APPENDIX D

CALPUFF Dispersion Model

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1.0 MODEL REQUIREMENTS

For the area of concern for the Project, the following model attributes are required:

1) Ability to handle multiple emissions sources of varying geometry, (point, area, line volume), located in the study area;
2) Ability to handle both flat and elevated terrain features;
3) Ability to convert SO_2 to sulphate (SO_4^{2-}), and NO_x to nitrate (NO_3^-); and
4) Ability to simulate boundary layer mechanics and dispersion in coastal areas.

In accordance with recent assessments of proposed projects in BC, for example the BC Hydro Vancouver Island Generation Project at Duke Point, and in consultation with regulatory agencies, CALPUFF was chosen as the model with which to perform air quality modelling in the Local Study Area (LSA). CALPUFF contains the attributes outlined above and, when applied in full 3-D CALMET mode, it has the ability to assimilate multiple meteorological stations and to simulate the changes in mixing height and boundary layer mechanics that result from the variable land use and terrain in the study region.

Due to the expected changes in traffic patterns resulting from the project, the California Line source model (CALINE) was suggested for modelling roadway emissions in the study area. Although CALINE was developed expressly for this purpose, it is an older generation, Gaussian plume model and has several limitations:

1) It is a plume rather than a puff model. Unlike CALPUFF it can not account for changes in plume trajectory and boundary layer properties once emissions have travelled away from the source. Also, CALINE does not account for causality, i.e. it does not track plumes over several consecutive hours.

2) It is driven by point meteorology. Though point source meteorology can be extracted from CALMET outputs, by and large CALINE cannot make full use of the CALMET meteorological fields.

3) CALINE can only simulate dispersion of primary pollutants. It has no mechanisms for chemical transformation, such as the formation of secondary particulate.

4) It cannot include temporal variation of emission rates.

5) It does not accept area sources and therefore the cumulative contribution of other sources cannot easily be derived.

Due to these limitations, CALINE was not selected for this study.

As described below, road and rail emissions were incorporated into CALPUFF in a manner that should provide at least as much information about road emissions impacts as would have been obtained using CALINE. In addition, CALPUFF does not share the limitations described above. A comparison of CALINE and CALPUFF for line segments is given in Appendix E.

CALPUFF has two major options with respect to the meteorology used to drive the dispersion calculations:

- The **ISC mode** assumes a uniform meteorological field over the modelling domain during a given hour. While this is consistent with the ISC-PRIME and AERMOD models, CALPUFF has the advantage of allowing the plume trajectory to vary from hour-to-hour in a systematic manner.
- The **CALMET mode** allows for the use of a three-dimensional meteorological field over the modelling domain during a given hour.

For this assessment, the CALPUFF model was applied using the CALMET mode option. The methods employed in the development of the CALMET meteorological fields are described in Appendix C.

1.1 CALPUFF MODEL DESCRIPTION

CALPUFF (Scire *et al.,* 2000) is a multi-layer, multi-species, non-steady-state puff dispersion model. It simulates the effects of time- and space-varying meteorological conditions on pollutant transport, transformation and deposition. CALPUFF can use three-dimensional meteorological fields developed by the CALMET model, or simple, single-station winds in a format consistent with the meteorological files used to drive the ISCST3 steady-state Gaussian model. However,

single-station ISCST3 winds do not allow CALPUFF to take advantage of its capabilities to treat spatially varying meteorological fields.

CALPUFF contains algorithms for near-source effects such as building downwash, transitional plume rise, partial plume penetration, sub-grid scale terrain interactions as well as longer-range effects such as pollutant removal (wet scavenging and dry deposition), chemical transformation, vertical wind shear, over-water transport, and coastal interaction effects. It can accommodate arbitrarily varying point source and gridded area source emissions. Most of the algorithms contain options to treat the physical processes at different levels of detail depending on the model application.

The major features and options of the CALPUFF model are summarized in Table D-1. Some of the technical algorithms of relevance include:

- **Chemical Transformation**: CALPUFF includes options to parameterize chemical transformation using the five species scheme (SO_2, SO_4^{2-}, NO_X, HNO_3, and NO_3^-) employed in the MESOPUFF II model, a modified six-species scheme (SO_2, SO_4^{2-}, NO, NO_2, HNO_3, and NO_3^-) adapted from the RIVAD/ARM3 method, or a set of user-specified, diurnally-varying transformation rates.

- **Dispersion Coefficients**: Several options are provided in CALPUFF for the computation of dispersion coefficients: the use of turbulence measurements (σ_v and σ_w), similarity theory to estimate σ_v and σ_w from modelled surface heat and momentum fluxes, Pasquill-Gifford (PG) or McElroy-Pooler (MP) dispersion coefficients, or dispersion equations based on the Complex Terrain Dispersion Model (CDTM). Options are provided to apply an averaging time correction or surface roughness length adjustments to the PG coefficients.

- **Thermal Internal Boundary Layer (TIBL)**: For areas with transitions between water and land, the model has the ability to simulate the growth of a thermal internal boundary layer as the modelled air mass passes over the water/land interface.

- **Post Run Speciation**: By using some of the post-processing options, the user can re-group model species into derived secondary species. For example, an estimate of secondary fine particulate can be derived by adding the SO_4^{2-} and NO_3^- species output by the MESOPUFF/RIVAD chemical schemes.

Table D-1: Major Features of the CALPUFF Model (continued on next page)

Source Types	Point sources (constant or variable emissions) Line sources (constant or variable emissions) Volume sources (constant or variable emissions) Area sources (constant or variable emissions)
Non-steady-state emissions and meteorological conditions	Gridded 3-D fields of meteorological variables (wind speed and direction, temperature) Spatially-variable fields of mixing height, friction velocity scale, Monin-Obukhov length, precipitation rate Vertically and horizontally-varying turbulence and dispersion rates Time-dependant source and emissions data
Efficient sampling functions	Integrated puff formulation Elongated puff (slug) formulation
Dispersion coefficient (σ_y, σ_z) options	Direct measurements of σ_v and σ_w Estimated values of σ_v and σ_w based on similarity theory PG dispersion coefficients (rural areas) MP dispersion coefficients (urban areas) CTDM dispersion coefficients (neutral/stable) PDF formulation for the convective boundary layer
Vertical wind shear	Puff splitting Differential advection and dispersion
Plume rise	Partial penetration Buoyant and momentum rise Stack tip effects Vertical wind shear Building downwash effects
Building downwash	Huber-Snyder method Schulman-Scire method

Table D-1: Major Features of the CALPUFF Model (concluded)

Sub-grid scale complex terrain	CTDM flow module Dividing streamline, H_d - Above H_d puff flows over the hill and experiences altered diffusion rates - Below H_d puff deflects around the hill, splits, and wraps around the hill
Interface to the Emissions Production Model (EPM)	Time-varying heat flux and emissions from controlled burns and wildfires
Dry Deposition	Gases and particulate matter Three options: - Full treatment of space and time variations of deposition with a resistance model - User-specified diurnal cycles for each pollutant - No dry deposition
Over water and coastal interaction effects	Over-water boundary layer parameters Abrupt change in meteorological conditions, plume dispersion at coastal boundary Plume fumigation Option to introduce sub-grid scale Thermal Internal Boundary Layers (TIBL's) into coastal grid cells
Chemical transformation options	Pseudo-first-order chemical mechanism for SO_2, SO_4^{2-}, NO_X, HNO_3, and NO_3^- (MESOPUFF II method) Pseudo-first-order chemical mechanism for SO_2, SO_4^{2-}, NO, NO_2, HNO_3, and NO_3^- (RIVAD/ARM3 method) User-specified diurnal cycles of transformation rates No chemical conversion
Wet removal	Scavenging coefficient approach Removal rate a function of precipitation intensity and precipitation type
Graphical User Interface	Point-and-click set-up and data input Enhanced error checking of model inputs On-line help files

2.0 MODEL APPLICATION

2.1 MODEL DOMAIN

The CALPUFF model domain was chosen to coincide with the CALMET model boundaries. The coordinates of the domain vertexes are given in Table D-2. The extent of the model domain is shown in Figure D-1.

