of the ambient air standard may have occurred in an area where a monitor was not located.

To address compliance with the ambient standards, the Department of Environment and Conservation developed guidance document *GD-PPD-009.3 Compliance Determination*. In that guidance document, compliance is to be determined by a registered dispersion model, or more specifically, in accordance with the terms and conditions of this particular guidance document.

In the 1st revision of this guidance document, numerous conditions were adjusted to account for model updates and improved algorithms in the approved models and associated preprocessors. As well, various usage conditions were modified to account for new technologies.

For this 2nd revision, numerous conditions were again adjusted to account for model updates, newer datasets and improved algorithms in the approved models, including implementation of the RIVAD / ISORROPIA chemistry. This revision also clarifies questions that have been raised since the previous revision and defines some standardized approaches applicable to all modelling applications thereby minimizing discontinuities across various industrial sectors.

DEFINITIONS

In this guidance document:

a) "administrative boundary" means the boundary, as defined in a Certificate of Approval, for the administration of the *Air Pollution Control Regulations, 2004*;

b) "AERMOD modelling system" means the modelling system developed by United States Environmental Protection Agency (US EPA) in conjunction with the American Meteorological Society (AMS) and includes the AERMET meteorological preprocessor, the AERMAP terrain preprocessor, and the AERMOD dispersion model;

c) "AERSCREEN" is the recommended screening model based on AERMOD;

d) "air contaminant" means any discharge, release, or other propagation into the air and includes, but is not limited to, dust, fumes, mist, smoke, particulate matter, vapours, gases, odours, odorous substances, acids, soot, grime or any combination of them;

e) "air zone" is a finite geographic area, within the province that typically exhibits similar air quality issues and trends throughout;

f) "CALPUFF modelling system" means the modelling system developed by scientists at the Atmospheric Studies Group and includes the CALMET meteorological preprocessor, the CALPUFF dispersion model, the CALPOST postprocessor, and associated preprocessing programs;

g) "Department" means the Department of Environment and Conservation and its successors.

1. APPROVED MODELS

For all regulatory applications, the CALPUFF modelling system is approved, subject to the terms and conditions outlined in Section 4. Under special circumstances outlined in Sections 1.4 and 1.5, and with the prior approval of the Department, the US EPA model AERSCREEN and the AERMOD modelling system, may be approved for regulatory applications. If a circumstance exists where the CALPUFF modelling system, or alternatively the AERMOD modelling system or the AERSCREEN model is not appropriate, the Department will review, on a case by case basis, the appropriateness of alternate models and define the terms and conditions under which an alternate model will be employed.

1.1 CALPUFF MODEL - OVERVIEW

The CALPUFF modelling system includes three main components: CALMET, CALPUFF and CALPOST, and a series of preprocessing programs designed to interface the model with routinely-available meteorological and geophysical datasets. CALMET is a meteorological model that develops hourly wind and temperature fields on a three-dimensional gridded modelling domain. Associated two-dimensional fields such as mixing heights, surface characteristics and dispersion properties are also included in the file produced by CALMET. CALPUFF is a transport and dispersion model that advects puffs of material emitted from modelled sources, simulating dispersion and transformation processes along the way. It typically uses the fields generated by CALMET, or as an option, uses simpler non-gridded meteorological data much like the existing plume models. Temporal and spatial variations in the meteorological fields selected are explicitly incorporated in the resulting distribution of puffs throughout a simulation period. The primary output files from CALPUFF contain either hourly concentrations or hourly deposition fluxes evaluated at selected receptor locations. CALPOST is used to process these files, producing tabulations that summarize the results of the simulation, identifying, for example, the highest and second highest 1-hour average concentrations at each receptor. When performing visibility-related modelling, CALPOST uses concentrations from CALPUFF to compute extinction coefficients and related measures of visibility, reporting these for selected averaging times and location. [1]

1.2 AERMOD MODEL – OVERVIEW

The AERMOD modelling system includes three main components: AERMET, AERMAP and AERMOD. AERMET is a general purpose meteorological preprocessor for organizing available meteorological data, and requires the input of surface roughness, Bowen ratio and albedo together with morning upper air soundings and hourly observations of wind speed, wind direction, cloud cover and temperature. AERMAP is a terrain preprocessor whose primary purpose is to determine the height scale for each receptor in the modelling domain. AERMOD is a steady-state plume dispersion model for assessment of pollutant concentrations from a variety of sources. AERMOD simulates transport and dispersion from multiple point, area, or volume sources based on an up-to-date characterization of the atmospheric boundary layer. [2,3]

1.3 AERSCREEN MODEL - OVERVIEW

AERSCREEN is a screening-level air quality model based on AERMOD (U.S. EPA, 2004a), and includes averaging time factors for worst-case 1-hr, 3-hr, 8-hr, 24-hr and annual averages. Three areas where AERSCREEN deviates significantly from SCREEN3, which was the previously approved screening model, are:

1) Building wake effects – AERSCREEN utilizes all the advantages of PRIME (Schulman et al., 2000) including stacks detached from the building;
2) Meteorology – AERSCREEN provides three options for generating the screening meteorology. One option allows for user-specified surface characteristics; the second option is to use seasonally varying surface characteristics for generic land use classifications; and the third option is to use surface characteristics listed in an external file; and
3) Terrain – AERSCREEN provides the option for incorporating terrain impacts on the screening analysis.[4]

1.4 AERSCREEN MODEL - SPECIAL CIRCUMSTANCES

The AERSCREEN model may be approved for regulatory applications provided the application does not involve multiple source or complex fumigation calculations and has annual emissions lower than the thresholds denoted in Table 1.4.1. AERSCREEN may also be approved if the annual emissions of at least one pollutant of the application are in excess of those denoted in Table 1.4.1, and the Department has deemed the use of the model as adequate for the application. Only results from the latest version of AERSCREEN shall be acceptable. As of the date of this guidance document, the version was 11126. The Department shall be contacted prior to undertaking compliance modelling to confirm the latest acceptable version.