Table D-2: Model Domain (All Coordinates are for UTM Zone 10)

DOMAIN VERTEX	UTM EASTING (KM)	UTM NORTHING (KM)
Southwest	478	5419
Northwest	478	5449
Southeast	508	5419
Northeast	508	5449

2.2 RECEPTOR LOCATIONS

Two types of receptors within the modelling domain were selected:

- A series of nested Cartesian grid points, and
- Specific receptors for the human health risk assessment.

Figure D-1 shows the nested Cartesian receptor grids used for the modelling. The grid spacing is as follows:

- 100 m for a 2 by 2 km area centred on the Roberts Bank project;
- 200 m for an area from 2 km to the north and west of the project to approximately 1 km inland;
- 500 m for areas over land up to approximately 15 km north and east of the Project; and
- 1 km for the rest of the domain and for areas over open water.

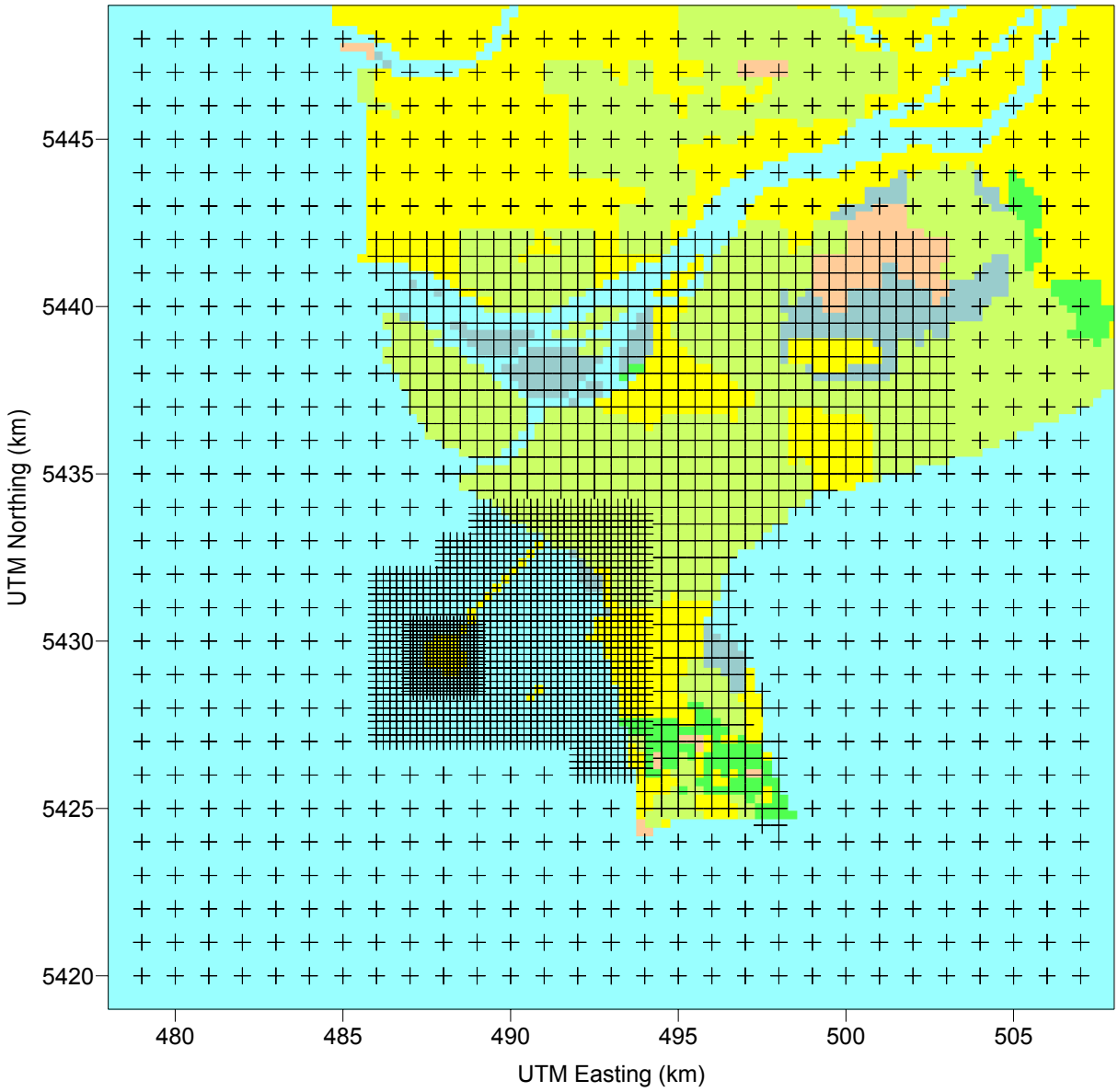

Figure D-1: Location of receptors used for the CALPUFF dispersion model. Crosses indicate Cartesian grid points.

To avoid including receptors that are within the right-of-way of road and rail sources, receptors that were located within 100 m of a road or railway were excluded from the analysis. This also corresponds roughly to the distance at which CALPUFF predictions match those from CALINE (see Appendix E).

Table D-3 and Figure D-2 indicate the locations of community and recreation receptors near the Roberts Bank facility that were used for the human health and ecological risk assessments. The table also provides the coordinates of the receptors.

Table D-3: Specific Receptors for the Human Health and Ecological Risk Assessments

ID	RECEPTOR DESCRIPTION	RISK ASSESSMENT	UTM (KM E)	UTM (KM N)	ELEVATION (M ASL)
R1	Steveston	Human Health	486.500	5441.700	3.0
R2	Ladner	Human Health	493.850	5436.550	0.0
R3	Farmer 1	Human Health	491.150	5434.600	2.8
R4	Tsawwassen First Nations	Human Health	492.500	5432.500	3.5
R5	Farmer 2	Human Health	492.050	5433.100	3.3
R6	Farmer 3	Human Health	489.800	5434.050	2.0
R7	Tsawwassen Beach Campsite	Human Health	493.250	5431.050	2.8
R8	Beach Grove	Human Health	495.800	5431.350	5.0
R9	Boundary Bay	Human Health	497.100	5427.950	4.0
R10	Tsawwassen	Human Health	493.575	5429.350	55.7
R11	Point Roberts 1	Human Health	497.125	5426.100	62.0
R12	Point Roberts 2	Human Health	493.875	5427.600	52.0
R13	Reifel Bird Sanctuary	Ecological	486.900	5438.150	0.0
R14	Boundary Bay GVRD Park	Ecological	496.350	5429.850	4.3
R15	English Bluffs Beach	Ecological	492.760	5429.900	0.0
R16	South Arm Marsh	Ecological	490.810	5437.300	0.8

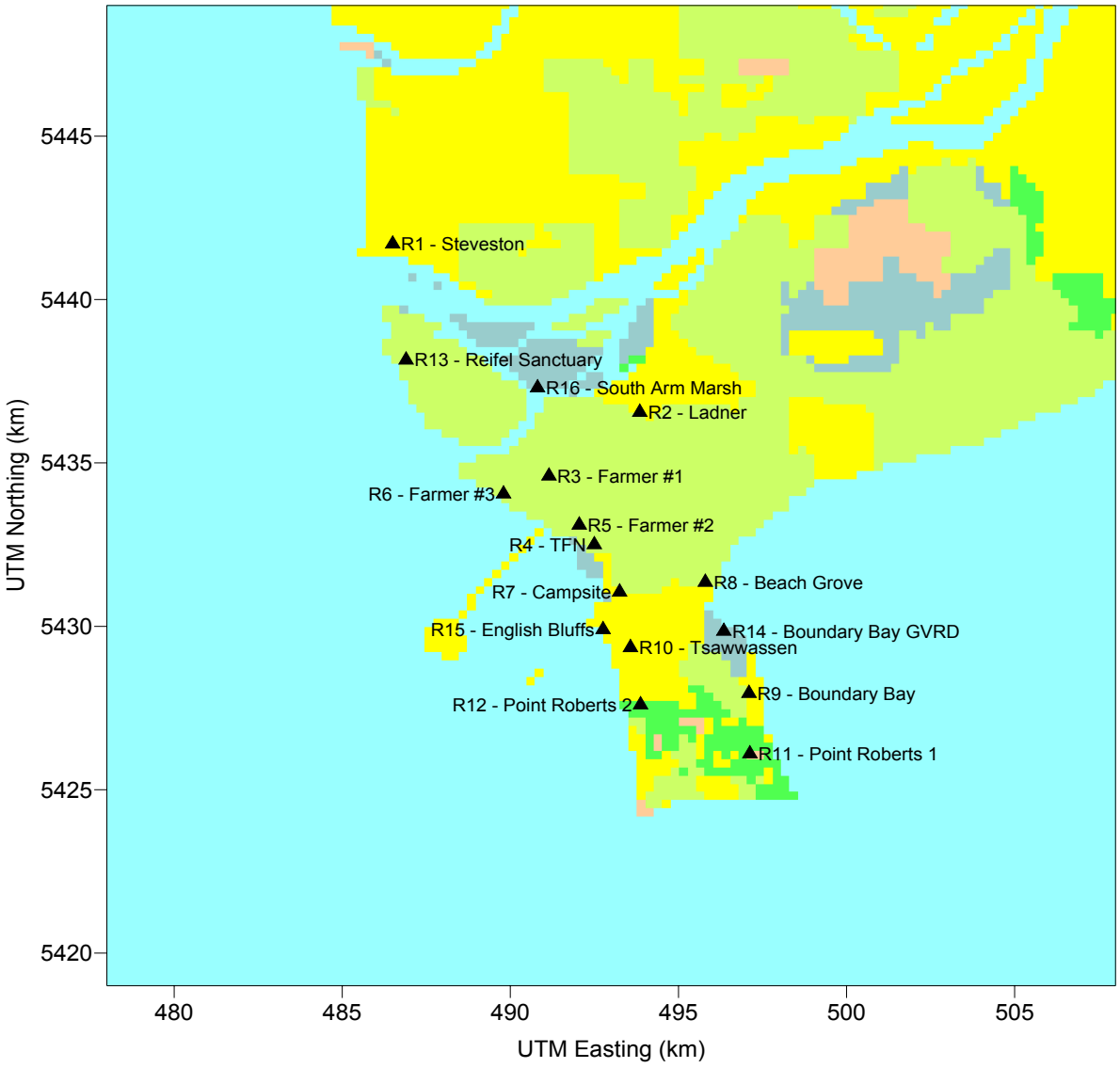

Figure D-2: Location of Specific Receptors for the Human Health and Ecological Risk Assessments

2.3 COMPOUNDS MODELLED

There were 11 compounds included in the model runs. The following 10 compounds were modelled for both the gridded receptors and the specific receptors for the human health and ecological risk assessments:

SO_2, SO_4^{2-}, NO_x , NO^-_3, HNO_3, $PM_{2.5}$, PM_{10}, TSP, VOCs and CO.

For the receptor grid runs, non-reactive inert NO_x (i.e., emitted at the same rate as NO_x but not included in the chemical transformations) was included as an 11th compound. For the human health assessment, Diesel PM ($PM_{2.5}$ resulting from combustion of diesel fuels only) was included as the 11th compound.

For all sources, the emissions rates of SO_4^{2-}, NO^-_3 and HNO_3 were set to zero. Predicted concentrations of these compound are purely the result of secondary chemical reactions.

2.4 MESOPUFF CHEMISTRY

The MESOPUFF II chemistry option was used to calculate concentrations of secondary nitrate and sulphate. This option is the US EPA regulatory default. Hourly observed ozone concentrations from GVRD station T17 were used to supply the background ozone concentration required by the MESOPUFF II scheme. The model also requires background concentrations of ammonium. A wide range of ammonium concentrations have been measured in the Lower Fraser Valley. As part of a field campaign in July and August 1993, ammonium concentrations ranging from 0 to 4 $\mu g/m^3$ were observed at three sites: Chilliwack, Clearbrook and Pitt Meadows (Barthelmie and Pryor, 1998). Ammonium concentrations were also measured at two sites in the eastern past of the Lower Fraser Valley, an area known for its high ammonia emissions from agricultural sources, from February 1996 to March 1997 (Belzer et al., 1997). Ammonia concentrations ranged from about 8 to 30 $\mu g/m^3$ at the Abbotsford site, and from about 2 to 10 $\mu g/m^3$ at the Agassiz site. The CALPUFF default background ammonium concentration of 10 ppb (7 $\mu g/m^3$) is bracketed by these historical observations and was used for this project.

2.5 POINT SOURCE PARAMETERS

Ships at dockside were modelled as point sources. These sources include ships loading coal at Westshore Terminals, BC Ferries loading and unloading at the Tsawwassen terminal, and container ships calling at the Deltaport Terminal. In reality, emissions parameters such as stack height, stack diameter, exit temperature, exit velocity and actual emission rate will vary somewhat from ship to ship. For modelling purposes a 'typical' stack was chosen to represent all ships at a given port. These parameters were based on previous studies done for the Roberts Bank Port (Jacques Whitford, 2002; Hrebenyk, 2004). The parameters used are consistent with recommendations found in similar studies described elsewhere (Cooper, 2003). The point source parameters used for the project are given below in Table D-4.

Table D-4: Point Source Paramters for Dockside Emissions

POINT SOURCE PARAMETER	VALUE USED IN MODELLING
Stack Height	36.5 m
Stack Diameter	1.5 m
Exit Velocity	5.0 m/s
Exit Temperture	373 °K
Emission Rate	Varies by individual source

2.6 AREA SOURCE PARAMETERS

Other than for ships at dockside and linear sources such as road and rail, the emission inventory consists mainly of annual emissions estimates over broad areas (e.g., annual emissions due to shipping traffic and the lanes in which ships operate; annual emissions due to trucks operating in the shipyard; total emissions from tugs working the Roberts Bank Port). These types of emissions are very difficult to define as individual sources, particularly individual point sources.

Even where the emissions are from a point source, such as the stack of a ship or ferry at sea, the location of the source varies too quickly to be defined on an hour-by-hour basis. All such emissions were treated as area sources.

Area source parameters were chosen so that the initial vertical plume sigma was the same as the assumed average emission height above ground. This effectively gives the plume an initial width of twice the emission source height. The emission source height was chosen to roughly represent the average height of emissions for that category. Typical area source emissions parameters are provided in Table D-5.

Table D-5: Typical Area Source Emissions Parameters

SOURCE TYPE	RELEASE HEIGHT (m)	INITIAL PLUME SIGMA (m)	INITIAL VERTICAL VELOCITY (m/s)
Shipping Lanes	10	10	0
Tugs	10	10	0
Dockyard	2	2	0

Fugitive coal dust emissions are dependent on ambient wind speed and vary arbitrarily by hour. Fugitive dust was estimated hour-by-hour (see Appendix A) and then incorporated through use of the option for an external BAEMARB.DAT file for arbitrarily varying buoyant area emissions. This file is mostly used for buoyant emission sources such as forest fires. To limit the buoyancy in this case, the vertical velocity was set to zero and the temperature of the emissions was set by extracting the ambient temperature for the location of the coal piles from the CALMET output meteorological fields.