Table 1.4.1

Pollutant	Annual Emission Limit for AERSCREEN (kilograms)
sulphur dioxide (SO_2)	5000
total suspended particulate (TSP)	1000
particulate matter less than 10 microns (PM_{10})	500
particulate matter less than 2.5 microns ($PM_{2.5}$)	250
nitrogen oxides (NO_x)	5000

For pollutants not listed in Table 1.4.1, but where the use of AERSCREEN may otherwise be approved, the Department shall determine, on a case by case basis, if AERSCREEN may be applied. If AERSCREEN indicates a potential violation of the *Air Pollution Control Regulations, 2004* or a condition of a Certificate of Approval, then the Department may require the use of either the AERMOD modelling system or the CALPUFF modelling system.

Examples of regulatory applications for which AERSCREEN may be approved include:

- single source diesel powered electrical generators
- space heating of small rectangular buildings
- VOC emissions from small industrial facilities

1.5 AERMOD MODEL – SPECIAL CIRCUMSTANCES

The AERMOD modelling system may be approved for regulatory application if the application does not involve situations denoted in Table 1.5.1. If an application involves a circumstance denoted in Table 1.5.1, the application shall adhere to the provisions of the CALPUFF modelling system detailed in Section 4.

Table 1.5.1

Applications where the AERMOD modelling system is not acceptable	
Long range transport (> 50km)	Visibility-related postprocessing
Overwater and coastal interaction effects	Chemical transformations present
Variable land use about the source	Subgrid scaling of complex terrain

2. MODEL PARAMETERS

2.1 POLLUTANTS

Unless otherwise specified under a Certificate of Approval issued by the Department, the minimum number of pollutants to be modelled is listed in Table 2.1.1.

Table 2.1.1

Pollutant	Combustion Sources	Non-Combustion Sources
sulphur dioxide (SO_2)	✓	✗
total suspended particulate (TSP)	✓	✓
particulate matter less than 10 microns (PM_{10})	✓	✓
particulate matter less than 2.5 microns ($PM_{2.5}$)	✓	✓
nitrogen dioxide (NO_2)	✓	✗
carbon monoxide (CO)	✓	✗

Where other pollutants are deemed by the Department to have the potential to exceed the limits established in the *Air Pollution Control Regulations, 2004* or otherwise have an adverse effect on the environment, the Department reserves the right to require the modelling of these other pollutants.

When modelling for NO_2, refer to Appendix A for further guidance.

2.2 AVERAGING PERIODS

For all regulatory applications, the averaging periods to be modelled for all pollutants denoted in Section 2.1 are contained in Table 2.2.1. Where concentrations are modelled, the results shall be reported in micrograms per cubic metre ($\mu g/m^3$). Where deposition is modelled, the results shall be reported in micrograms per square metre ($\mu g/m^2$). The minimum output requirement is the maximum concentration at each receptor for the time frames denoted in Table 2.2.1 over the meteorological period defined in Section 2.3.

Table 2.2.1

Pollutant	Averaging Period
sulphur dioxide (SO_2)	1 hour, 3 hour, 24 hour, annual
total suspended particulate (TSP)	1 hour, 24 hour, annual
particulate matter less than 10 microns (PM_{10})	1 hour, 24 hour
particulate matter less than 2.5 microns ($PM_{2.5}$)	1 hour, 24 hour, annual
nitrogen dioxide (NO_2)	1 hour, 24 hour, annual
carbon monoxide (CO)	1 hour, 8 hour

Where modelling of other pollutants is required under Section 2.1, such modelling shall be conducted for the averaging periods specified by the Department.

2.3 MODELLING TIME PERIOD

2.3.1 COMPLIANCE MODELLING

With reference to guidance document *GD-PPD-009.3 Compliance Determination* or its successor, a facility is required to demonstrate compliance with the ambient air quality standards in the *Air Pollution Control Regulations, 2004* via a registered dispersion model on a two-year cycle if the facility is non-compliant with the standards or four-year cycle if the facility is compliant with the standards. Compliance determination, irrespective of the two-year or four-year cycle will be based on the modelling of the actual emissions profile and meteorological conditions for the previous four years. In the case of the two-year cycle this means that the model outcomes for the last two years of a prior cycle will be considered in compliance determination. Reporting of modelling results for the pollutants and timeframes listed in Table 2.2.1 from either the two-year or four-year cycle is required to be presented on an annual basis.

For example, a facility determined to be non-compliant in 2010 would have to determine compliance again in 2012 based on the actual emission profiles and meteorological conditions for 2008, 2009, 2010 and 2011. The non-compliance determined in 2010 would have been based on the actual emission profiles and meteorological conditions from 2006, 2007, 2008 and 2009. For each of these years, the pertinent 1-hour, 3-hour, 8-hour, 24-hour and annual results would have to be presented. Since modelling for both 2010 and 2012 would have included 2008 and 2009, subject to a significant model upgrade, it would only be necessary to model

2010 and 2011 emissions in 2012, though compliance would be based on the results for the years 2008, 2009, 2010 and 2011.

The minimum requirement for the generation of the actual emission profile is daily production information. Where available, hourly production information is preferred.

2.3.2 ASSESSMENT MODELLING

All assessment modelling required by the Department, such as modelling required for an Environmental Impact Statement, or modelling undertaken for evaluating process changes or control equipment, shall be based on, as a minimum, the three most recent years of meteorological data.

2.4 RECEPTOR GRID

All receptors shall incorporate a rectangular Cartesian grid coupled with discrete receptors. The maximum spacing, on and off the administrative boundary, shall be:

- 50 metre spacing from the centre of the operation out to 500 metres;
- 100 metre spacing from 500 metres out to 1000 metres;
- 200 metre spacing from 1000 metres out to 2000 metres;
- 500 metre spacing beyond 2000 metres;
- 50 metre spacing within all residential areas located less than 1000 metres of the administrative boundary;
- 100 metre spacing within all residential areas located beyond 1000 metres of the administrative boundary, but located within 2000 metres of the administrative boundary;
- 200 metre spacing within all residential areas located beyond 2000 metres of the administrative boundary.

Discrete receptors are to be placed along the property's administrative boundary at 20 metre intervals or less.

Unless otherwise indicated by the Department, all model outcomes are to be determined based on a flagpole height of 0.0 metres, or ground-level at any given receptor.

The physical extent of the modeling domain shall be determined after consultation with the Department.

2.5 BUILDING DOWNWASH

Building downwash must be accounted for when it exists. As a general rule of thumb, if a building height is greater than 40% of the source emission height, then there is building downwash.

Building downwash variables shall be calculated for the Plume Rise Model Enhancements (PRIME) algorithm with the appropriate output variables serving as inputs. These variables are (variable name):

- direction specific building height (BUILDHGT);
- direction specific building width (BUILDWID);
- direction specific along flow building length (BUILDLEN);
- along flow distance from stack to centre of upwind face of projected building (XBADJ);
- across flow distance from stack to centre of upwind face of projected building (YBADJ).

The Building Projection Input Program (BPIP) has been traditionally used to determine the building wake effects. However, it has been demonstrated that in certain circumstances, particularly for complex structures, that BPIP may produce a result that is not entirely accurate for the structure being modelled. To account for this problem, the following step-wise approach is approved:

Step 1: Run BPIP treating the entire building complex as one building, using the coordinates of the perimeter. Building heights are irrelevant.

Step 2: Run BPIP with each unique building section defined as a separate building with its correct building dimensions, including height.

Step 3: Merge the BUILDWID, BUILDLEN, XBADJ and YBADJ values from step one with the BUILDHGT values from step two to generate the appropriate downwash parameterization.

All building downwash input must be approved by the Department prior to modelling to ensure it conforms to this approach.

2.6 PARTICULATE MATTER

When modelling for primary particulate matter, both the size of the particulate and its density must be accounted for. For size, the parameterization in Table 2.6.1 is preferred.

Table 2.6.1 – Particulate Sizing

Particle #	Geometric mass mean diameter (microns)	Geometric standard deviation (microns)	Particle size intervals (NINT)	Effective particle minimum (microns)	Effective particle maximum (microns)
P1	1.25	1.2418578	5	0.625	2.5
P2	5	1.2418578	5	2.5	10
P3	20	1.2418578	5	10	40

Under such parameterization, emission rates for $PM_{2.5}$, PM_{10} and TPM would be defined as follows:

$$PM_{2.5} = P1$$

$$PM_{10} = P1 + P2$$

$$TPM = P1 + P2 + P3$$

For particulate matter density, the latest version of CALPUFF is currently hard-coded for a density of 1 g/cm^3. In many instances, this may not be an issue, however, when modelling emissions of a heavier particulate such as iron which has a density of nearer 5 g/cm^3, the hard-coded density is not appropriate.

To overcome this issue, pseudo particulate parameterizations have to be established. This is done by retaining the geometric standard deviation but adjusting the geometric mass mean diameter to simulate how a particle would react if it had a density of 1 g/cm^3. Table 2.6.2 provides illustrative modifications to the input that would be required to model particles which have a density significantly different than 1 g/cm^3.

Table 2.6.2 – Particulate Density Adjustments

Particle #	Particle density (g/cm^3)	Geometric mass mean diameter (microns)	Geometric standard deviation (microns)	Particle size intervals (NINT)
P1	0.5	0.87	1.2418578	5
P1	1	1.25	1.2418578	5
P1	2	1.79	1.2418578	5
P1	3	2.20	1.2418578	5
P1	4	2.55	1.2418578	5
P1	5	2.86	1.2418578	5
P2	0.5	3.52	1.2418578	5
P2	1	5.00	1.2418578	5
P2	2	7.09	1.2418578	5
P2	3	8.70	1.2418578	5
P2	4	10.05	1.2418578	5
P2	5	11.25	1.2418578	5
P3	0.5	14.13	1.2418578	5
P3	1	20.00	1.2418578	5
P3	2	28.31	1.2418578	5
P3	3	34.68	1.2418578	5
P3	4	40.05	1.2418578	5
P3	5	44.79	1.2418578	5

3. GEOPHYSICAL PARAMETERS

3.1 LAND USE

The Canadian Forest Service's project entitled Earth Observation for Sustainable Development of Forests (EOSD) is to be used as the basis for all land use parameterization. For major industrial locations in the province, the Department has derived a land use dataset from EOSD to be compatible with the US Geological Survey Land Use and Land Cover Classification System, and it is this dataset that is to be used for compliance modelling. The datasets, with an approximate 25 metre resolution and containing up to 18 land use classifications, are input ready into the CTGPROC land use data processor of the CALPUFF modelling system and can be obtained from the Department upon request. Figure 3.1.1 indicates for the island of Newfoundland, the available land use datasets from the Department as of the date of this guidance document, while Figure 3.1.2 indicates the available land use datasets for Labrador. For other regions of the province which are currently not processed, the Department shall be contacted for appropriate guidance.