2.7 LINE SOURCES (ROADS AND RAIL)

The emissions inventory included baseline and predicted changes to railway and road traffic due to the Project. The modelling incorporated predicted incremental changes in road and rail traffic due to Project operation only; i.e. emissions due to existing or projected background traffic were

not included in the modelling as they were accounted for by adding the 98th percentile ambient observed values. Rail and roadway emissions were implemented in CALPUFF as line sources. CALPUFF uses the Buoyant Line Source Algorithm (Scire, 2000). The model developers intended for this algorithm to be used for elongated buoyant line sources (such as building roof vents) and recommend using area or volume sources to model road sources.

However, CALPUFF uses the ISC2 area source algorithm (Scire, 2000). Model guidance for use of this algorithm dictates that the ratio of length to width for rectangular area sources should not exceed 10:1. There are over 80 km of road and railway included in each scenario. Even assuming a rather wide average source width of 50 m would result in upwards of 160 area sources in addition to those from non-road and rail emissions. Area sources are very computationally expensive and this many sources would make model run times untenable.

Although the line source algorithm used in CALPUFF was not designed for modelling road sources, by selecting parameters to limit the buoyancy of the line source plume, the algorithm can be made to approximate results obtained from using line sources in ISC or AERMOD (Radonjic et al, 2003).

Use of line sources reduces the total number of separate road and rail segments to a maximum of 35. In addition, each individual line source is not as computationally intensive as a corresponding area source. Although each line source still releases a very large number of puffs at each hour and the CALPUFF simulation requires very significant computer resources, the resulting run time is about an order of magnitude less than would be required for modelling using area sources.

A comparison of resulting predicted concentrations from road emissions using CALPPUFF line sources versus the same sources in CALINE is provided in Appendix E. In general, CALPUFF was found to predict higher concentrations compared to CALINE for locations within approximately 200 m of the source centerline. For locations at 500 m from the source centerline and beyond, CALPUFF and CALINE provided similar results.

Line source parameters for input to CALPUFF were adjusted to mimic a non-buoyant plume. Also line sources were entered so as to avoid invoking calculations in the BLP algorithm for parameters such as building height and distance between line sources. This was done by defining each individual line segment as its own source group containing just the one line segment, and incorporating all line sources through use of the external LNEMARB.DAT emissions file. This required recompiling CALPUFF to allow for more line source groups than the default configuration. This change in array size only affects the number of sources that may be included and does not affect any of the actual plume dispersion calculations.

2.8 TECHNICAL DISPERSION OPTIONS

In the absence of regulatory guidance to the contrary, all technical options relating to the CALPUFF dispersion calculation were set to the model defaults. These include parameters and options such as the calculation of plume dispersion coefficients, the plume path coefficients used for terrain adjustments, exponents for the wind speed profile, and wind speed categories. These options are listed in their entirety in Tables D-8 through D-15.

2.9 BUILDING EFFECTS

All sources in the models were entered as area or line sources. No building downwash information was required.

2.10 WET AND DRY DEPOSITION

Wet and dry deposition was not modelled for this assessment. As a result, with no removal processes, predicted concentrations, most notably of particulate, are conservative in nature.

3.0 MODEL OUTPUT INTERPRETATION

3.1 SECONDARY PARTICULATE

In addition to the compounds explicitly included in the model, secondary particulate species were derived from the outputs of secondary SO_4^{2-} and NO_3^-. To calculate the mass of secondary particulate matter, it was conservatively assumed that the sulphate and nitrate ions would combine with ambient ammonium ions (NH_4^+) to form $(NH_4)_2SO_4$ and $(NH_4)NO_3$. It was further assumed that the resulting $(NH_4)_2SO_4$ and $(NH_4)NO_3$ particles would be less than 2.5 microns in diameter and thus would add to the predicted primary $PM_{2.5}$ concentrations.

The calculated secondary $PM_{2.5}$ concentrations were then added to each of the primary $PM_{2.5}$, PM_{10} and TSP concentrations to estimate totals of primary plus secondary particulate (denoted $PM_{2.5}$sec, PM_{10}sec and TSPsec, respectively) for each of the three particulate size classes.

3.2 NO_X TO NO_2 CHEMISTRY

For this assessment, NO_2 concentrations were estimated from the predicted total NO_x concentrations using the ambient ratio method. The ambient ratio method relies on obtaining an estimate of the NO_2/NO_x ratio based on representative ambient observations. Ambient air quality data from GVRD station T17 (Richmond South) were used to calculate the NO_2/NO_x ratios. The resulting ratios were validated against ambient observations from GVRD stations T2 (Kitsilano) and T31 (Vancouver Airport).

For each averaging period (1-hour, 24-hour and annual), curves were fit to the upper-envelope of observed NO_2/NO_x versus NO_x. The resulting relationships are depicted in Figure D-3, D-4 and D-5 for the one-hour, 24-hour and annual average concentrations. The curve on each plot is an exponential of the form $y = ax^b$, where a and b are empirically determined parameters. The equation given for each averaging period is used to determine the ratio of NO_2/NO_x for a predicted NO_x concentration, subject to the conditions that: 1) The calculated NO_2/NO_x ratio may never exceed unity, and 2) the calculated NO_2/NO_x ratio may never be less than 0.10.

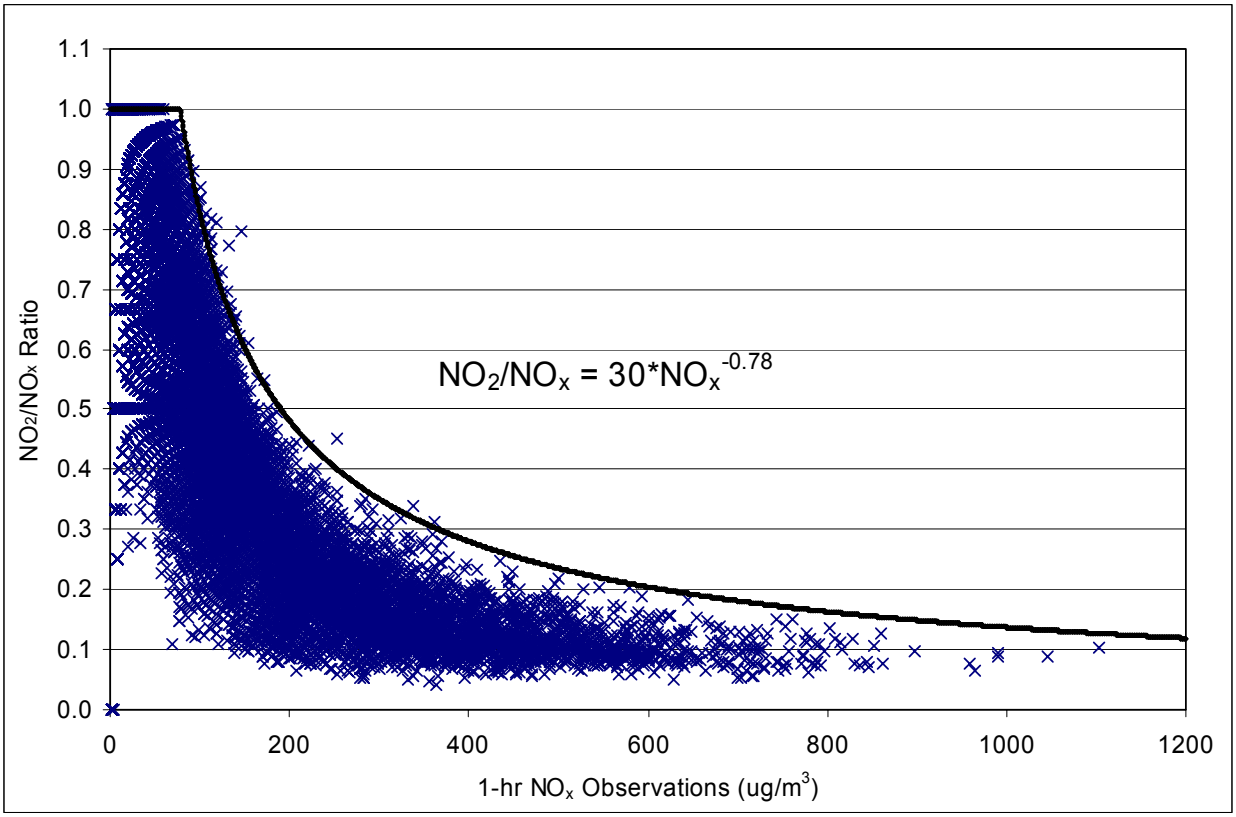

Figure D-3: Dependence of NO_2/NO_x Ratio on 1-hour Average NO_x Concentrations from GVRD Station T17 (Richmond South)