Figure 3.1.1 – Land Use Availability, Newfoundland

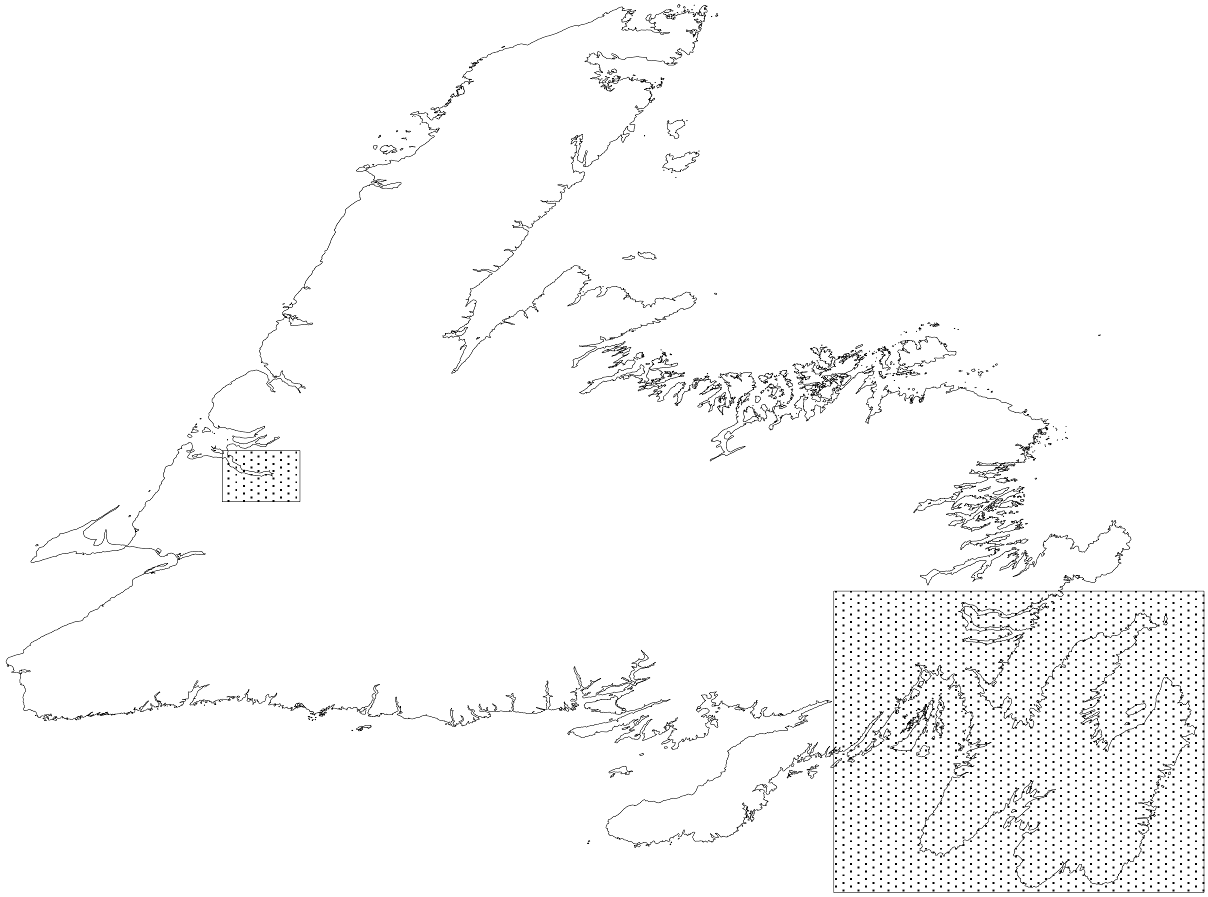
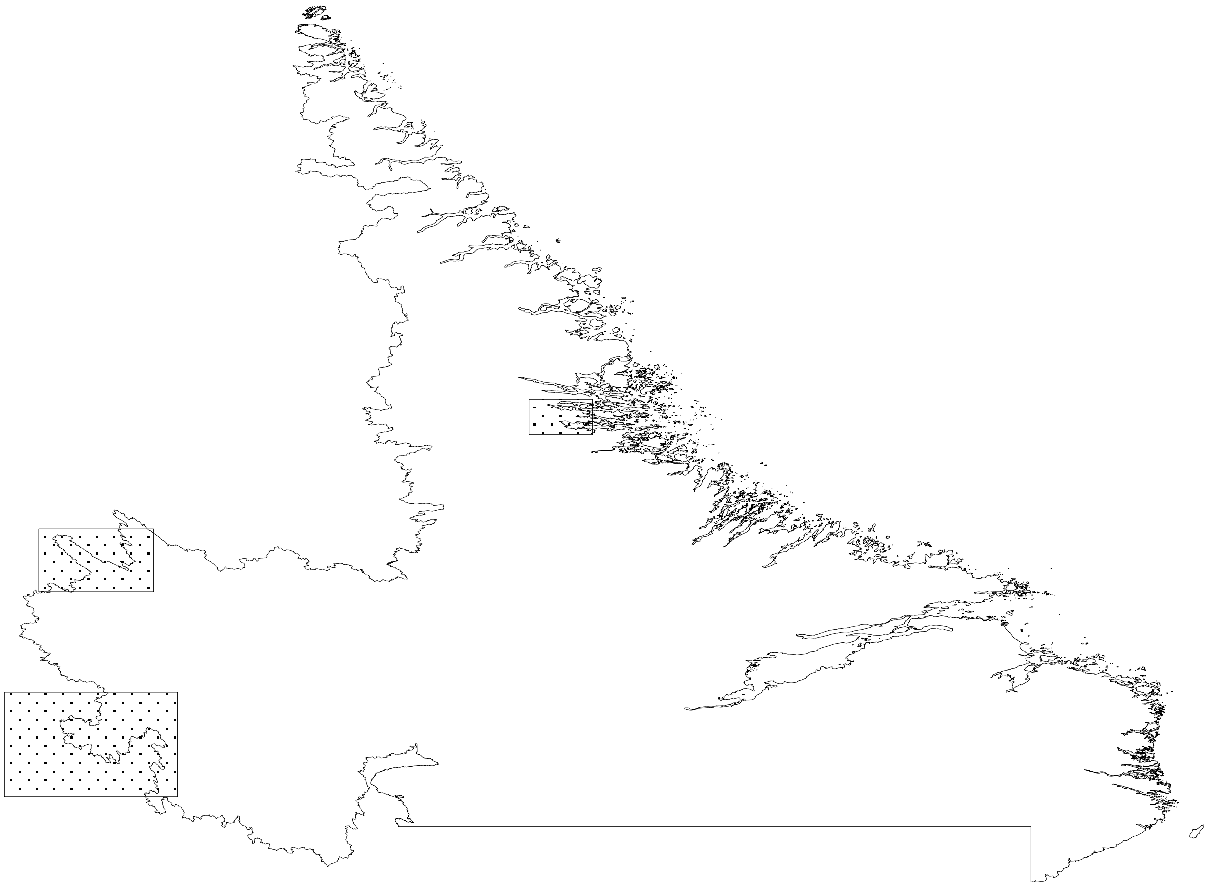


Figure 3.1.2 – Land Use Availability, Labrador



The land use classifications included in the datasets are listed in Table 3.1.1.

Table 3.1.1 – Land Use Classifications

11 – Residential	51 – Fresh Water
12 – Industrial / Commercial	55 – Salt Water
21 – Cropland and Pasture	61 – Forested Wetland
31 – Herbaceous Rangeland	62 – Non-forested Wetland
32 – Shrub and Brush Rangeland	74 – Bare Exposed Rock
33 – Mixed Rangeland	77 – Mixed Barren Land
41 – Deciduous Forest Land	81 – Shrub and Brush Tundra
42 – Evergreen Forest Land	82 – Herbaceous Tundra
43 – Mixed Forest Land	91 – Perennial Snow

Surface roughness, albedo, Bowen ratio, soil heat flux, anthropogenic heat flux, and leaf area index parameters are to be determined for each node of the meteorological grid and incorporate seasonality. Tables 3.1.2 to 3.1.4 define the acceptable values for each of these parameters, while Table 3.1.5 defines the timeframes for the various regions of the province where the seasonal parameterization will be applicable. By extension, Table 3.1.5 also implies that four GEO.DAT files will have to be generated for any given year. Where ambiguity may exist in determining which region a particular application may lie, the Department shall be contacted for appropriate guidance.

Table 3.1.2 – Land Use Parameterization – non-winter

Input Category ID	z0 (m)	Albedo (0 to 1)	Bowen Ratio	Soil Heat Flux Parameter	Anthropogenic Heat Flux (W/m^2)	Leaf Area Index	Output Category ID
11	0.5	0.18	1.0	0.20	0.0	1.0	10
12	1.0	0.18	1.5	0.25	0.0	0.2	10
21	0.25	0.15	1.0	0.15	0.0	3.0	20
31	0.05	0.25	1.0	0.15	0.0	0.5	30
32	0.05	0.25	1.0	0.15	0.0	0.5	30
33	0.05	0.25	1.0	0.15	0.0	0.5	30
41	1.0	0.1	1.0	0.15	0.0	7.0	40
42	1.0	0.1	1.0	0.15	0.0	7.0	40
43	1.0	0.1	1.0	0.15	0.0	7.0	40
51	0.001	0.1	0.0	1.00	0.0	0.0	51
55	0.001	0.1	0.0	1.00	0.0	0.0	55
61	1.0	0.1	0.5	0.25	0.0	2.0	61
62	0.2	0.1	0.1	0.25	0.0	1.0	62
74	0.05	0.3	1.0	0.15	0.0	0.05	70
77	0.05	0.3	1.0	0.15	0.0	0.05	70
81	0.2	0.3	0.5	0.15	0.0	0.0	80
82	0.2	0.3	0.5	0.15	0.0	0.0	80
91	0.05	0.7	0.5	0.15	0.0	0.0	90

Table 3.1.3 – Land Use Parameterization – winter without snow cover

Input Category ID	z0 (m)	Albedo (0 to 1)	Bowen Ratio	Soil Heat Flux Parameter	Anthropogenic Heat Flux (W/m^2)	Leaf Area Index	Output Category ID
11	0.5	0.18	1.0	0.20	0.0	1.0	10
12	1.0	0.18	1.5	0.25	0.0	0.2	10
21	0.02	0.18	0.7	0.15	0.0	3.0	20
31	0.01	0.20	1.0	0.15	0.0	0.5	30
32	0.01	0.20	1.0	0.15	0.0	0.5	30
33	0.01	0.20	1.0	0.15	0.0	0.5	30
41	0.6	0.17	1.0	0.15	0.0	7.0	40
42	1.3	0.12	0.8	0.15	0.0	7.0	40
43	0.95	0.14	0.9	0.15	0.0	7.0	40
51	0.001	0.10	0.0	1.00	0.0	0.0	51
55	0.001	0.10	0.0	1.00	0.0	0.0	55
61	0.6	0.14	0.3	0.25	0.0	2.0	61
62	0.2	0.14	0.1	0.25	0.0	1.0	62
74	0.05	0.20	1.5	0.15	0.0	0.05	70
77	0.05	0.20	1.5	0.15	0.0	0.05	70
81	0.1	0.20	1.0	0.15	0.0	0.0	80
82	0.1	0.20	1.0	0.15	0.0	0.0	80
91	0.002	0.70	0.5	0.15	0.0	0.0	90

Table 3.1.4 – Land Use Parameterization – winter with snow cover

Input Category ID	z0 (m)	Albedo (0 to 1)	Bowen Ratio	Soil Heat Flux Parameter	Anthropogenic Heat Flux (W/m^2)	Leaf Area Index	Output Category ID
11	0.5	0.45	0.5	0.15	0.0	1.0	10
12	1.0	0.35	0.5	0.15	0.0	0.2	10
21	0.01	0.7	0.5	0.15	0.0	0.0	20
31	0.005	0.7	0.5	0.15	0.0	0.5	30
32	0.005	0.7	0.5	0.15	0.0	0.5	30
33	0.005	0.7	0.5	0.15	0.0	0.5	30
41	0.5	0.5	0.5	0.15	0.0	0.0	40
42	1.3	0.35	0.5	0.15	0.0	7.0	40
43	0.9	0.42	0.5	0.15	0.0	3.5	40
51	0.001	0.7	0.5	0.15	0.0	0.0	51
55	0.001	0.7	0.5	0.15	0.0	0.0	55
61	0.5	0.3	0.5	0.15	0.0	0.0	61
62	0.2	0.6	0.5	0.15	0.0	0.0	62
74	0.002	0.7	0.5	0.15	0.0	0.0	70
77	0.002	0.7	0.5	0.15	0.0	0.0	70
81	0.005	0.7	0.5	0.15	0.0	0.0	80
82	0.005	0.7	0.5	0.15	0.0	0.0	80
91	0.05	0.7	0.5	0.15	0.0	0.0	90

Table 3.1.5 – Seasonal Land Use Timeframes

Geographic Area	Non-winter	Winter – without snow cover	Winter – with snow cover
Avalon Peninsula, Burin Peninsula and South Coast	May 16 to October 31	April 1 to May 15 & November 1 to December 31	January 1 to March 31
Central and Western Newfoundland	May 16 to October 31	April 16 to May 15 & November 1 to December 15	December 16 to April 15
Northern Peninsula and Southern Labrador	June 1 to October 15	May 1 to May 31 & October 16 to November 30	December 1 to April 30
Western and Central Labrador	June 1 to September 30	May 1 to May 31 & October 1 to October 31	November 1 to April 30
Northern and Coastal Labrador	June 16 to September 30	May 16 to June 15 & October 1 to October 31	November 1 to May 15

3.2 TERRAIN ELEVATION

Digital elevation data can take the form of digital surface data or digital terrain data. Digital surface data, such as Shuttle Radar Topography Mission (SRTM) or Advanced Spaceborne Thermal Emission and Reflection Radiometer (ASTER) are reflective datasets and as such indicate elevation including treetops / canopy heights and building heights when present. Digital terrain information, such as the Canadian Digital Elevation Data (CDED) is based on hypsographic and hydrographic data and is representative of the ground-level elevation. In situations where there is minimal ground cover, the digital surface and digital terrain data should be very consistent. However in forested or urbanized areas, large discrepancies can exist.