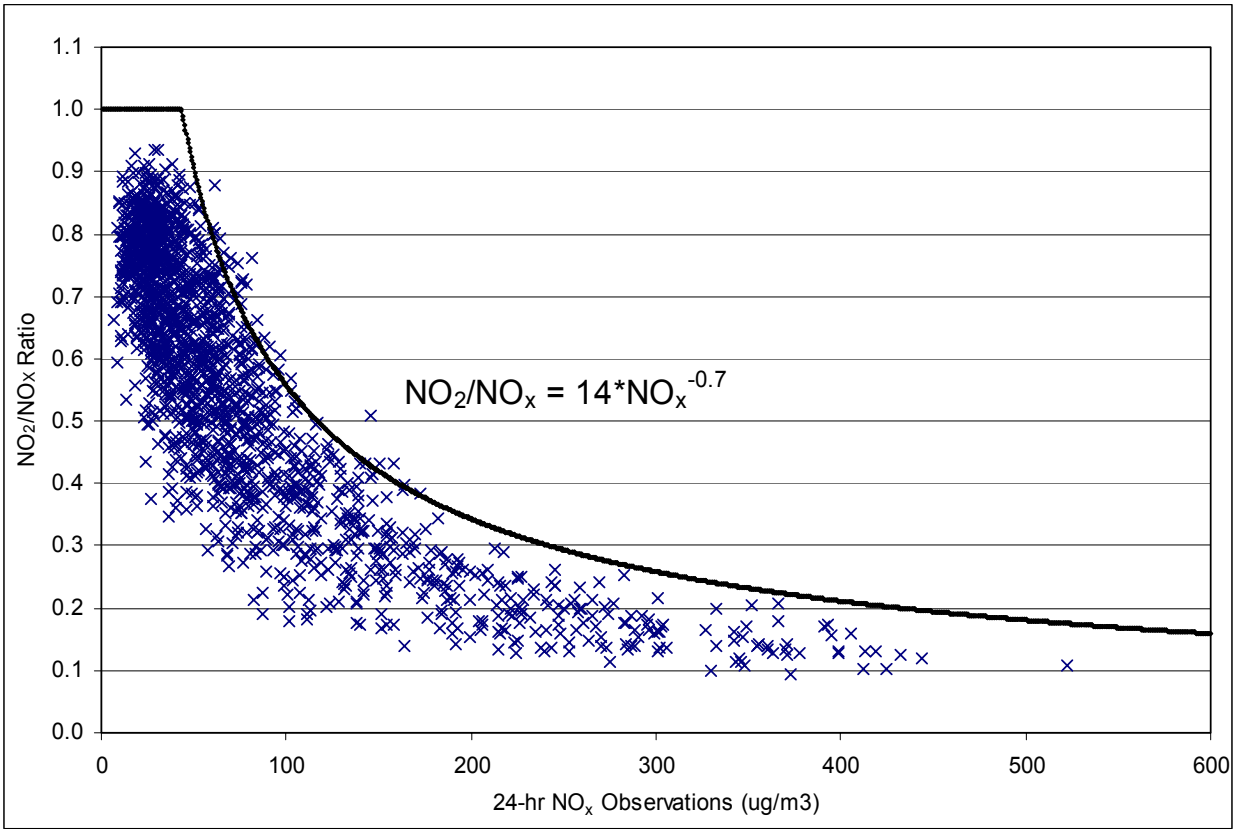

Figure D-4: Dependence of NO_2/NO_x Ratio on 24-hour Average NO_x Observations from GVRD Station T17 (Richmond South)

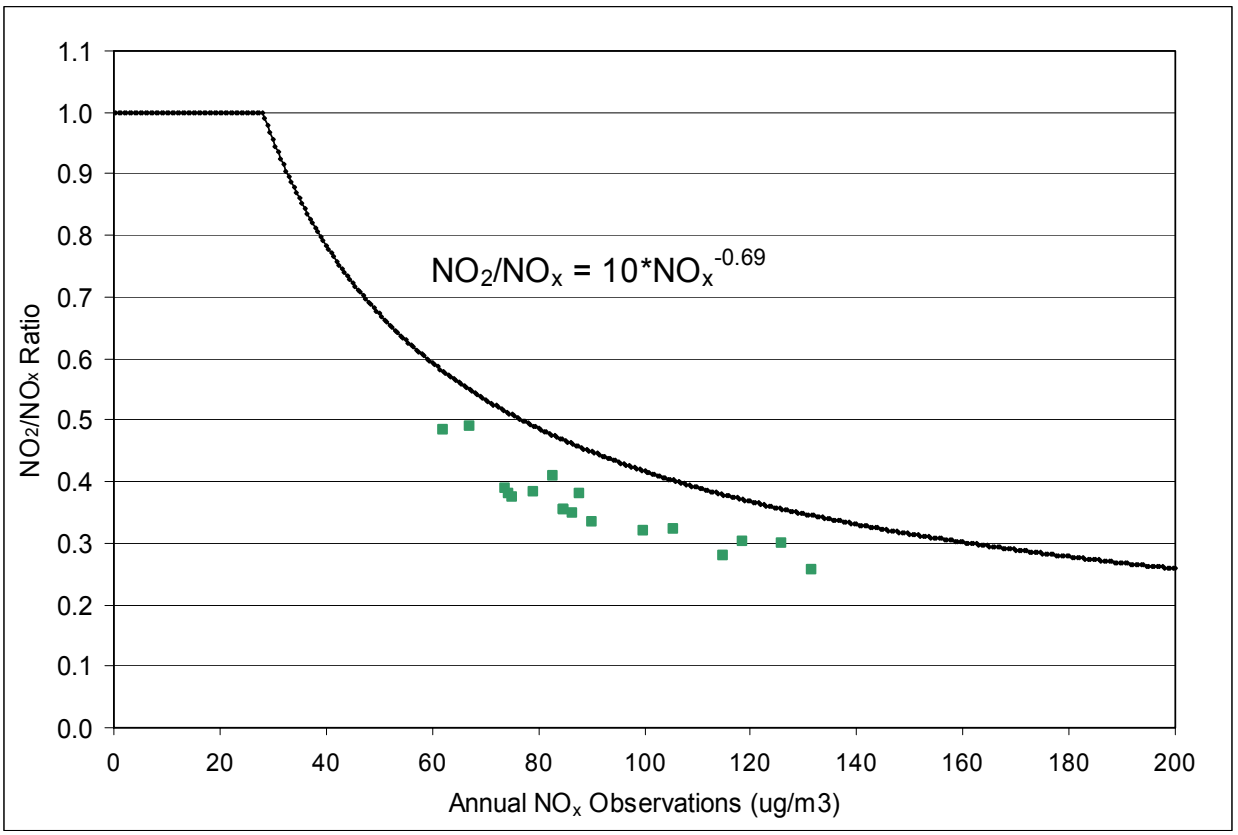

Figure D-5: Dependence of NO_2/NO_x Ratio on Annual Average NO_x Observations from GVRD Station T17 (Richmond South)

3.3 SPECIATION OF VOCS, PAHS AND METALS

Concentrations of Volatile Organic Compounds (VOCs), Poylcyclic Aromatic Hydrocarbons (PAHs) and metals were estimated at 12 human health receptors and 4 ecologically sensitive receptors. The VOC, PAH and metal species that were estimated and used in the health risk and ecological assessments are summarized in Section 5 of the main report. These species were not modelled individually; instead, particulate matter (PM_{10} and $PM_{2.5}$) and total VOC concentrations predicted at the receptors were used to estimate concentrations of individual VOCs and PAHs using speciation data specific to the different emission source types.