As noted in Section 3.1, land use parameterization is to be incorporated in all modelling applications. Given the land use parameterization defines surface roughness, albedo, etc. which effectively defines the canopy height of the domain, data elements from a digital terrain dataset are more appropriate than those from a digital surface dataset.

Thus for modeling purposes, terrain elevation data is to be taken from an approved digital elevation dataset, with a resolution equal to or better than the CDED dataset. CDED is approved for all modelling applications. The reference datum is to be WGS84.

4. MODELLING PROVISIONS

4.1 CALMET

4.1.1 PARAMETERIZATION

All parameters of the input file are to be set at default unless justification exists to the contrary or otherwise defined in the guidance document. In situations where the default parameters are not justified for modelling, the Department shall be contacted for guidance.

For all applications, precipitation rates are to be included for the generation of wet deposition as detailed in Section 4.2. Preferably, precipitation should be obtained from an on-site or nearby meteorological station, however, precipitation generated from a meteorological model is acceptable.

Where sea breezes are likely to affect the dispersion of a pollutant from a facility located in close proximity to the ocean, the effects must be considered. In this case, sea surface meteorological parameters must be extracted from a representative station or meteorological model. Though hourly is preferred, parameters recorded weekly or monthly may be acceptable.

4.1.2 MESOSCALE / PROGNOSTIC METEOROLOGICAL MODELS

It is recognized that CALMET can accept mesoscale meteorological model inputs such as those from the Rapid Refresh Model (RAP), the Weather Research and Forecasting Model (WRF) and the Mesoscale Model Interface Program (MMIF), and is the preferred approach for the generation of windfields in all modelling applications when supplemented with data measured from an on-site or nearby meteorological station. No differentiation is made herein for applying the mesoscale model outputs directly into CALMET or using the mesoscale model outputs to generate hourly upper air profiles, however, it is expected that the minimum resolution to be used will be equivalent to the highest resolution available. As of the date of this guidance document, the minimum acceptable resolution is 12 kilometres.

Research has also shown, however, that for coastal applications in particular, such an approach may introduce "mathematical" meteorological conditions, such as the generation of a shallow inversion layer, which may not have occurred in reality. It is therefore imperative that all mesoscale meteorological data be assessed against the on-site or nearby meteorological data to ensure consistency.

4.1.3 GENERIC CONDITIONS

For applications where the data from a mesoscale meteorological model is unavailable or inappropriate, the following specifications for CALMET are required:

(a) Meteorological data inputs shall consist of observations extracted from twice daily upper air soundings together with hourly surface data from an on-site meteorological station and/or nearest Environment Canada meteorological station. Data extracted from the twice daily upper air soundings shall extend to the 500 millibar (mb) level and shall incorporate all sounding levels (mandatory, significant, etc.), including the surface level and 500 mb level. Data to be extracted at each level includes, pressure, altitude, temperature, dew point temperature, wind direction and wind speed. The upper air soundings are to be taken from the most representative upper air station. Where a facility is approximately equidistant from 2 or more upper air stations, the choice of the upper air station will be dependent on the direction of the upper air stations from the facility, the terrain elevation of the facility, the terrain elevation of the upper air station, and the proximity of the facility and upper air station to large water bodies. Table 4.1.1 provides general guidance on choosing the appropriate upper station, however since CALMET can accommodate data from multiple upper air stations, it is advisable to incorporate data from all relevant stations.

Table 4.1.1

Location	Upper Air Station	Latitude / Longitude
Eastern Newfoundland	71801 – St. John's	47.61 N -52.75 W
Central and Western Newfoundland	71815 – Stephenville	48.56 N -58.56 W
Coastal and Central Labrador	71816 – Goose Bay	53.30 N -60.36 W
Western Labrador	71823 – La Grande IV	53.75 N -73.66 W
Alternate 1	71811 – Sept-Isle	50.21 N -66.25 W
Alternate 2	71906 – Kuujjuaq	58.11 N -68.41 W

(b) The meteorological grid shall be rectangular Cartesian, and shall be sufficiently large to encompass the entire modelling domain. Nodal spacing within the grid shall be a maximum of 500 metres, but where terrain varies significantly about the facility, a meteorological grid of a smaller spacing may be required. In the vertical, a minimum of 7 cell face heights are required, the heights of which are dependent on the nature of the facility being modelled and the surrounding terrain. The BIAS at each cell face height shall be determined only after consultation with the Department.

(c) Wind directions are to be randomized to 1^o or better.

(d) Where only one surface meteorological station exists in the meteorological grid, the LVARY variable, specifying the radius of influence of the meteorological data, shall be set to true. If more than one surface meteorological station exists, then appropriate values of RMAX1, RMAX2 and RMAX3 need to be defined based on the topography of the meteorological grid.

4.1.5 CALMET VERSION

Only results from the latest version of CALMET shall be acceptable. As of the date of this guidance document, the version was 6.334, level 110421. The Department shall be contacted prior to undertaking compliance or assessment modelling to confirm the latest acceptable version.

4.2 CALPUFF

4.2.1 PARAMETERIZATION

All parameters of the input file are to be set at default unless justification exists to the contrary or otherwise defined in this guidance document. In situations where the default parameters are not justified for modelling, the Department shall be contacted for guidance. Table 4.2.1 summarizes the required parameterizations for the modelling of all pollutants.

Table 4.2.1 – CALPUFF Coding Requirements

Parameter Name	Parameter Interpretation	Value Required	Value Interpretation
MBDW	Method used to simulate building downwash	2	PRIME method
MSHEAR *	Vertical wind shear modeled above stack top	0	no
MSPLIT	Puff splitting allowed	1	yes
MCHEM	Chemical mechanism	6	updated RIVAD scheme with ISORROPIA equilibrium
MAQCHEM	Aqueous phase transformation	1	transformation rates and wet scavenging coefficients adjusted for in-cloud aqueous phase reactions
MLWC	Liquid water content	0	water content estimated from cloud cover and presence of precipitation
MWET	Wet removal modeled	1	yes
MDRY	Dry deposition modeled	1	yes
MDISP	Method used to compute dispersion coefficients	2	Dispersion coefficients from internally calculated sigma v, sigma w using micrometeorological variables (u*, w*, L, etc.)
MPDF	PDF used for dispersion under convective conditions	1	yes
MREG	Test options specified to see if they conform to regulatory values	0	no checks are made
MOZ	Ozone data input option	0	use a monthly background ozone value
MNH3	Ammonia data option	0	use monthly background ammonia values (BCKNH3) - no vertical variation
MAVGNH3	Ammonia vertical averaging option	1	average NH3 values over vertical extent of puff
MH2O2	H2O2 data input option	0	use a monthly background H2O2 value

* It is noted that in the revision #1 of this guidance document, the MSHEAR was required to be turned on. Upon further evaluation, a coding error exists which leads to inaccurate results and is therefore not to be activated at this time.

4.2.2 BACKGROUND CONCENTRATIONS

The monthly background ozone concentrations (in ppb) for inclusion in the BCKO3 parameter have been derived for the province as a 5-year weighted average over all ozone monitoring stations. These concentrations are provided in Table 4.2.1 and are to be used in all applications. Table 4.2.1 also provides estimated monthly background concentrations for ammonia and hydrogen peroxide for inclusion in the BCKNH3 parameter and the BCKH2O2 parameter respectively.

Table 4.2.2 – Background Concentrations

Month	O_3 Concentration (ppb)	NH_3 Concentration (ppb)	H_2O_2 Concentration (ppb)
Parameter	BCKO3	BCKNH3	BCKH2O2
January	32	0.5	0.2
February	34	0.5	0.2
March	37	0.5	0.2
April	38	0.5	0.2
May	32	0.5	0.2
June	26	0.5	0.2
July	23	0.5	0.2
August	21	0.5	0.2
September	23	0.5	0.2
October	25	0.5	0.2
November	28	0.5	0.2
December	31	0.5	0.2

4.2.3 RIVAD / ISORROPIA

The RIVAD / ISORROPIA chemical transformation module, inclusive of wet and dry deposition, is to be invoked for both compliance and assessment modelling. In addition to the parameterization provided in Tables 4.2.1 and Table 4.2.2, Table 4.2.3 provides the sequencing for the six pollutants required to invoke the module in section 3a of the CALPUFF input file.

For wet deposition, both hourly precipitation rates and precipitation codes are required in CALMET. As wet deposition can be significant especially when considering SO_2 emissions, it is suggested that the IMBAL parameter be activated as a means to validate results.

Table 4.2.3 – RIVAD / ISORROPIA Pollutant Sequencing

Species	Modelled	Emitted	Dry Deposited
SO2	Yes	Yes	Computed gas
SO4	Yes	No	Computed particle
NO	Yes	Yes	Computed gas
NO2	Yes	Yes	Computed gas
HNO3	Yes	No	Computed gas
NO3	Yes	No	Computed particle

4.2.4 SOURCE EMISSION DATA

All source emission parameters shall be based on results taken from the stack testing conducted in accordance with Departmental guidance document *GD-PPD-016.1 Procedural Guide for Source Emission Testing* or its successor. If no stack parameters exist, then source inputs to the model shall be made only in consultation with the Department.

4.2.5 CALPUFF VERSION

Only results from the latest version of CALPUFF shall be acceptable. As of the date of this guidance document, the version was 6.42, level 110325. The Department shall be contacted prior to undertaking either compliance or assessment modelling to confirm the latest acceptable version.

4.3 CALPOST

4.3.1 PARAMETERIZATION

All parameters of the input file are to be set at default unless justification exists to the contrary or otherwise defined in this guidance document. In situations where the default parameters are not justified for modelling, the Department shall be contacted for guidance.

4.3.2 CALPOST VERSION

Only results from the latest version of CALPOST shall be acceptable. As of the date of this guidance document, the version was 6.292, level 110406. The Department shall be contacted prior to undertaking compliance or assessment modelling to confirm the latest acceptable version.

5. REPORTING

The modelling report shall be submitted to the Department within 120 days of acceptance of a source emission test as defined in a Certificate of Approval issued to the industry, or in accordance with Departmental guidance document *GD-PPD-009.3 Compliance Determination* or its successor. The modelling report shall include:

(a) isopleths for the pollutants listed in Section 2.1 over the time frames specified in Table 2.2.1 and where the maximum concentration exceeds half of the associated standard, superimposed on a map defining major roads, buildings, structures, landmarks. This means for any given year up to 17 isopleths may be required to be generated;

(b) a listing of model input parameters including a copy of the input and output files;

(c) a top-50 summary table for pollutants and timeframes identified in (a); and

(d) an accompanying discussion of the results.

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APPENDIX A

A. NO_X VS NO_2

A.1 NO_X FORMATION AND PRIMARY CONTROL

In a combustion process, NO_x is produced through 3 mechanisms, namely thermal NO_x, fuel NO_x and prompt NO_x.

Thermal NO_x is the primary source of NO_x and is formed as a high temperature dissociation and subsequent reaction of nitrogen (N_2) and oxygen (O_2). It is produced in the hottest part of the flame and its formation increases exponentially with the flame temperature. The control of thermal NO_x is generally achieved through reducing the flame temperature, reducing the residence time, or by operating under fuel rich conditions.

Fuel NO_x is formed by the reaction of nitrogen compounds chemically bound in liquid or solid fuels with oxygen in the combustion air. In the combustion of such fuels, fuel NO_x can account for up to 50% of the total NO_x emissions. As heavier fuels tend to have higher levels of bound nitrogen, whereas gaseous fuels have minimal bound nitrogen, the principal control of fuel NO_x is through conversion to light fuels or gaseous fuels.

Prompt NO_x is formed from the rapid reaction of atmospheric nitrogen with hydrocarbon radicals, and typically under partially fuel-rich conditions. It can be reduced through combustion staging or by operating under highly oxidizing combustion conditions.