The five VOC species of interest were estimated from the maximum predicted VOC concentrations. Speciation for onroad mobile sources was conducted using the US EPA MOBILE6 model air toxics module. Nonroad VOC species including dockyard equipment, marine vessels and locomotives were estimated using fraction to total VOC ratios published by the US EPA (US EPA, 2004a and US EPA, 1998). Table D-6 summarizes the VOC speciation data used for the various emission sources.

Table D-6: Speciation Data for VOC (as a Fraction of Total VOC)

VOC SPECIES	MARINE VESSELS	BACKGROUND TRAFFIC	CONTAINER TRUCKS	PASSENGER CARS	NONROAD DIESEL ENGINES
Acetaldehyde	0.0743	0.00579	0.00577	0.00561	0.053
Acrolein	0.0035	0.00076	0.00070	0.00072	0.003
Benzene	0.02034	0.04210	0.00211	0.04258	0.02
1,3-Butadiene	0.002	0.00690	0.00122	0.00694	0.002
Formaldehyde	0.1496	0.01759	0.01568	0.01705	0.118

The sixteen PAH species were estimated from the maximum PM_{10} and $PM_{2.5}$ concentrations. PAH speciation data as a fraction of total $PM_{2.5}$ or PM_{10} for onroad mobile sources, locomotives and dockyard equipment were estimated based on published values from the US EPA (US EPA, 2001). PAH species for marine emission sources were estimated using the fraction to total $PM_{2.5}$ ratios provided by the US EPA (US EPA, 2001). Table D-7 summarizes the PAH speciation data used for the various emission sources.

Table D-7: Speciation Data for PAH (as a Fraction of PM_{10} or $PM_{2.5}$)

PAH	MARINE VESSELS ($PM_{2.5}$)	HEAVY DUTY DIESEL TRUCKS ($PM_{2.5}$)	PASSENGER CARS (PM_{10})	BACKGROUND TRAFFIC (PM_{10})	LOCOMOTIVE ENGINE (PM_{10})
Acenaphthylene	0.000037	0.000037	0.004083157	0.003964501	0.0004355
Acenaphthene	0.000024	0.000024	0.000722465	0.000702016	0.000037
Anthracene	0.000037	0.000037	0.000842184	0.000818584	0.0001042
Benz(a)anthracene	0.00004	0.00004	9.93916E-05	0.000097648	0.0000166
Benzo(a)pyrene	0.000013	0.000013	9.93565E-05	9.68185E-05	0.0000027
Benzo(b)fluoranthene	0.000011	0.000011	0.000119509	0.000116311	0.0000069

Benzo(k)fluoranthene	0.000011	0.000011	0.000119509	0.000116311	0.0000054
Benzo(g,h,i)perylene	0.000009	0.000009	0.000257578	0.000250293	0.0000034
Chrysene	0.000007	0.000007	9.94969E-05	9.67735E-05	0.0000129
Dibenzo(a,h)anthracene	0.00	0.00	2.34E-08	0.000000022	0.00
Fluoranthene	0.000022	0.000022	0.000905624	0.000879599	0.0000781
Fluorene	0.000049	0.000049	0.001496791	0.001454331	0.0001551
Indeno(1,2,3-cd)pyrene	0.000001	0.000001	7.93097E-05	7.70125E-05	0.0000027
Naphthalene	0.001401	0.001401	0.089711316	0.087127985	0.0025885
Phenanthrene	0.000056	0.000056	0.002522661	0.002450166	0.0006106
Pyrene	0.000039	0.000039	0.001233553	0.001198386	0.0001136

The five metal concentrations were estimated from the maximum total $PM_{2.5}$ concentrations. Speciation for onroad mobile sources was conducted using the US EPA SPECIATE 3.2 Model (US EPA, 2004b). Nonroad VOC species including all other emission sources were estimated using data published by the US EPA for gasoline and diesel engines (US EPA, 1996). Table D-8 summarizes the metal speciation data used for the various emission sources.

Table D-8: Speciation Data for Metals (as a Fraction of $PM_{2.5}$)

METALS	BACKGROUND TRAFFIC	DIESEL ENGINES
Arsenic	8.00E-05	3.76471E-05
Cadmium	0.00E-00	3.52941E-05
Chromium	1.00E-05	1.41176E-05
Manganese	9.30E-04	7.29412E-05
Nickel	3.00E-05	9.17647E-05

4.0 MODEL LIMITATIONS

By definition, air quality models can only approximate atmospheric processes. Many assumptions and simplifications are required to describe real phenomena in mathematical equations. Model uncertainties can result from:

- Simplifications and accuracy limitations related to source data;
- Extrapolation of meteorological data from selected locations to a larger region; and

- Simplifications to model physics to replicate the random nature of atmospheric dispersion processes.

Models are reasonable and reliable in estimating the maximum concentrations occurring on an average basis. That is, the maximum concentration that may occur at a given time somewhere within the model domain, as opposed to the exact concentration at a point at a given time will usually be within the ±10% to ±40% range (US EPA, 2003). Typically, a model is viewed as replicating dispersion processes if it can predict within a factor of two, and if it can replicate the temporal and meteorological variations associated with monitoring data. Model predictions at a specific site and for a specific hour, however, may correlate poorly with the associated observations due to the above-indicated uncertainties. For example, an uncertainty of 5° to 10° in the measured wind direction can result in concentration errors of 20% to 70% for an individual event (US EPA, 2003).

5.0 SUMMARY AND CONCLUSIONS

The CALPUFF dispersion model was selected as the primary air quality assessment tool to predict ambient concentrations and deposition. The following were adopted for the application of the model:

- Receptor spacing varies from 100 m to 1,000 m;
- An additional 16 community, recreation or wildlife receptors;
- One year of meteorological data for the period January 2003 to December 2003;
- Hourly ozone concentrations from GVRD station T17 in South Richmond;
- The ambient ratio method was selected to convert predicted ground-level NO_x concentrations to NO_2 concentrations; and
- The majority of emissions were incorporated as area sources. Emissions from railways and roads traffic were modelled as line sources.

6.0 FULL CALPUFF MODEL OPTIONS LISTING

The CALPUFF control file defines 17 input groups as identified in Table D-9. For many of the options, default values were used in the absence of site/project specific data. Tables D-10 to D-16 identify the input parameters, the default options, and the values used for those input groups relevant to the Roberts Bank project.

Table D-9: Input Groups in the CALPUFF Control File.

INPUT GROUP	DESCRIPTION	APPLICABLE TO ROBERTS BANK PROJECT
0	Input and output file names	Yes
1	General run control parameters	Yes
2	Technical options	Yes
3	Species list	Yes
4	Grid control parameters	Yes
5	Output options	Yes
6	Sub grid scale complex terrain inputs	No
7	Dry deposition parameters for gases	No
8	Dry deposition parameters for particles	No
9	Miscellaneous dry deposition for parameters	No
10	Wet deposition parameters	No
11	Chemistry parameters	Yes
12	Diffusion and computational parameters	Yes
13	Point source parameters	No
14	Area source parameters	Yes
15	Line source parameters	No
16	Volume source parameters	No
17	Discrete receptor information	Yes

Table D-10: CALPUFF Model Options Groups 1 and 2.

Input Group 1: General run control parameters.