A.2 NO_X FROM INDUSTRIAL SOURCES

The main industrial sources of NO_x emissions in Newfoundland and Labrador are from the burning of fossil fuels to either generate steam for assorted processes or to generate electricity.

In power boilers:

NO_x formation is primarily through thermal NO_x and fuel NO_x, with minimal prompt NO_x.

Thermal NO_x formation is dependent on peak temperature, and proportional to the nitrogen concentration in the flame, the oxygen concentration in the flame, and the residence time. Increases in flame temperature, oxygen availability, and/or residence time at high temperatures leads to an increase in NO_x production. It is the dominant NO_x forming mechanism in units firing distillate oils primarily because of the negligible nitrogen content in these fuels.

Fuel nitrogen conversion is the more important NO_x forming mechanism in residual oil boilers. The percent conversion of fuel nitrogen to NO_x varies, however, typically from 20 to 90 percent of nitrogen in oil is converted to NO_x.

In gas turbines:

NO_x formation occurs by all three mechanisms.

Thermal NO_x, arises from the thermal dissociation and subsequent reaction of nitrogen and oxygen molecules in the combustion air. Most thermal NO_x is formed in high temperature stoichiometric flame pockets downstream of the fuel injectors where combustion air has mixed sufficiently with the fuel to produce the peak temperature fuel / air interface.

Prompt NO_x is formed from early reactions of nitrogen molecules in the combustion air and hydrocarbon radicals from the fuel. It is formed within the flame and is usually negligible when compared to the amount of thermal NO_x formed.

Fuel NO_x stems from the evolution and reaction of fuel-bound nitrogen compounds with oxygen. Fuel NO_x from distillate oil-fired turbines may become significant in turbines equipped with a high degree of thermal NO_x controls.

The maximum thermal NO_x formation occurs at a slightly fuel-lean mixture because of excess oxygen available for reaction. The control of stoichiometry is critical in achieving reductions in thermal NO_x. Thermal NO_x formation also decreases rapidly as the temperature drops below the adiabatic flame temperature for a given stoichiometry. Maximum reduction of thermal NO_x can be achieved by control of both the combustion temperature and the stoichiometry. Gas turbines operate with high overall levels of excess air because they use combustion air dilution as the means to maintain the turbine inlet temperature below design limits. In older gas turbines, where combustion is in the form of a diffusion flame, most of the dilution occurs downstream of the primary flame, which does not minimize peak temperature in the flame and suppress NO_x formation.

In internal combustion engines:

NO_x formation occurs primarily as thermal NO_x which arises from the thermal dissociation and subsequent reaction of nitrogen and oxygen molecules in the combustion air. Most thermal NO_x is formed in the high-temperature region of the flame from dissociated molecular nitrogen in the combustion air. Some prompt NO_x is formed in the early part of the flame from reaction of nitrogen intermediary species, and hydrocarbon radicals in the flame. Fuel NO_x is virtually non-existent.

A.3 BASIC NO_X CHEMISTRY IN THE ATMOSPHERE

In its simplest form, the basic NO_x chemistry can be considered a cycle of continual reactions.

NO_x emissions from a source are typically considered to be a combination of NO and NO_2. As the exhaust leaves the stack and mixes with the ambient air, the NO reacts with ambient ozone (O_3) to form NO_2 and O_2. In the presence of ultraviolet radiation from the sun, NO_2 gets broken down into NO and O. O and O_2 react with a third molecule (M) such as O_2 or N_2 to form O_3 and the third molecule.

$$NO + O_3 \rightarrow NO_2 + O_2$$

$$NO_2 + \mu v \rightarrow NO + O$$

$$O + O_2 + M \rightarrow O_3 + M$$

In the presence, of hydrocarbons (HCs), NO may also react to also form NO_2 via the following reaction:

$$NO + HC \rightarrow NO_2 + HC'$$

A.4 NO_2

NO_2 is the primary component of concern in NO_x. NO_2 is a reddish brown gas with a pungent odour, which upon reaction with other atmospheric compounds, becomes a major contributor to smog, acid rain, inhalable particulates and reduced visibility. At significant levels and exposure, inhalation may result in irritation and burning to the skin and eyes, nose and throat. Prolonged exposure may result in permanent lung damage.

A.5 DISPERSION MODELLING INTERPRETATION

The assumption historically has been that all of the NO_x being emitted from a source has been in the form of NO_2. Research, however, has indicated that this approach is conservative and that in reality only a relatively small fraction of the total NO_x emissions are in the form of NO_2. Further NO_2 will be produced however, based on the above noted reactions once the NO_x plume leaves the stack, the extent to which is largely dependent on the level of O_3 in the atmosphere. Consequently when a source was being modelled for compliance with the *Air Pollution Control Regulations, 2004*, results may have shown non-compliance when in actuality there may have been compliance.

The other major contributing factor to the determination of the concentration of NO_2 is the lack of actual in-stack emission data which speciates NO_x into NO_2 and NO. Both stack sampling programs and combustion equipment manufacturers cite emissions as total NO_x, not NO_2 or NO. Consequently there is only a small volume of information readily available to draw upon to determine the baseline emission rates and subsequent atmospheric emission rates.

A.6 GUIDANCE

For all CALPUFF compliance and assessment applications, the RIVAD / ISORROPIA chemistry is the approved method, subject to the terms and conditions provided in Section 4.2 of this guidance document. For all AERMOD and AERSCREEN applications, the Plume Volume Molar Ratio Method (PVMRM) is the preferred approach to evaluate NO_2 emissions.

All facilities will be required to measure the in-stack ratio of NO_2 / NO_x for combustion sources which meet the requirements of guidance document *GD-PPD-009.3 Compliance Determination* or its successor. Where in-stack emissions of NO and NO_2 are not available, the acceptable in-stack ratios for modelling purposes are listed in Table A.1.

All in-stack data shall be obtained using methods acceptable to the Department in accordance with guidance document *GD-PPD-016.1 Procedural Guide for Source Emission Testing* or its successor.

Table A.1

Emission Source	In-stack NO_2 / NO_x ratio
Power Boilers	0.1
Compressors and Gas Turbines	0.6
Diesel Power Generating Units	0.2