PARAMETER	DEFAULT	ROBERTS BANK	COMMENTS
METRUN	0	0	All model periods in met file(s) will be run
IBYR	-	2003	Starting year
IBMO	-	1	Starting month
IBDY	-	1	Starting day
IBHR	-	1	Starting hour
IRLG	-	8759	Length of run
NSPEC	5	11	Number of chemical species
NSE	3	8	Number of chemical species to be emitted
ITEST	2	2	Program is executed after SETUP phase
MRESTART	0	2	Write a restart file during run
NRESPD	0	24	Restart file written every 24 hours
METFM	1	1	CALMET binary file (CALMET.MET)
AVET	60	60	Averaging time in minutes
PGTIME	60	60	PG Averaging time in minutes

Input Group 2: Technical Options

PARAMETER	DEFAULT	ROBERTS BANK	COMMENTS
MGAUSS	1	1	Gaussian distribution used in near field
MCTADJ	3	3	Partial plume path terrain adjustment
MCTSG	0	0	Scale-scale complex terrain not modelled
MSLUG	0	0	Near-field puffs not modelled as elongated
MTRANS	1	1	Transitional plume rise not modelled
MTIP	1	1	Stack tip downwash used
MSHEAR	0	0	Vertical wind shear not modelled
MSPLIT	0	0	Puffs are not split
MCHEM	1	1	Transformation rates computed internally using MESOPUFF II scheme
MAQCHEM	0	0	Aqueous phase transformation not modelled
MWET	1	0	Wet removal modelled
MDRY	1	0	Dry deposition modelled
MDISP	3	3	PG dispersion coefficients for RURAL areas (computed using the ISCST multi-segment approximation) and MP coefficients in urban areas
MTURBVW	3	3	Use both σ_v and σ_w from PROFILE.DAT to compute σ_y and σ_z (n/a)
MDISP2	3	3	PG dispersion coefficients for rural areas (computed using ISCST3 approximation) and MP coefficients in urban areas when measured turbulence data is missing
MROUGH	0	0	PG σ_y and σ_z not adjusted for roughness
MPARTL	1	1	No partial plume penetration of elevated inversion
MTINV	0	0	Strength of temperature inversion computed from default gradients
MPDF	0	0	PDF not used for dispersion under convective conditions
MSGTIBL	0	0	Sub-grid TIBL module not used for shoreline
MBCON	0	0	Boundary concentration conditions not modelled
MFOG	0	0	Do not configure for FOG model output
MREG	1	0	Do not test options specified to see if they conform to regulatory values

Table D-11: CALPUFF Model Options Groups 3 and 4

Input Group 3: Species List-Chemistry options

CSPEC	MODELLED (0=no, 1=yes)	EMITTED (0=no, 1=yes)	DRY DEPOSITION (0=none, 1=computed-gas, 2=computed particle, 3=user-specified)	OUTPUT GROUP NUMBER
SO_2	1	1	0	0
SO_4^{2-}	1	1	0	0
NO_x	1	1	0	0
HNO_3	1	1	0	0
NO_3^-	1	1	0	0
CO	1	1	0	0
PM_{10}	1	1	0	0
$PM_{2.5}$	1	1	0	0
TSP	1	1	0	0
VOC	1	1	0	0
InertNOx or DieselPM*	1	1	0	0

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Input Group 4: Grid Control Parameters.

PARAMETER	DEFAULT	ROBERTS BANK	COMMENTS
NX	-	120	Number of X grid cells in meteorological grid
N		120	Number of Y grid cells in meteorological grid
NZ	-	8	Number of vertical layers in meteorological grid
DGRIDKM	-	.250	Grid spacing (km)
ZFACE	-	0, 20, 50, 100, 250, 500, 1000, 2000, 3000.	Cell face heights in meteorological grid (m)
XORIGKM	-	478	Reference X coordinate for SW corner of grid cell (1,1) of meteorological grid (km)
YORIGKM	-	5419	Reference Y coordinate for SW corner of grid cell (1,1) of meteorological grid (km)
IUTMZN	-	10	UTM zone of coordinates
IBCOMP	-	1	X index of lower left corner of the computational grid
JBCOMP	-	1	Y index of lower left corner of the computational grids
IECOMP	-	120	X index of the upper right corner of the computational grid
JECOMP	-	120	Y index of the upper right corner of the computational grid
AqLSAMP	T	F	Sampling grid is not used
IBSAMP	-	1	X index of lower left corner of the sampling grid
JBSAMP	-	1	Y index of lower left corner of the sampling grid
IESAMP	-	120	X index of upper right corner of the sampling grid
JESAMP	-	120	Y index of upper right corner of the sampling grid
MESHDN	1	1	Nesting factor of the sampling grid

Table D-12: CALPUFF Model Option Group 5

Input Group 5: Output Option

PARAMETER	DEFAULT	ROBERTS BANK	COMMENTS
ICON	-	1	Output file CONC.DAT containing concentrations is created
IDRY	-	0	Output file DFLX.DAT containing dry fluxes is created
IWET	-	0	Output file WFLX.DAT containing wet fluxes is created
IVIS	-	0	Output file containing relative humidity data is not created
LCOMPRS	T	T	Perform data compression in output file
IMFLX	0	0	Do not calculate mass fluxes across specific boundaries
IMBAL	0	0	Do not report mass balances
ICPRT	0	0	Do not print concentration fields to the output list file
IDPRT	0	0	Do not print dry flux fields to the output list file
IWPRT	0	0	Do not print wet flux fields to the output list file
ICFRQ	1	1	Concentration fields are printed to output list file every 1 hour
IDFRQ	1	1	Dry flux fields are printed to output list file every 1 hour
IWFRQ	1	1	Wet flux fields are printed to output list file every 1 hour
IPRTU	1	1	Units for line printer output are in ug/m_3 for concentration and $ug/m_2/s$ for deposition
IMESG	1	2	Messages tracking the progress of run are written on screen

SPECIES	**CONCENTRATIONS PRINTED** (0=no, 1=yes)		**DRY FLUXES PRINTED** (0=no, 1=yes)		**WET FLUXES PRINTED** (0=no, 1=yes)	
	output list file	saved to disk	output list file	saved to disk	output list file	saved to disk
SO_2	0	1	0	0	0	0
SO_4^{-2}	0	1	0	0	0	0
NO_x	0	1	0	0	0	0
HNO_3	0	1	0	0	0	0
NO_3^-	0	1	0	0	0	0
CO	0	1	0	0	0	0
PM_{10}	0	1	0	0	0	0
$PM_{2.5}$	0	1	0	0	0	0
TSP	0	1	0	0	0	0
VOC	0	1	0	0	0	0
InertNOx or DieselPM*	0	1	0	0	0	0

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LDEBUG	F	F	Logical value for debug output
IPFDEB	1	1	First puff to track
NPFDEB	1	1	Number of puffs to track
NN1	1	1	Meteorological period to start output
NN2	10	10	Meteorological period to end output

Table D-13: CALPUFF Model Option Groups 11

Input Group 11: Chemistry Parameters

PARAMETERS	DEFAULT	ROBERTS BANK	COMMENTS
MOZ	1	1	Hourly ozone values from GVRD T17 were used
BCKO3	-	-	Background ozone concentration (ppb)
BCKNH3	10	12*10	Background ammonia concentration (ppb)
RNITE1	0.2	0.2	Nighttime NO_2 loss rate in percent/hour
RNITE2	2	2	Nighttime NO_X loss rate in percent/hour
RNITE3	2	2	Nighttime HNO_3 loss rate in percent/hour
MH202	-	-	Background H_2O_2 concentrations (Aqueous phase transformations not modelled)
BCKH202	-	-	Background monthly H_2O_2 concentrations (Aqueous phase transformations not modelled)
BCKPMF	-	-	Fine particulate concentration for Secondary Organic Aerosol Option
OFRAC	-	-	Organic fraction of fine particulate for SOA Option
VCNX	-	-	VOC/NO_x ratio for SOA Option

Table D-14: CALPUFF Model Option Group 12.

Input Group 12: Diffusion/Computational Parameters

PARAMETERS	DEFAULT	ROBERTS BANK	COMMENTS
SYDEP	550	550	Horizontal size of a puff in metres beyond which the time dependant dispersion equation of Heffter (1965) is used
MHFTSZ	0	0	Do not use Heffter formulas for sigma z
JSUP	5	5	Stability class used to determine dispersion rates for puffs above boundary layer
CONK1	0.01	0.01	Vertical dispersion constant for stable conditions
CONK2	0.1	0.1	Vertical dispersion constant for neutral/stable conditions
TBD	0.5	0.5	Use ISC transition point for determining the transition point between the Schulman-Scire to Huber-Snyder Building Downwash scheme
IURB1	10	10	Lower range of land use categories for which urban dispersion is assumed
IURB2	19	19	Upper range of land use categories for which urban dispersion is assumed
ILANDUIN	20		Land use category for modelling domain
XLAIIN	3.0	*	Leaf area index for modelling domain
ZOIN	-0.25	*	Roughness length in metres for modelling domain
ELEVIN	0.0	*	Elevation above sea level
XLATIN	-999	-	North latitude of station in degrees
XLONIN	-999	-	South latitude of station in degrees
ANEMHT	10	-0	Anemometer height in metres
ISIGMAV	1	-	Sigma-v is read for lateral turbulence data
IMIXCTDM	0	-	Predicted mixing heights are used
XMXLEN	1	1	Maximum length of emitted slug in meteorological grid units
XSAMLEN	1	1	Maximum travel distance of slug or puff in meteorological grid units during one sampling unit
MXNEW	99	99	Maximum number of puffs or slugs released from one source during one time step
MXSAM	99	99	Maximum number of sampling steps during one time step for a puff or slug
NCOUNT	2	2	Number of iterations used when computing the transport wind for a sampling step that includes transitional plume rise
SYMIN	1	1	Minimum sigma y in metres for a new puff or slug
SZMIN	1	1	Minimum sigma z in metres for a new puff or slug
Values indicated by an asterisk (*) were allowed to vary spatially across the domain and were obtained from CALMET			

Stability Class	Parameter	
	SVMIN	SWMIN
	Minimum turbulence (σ_v) (m/s)	Minimum turbulence (σ_w) (m/s)
A	0.5	0.2
B	0.5	0.12
C	0.5	0.08
D	0.5	0.06
E	0.5	0.03
F	0.5	0.016

PARAMETERS	DEFAULT	ROBERTS BANK	COMMENTS
CDIV	0.0, 0.0	0.0, 0.0	Divergence criteria for dw/dz in met cells
WSCALM	0.5	1	Minimum wind speed allowed for non-calm conditions (m/s)
XMAXZI	3000	3000	Maximum mixing height in metres
XMINZI	50	50	Minimum mixing height in metres
WSCAT	-	1.54	wind speed category 1 [m/s]
	-	3.09	wind speed category 2 [m/s]
	-	5.14	wind speed category 3 [m/s]
	-	8.23	wind speed category 4 [m/s]
	-	10.80	wind speed category 5 [m/s]

STABILITY CLASS	PARAMETER	
	PLX0	PPC
	Wind speed profile exponent	Plume path coefficient
A	0.15	0.50
B	0.15	0.50
C	0.20	0.50
D	0.25	0.50
E	0.30	0.35
F	0.30	0.35

PTG0	0.020	0.020	potential temperature gradient for E stability [K/m]
	0.035	0.035	potential temperature gradient for F stability [K/m]
SL2PF	10	10	Slug-to-puff transition criterion factor equal to sigma y/length of slug
NSPLIT	3	3	Number of puffs that result every time a puff is split

PARAMETERS	DEFAULT	ROBERTS BANK	COMMENTS
IRESPLIT	0,0,0,0,0,0,0, 0,0,0,0,0,0,0, 0,0,0,1,0,0,0, 0,0,0	0,0,0,0,0,0,0, 0,0,0,0,0,0,0, 0,0,0,1,0,0,0, 0,0,0	Time(s) of day when split puffs are eligible to be split once again
ZISPLIT	100	100	Minimum allowable last hour's mixing height for puff splitting
ROLDMAX	0.25	0.25	Maximum allowable ratio of last hour's mixing height and maximum mixing height experienced by the puff for puff splitting
ASPLITH	5	5	Number of puffs that result every time a puff is horizontally split
SYSPLITH	1	1	Minimum sigma-y of puff before it may be horizontally split
SHSPLITH	2	2	Minimum puff elongation rate due to wind shear before it may be horizontally split
CNSPLITH	1.0e-7	1.0e-7	Minimum concentration of each species in puff before it may be horizontally split
EPSSLUG	1.00E-04	1.00E-04	Fractional convergence criterion for numerical SLUG sampling iteration
EPSAREA	1.00E-06	1.00E-06	Fractional convergence criterion for numerical AREA sampling iteration
DRISE	1.0	1.0	Trajectory step length for numerical rise
'-' symbol indicates that the parameter was not applicable to the Roberts Bank Project			

Table D-15: CALPUFF Model Option Groups 13, 14, and 15.

Input Group 13: Point Source Parameters

PARAMETERS	DEFAULT	ROBERTS BANK	COMMENTS
NPT1	-	Varies by scenario	Number of point sources with constant stack parameters or variable emission rate scale factors
NPTU	1	-	Units for point source emission rates are g/s
NSPT1	0	-	Number of source-species combinations with variable emissions scaling factors
NPT2	-	-	Number of point sources with variable emission parameters provided in external file
Point source parameters are given in Part A '-' symbol indicates that the parameter was not applicable to the Roberts Bank Project			

Input Group 14: Area Source Parameters

PARAMETERS	DEFAULT	ROBERTS BANK	COMMENTS
NAR1	-	Varies by scenario	Number of polygon area sources
IARU	1	-	Units for area source emission rates are $g/m^2/s$
NSAR1	0	-	Number of source species combinations with variable emissions scaling factors
NAR2	-	-	Number of buoyant polygon area sources with variable location and emission parameters
Area source parameters are given in Part A '-' symbol indicates that the parameter was not applicable to the Roberts Bank Project			

Input Group 15: Line Source Parameters

PARAMETERS	DEFAULT	ROBERTS BANK	COMMENTS
NLN2	-	-	Number of buoyant line sources with variable location and emission parameters
NLINES	-	-	Number of buoyant line sources
ILNU	1	-	Units for line source emission rates is g/s
NSLN1	0	-	Number of source-species combinations with variable emissions scaling factors
MXNSEG	7	-	Maximum number of segments used to model each line
NLRISE	6	-	Number of distance at which transitional rise is computed
XL	-	-	Average line source length (m)
HBL	-	-	Average height of line source height (m)
WBL	-	-	Average building width (m)
WML	-	-	Average line source width (m)
DXL	-	-	Average separation between buildings (m)
FPRIMEL	-	-	Average buoyancy parameter (m^4/s^3)
'-' symbol indicates that the parameter was not applicable to the Roberts Bank Project			

Table D-16: CALPUFF Model Option Groups 16 and 17

Input Group 16: Volume Source Parameters

PARAMETER	DEFAULT	ROBERTS BANK	COMMENTS
NVL1	-	-	Number of volume sources
IVLU	1	-	Units for volume source emission rates is grams per second
NSVL1	0	-	Number of source-species combinations with variable emissions scaling factors
IGRDVL	-	-	Gridded volume source data is not used
VEFFHT	-	-	Effective height of emissions (m)
VSIGYI	-	-	Initial sigma y value (m)
VSIGZI	-	-	Initial sigma z value (m)
'-' symbol indicates that the parameter was not applicable to the Roberts Bank Project			

Input Group 17: Discrete Receptor Information

PARAMETER	DEFAULT	ROBERTS BANK	COMMENTS
NREC	-	2989	Number of non-gridded receptors
Discrete receptors are identified on Figure 2-1 and Table 2-4			

7.0 REFERENCES

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