Assessment of Air Quality Impacts of Emissions from the Alcoa Aluminum Plant in Reydarfjordur, Iceland

January 2006

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1. INTRODUCTION

Earth Tech has been retained by Alcoa to conduct refined air quality dispersion modeling of the proposed Alcoa aluminum reduction facility at an industrial site in Fjardabyggd, located approximately 5 km east of the Reydarfjordur village in Iceland. The modeling analysis evaluates the air quality impacts due to emissions of particulate matter (PM_{10}), sulfur dioxide (SO_2), hydrogen fluoride (HF), hydrogen particulate (PF), Polycyclic Aromatic Hydrocarbons (PAHs) and benzo(a)pyrene (BaP). This study estimates the concentration of PM_{10}, SO_2, HF, PF, all PAHs and BaP and compares these concentrations with the corresponding ambient standards or air quality guidelines from the Norwegian guidelines, Icelandic regulation or European Union directive. In addition, both ambient air predictions and deposition predictions of these pollutants were provided to Exponent, for a risk assessment analysis.

The techniques used for this study involve the use of a comprehensive meteorological and dispersion modeling system representing the current state-of-the science in regulatory air quality modeling. The modeling approach is based on the CALMET diagnostic meteorological model (Scire et al., 2000a) and the CALPUFF non-steady-state dispersion model (Scire et al., 2000b). The U.S. Environmental Protection Agency (U.S. EPA) has adopted the CALPUFF modeling system as a *Guideline Model* for Class I impact ambient air quality assessments and other long range transport applications or, on a case-by-case basis, near-field applications involving complex flows, such as spatial changes in meteorological fields due to factors such as the presence of complex terrain or water bodies, plume fumigation (coastal fumigation or inversion break-up conditions), light wind speed or calm wind impacts, or other factors for which a steady-state straight-line modeling approach is not appropriate (U.S. EPA, Federal Register, April 15, 2003).

CALPUFF was designed to be a regulatory modeling tool that would treat multiple effects within a single modeling framework. It is consistent with Guideline plume modeling techniques where and when those techniques are valid (i.e., under steady-state conditions), but CALPUFF offers the advantage of accounting for non-steady-state effects when they exist. CALPUFF was developed to be suitable for use in the near-field (e.g., at the property fence line) at distances of tens of meters out to distances of several hundred kilometers. It includes near-field effects, such as transitional plume rise, building downwash effects, stack-tip downwash, momentum and buoyant plume rise, as well as far-field effects such as wet and dry deposition, chemical transformation, long range dispersion, and other factors (see Section 4). The model explicitly includes the buoyant line source algorithms in the Buoyant Line and Point Source (BLP) model (Schulman and Scire, 1980). BLP is accepted by the U.S. EPA as a *Guideline model* for buoyant line source emissions.

The CALPUFF model has been extensively evaluated and tested as part of the U.S. EPA Guideline model review process. The model has been subjected to extensive public review and comment through a public process mandated by the Clean Air Act. Evaluations of the CALPUFF model in near-field applications include an SO_2 evaluation for a pair of power plant stacks in a river valley with complex terrain and a tracer evaluation of a tall power plant stack in flat terrain (Strimaitis et al., 1998), near-field evaluation of smelter emissions in Canada (Morrison et al., 2003), a smelter-power plant facility in Texas (Robe et al., 2002), and an extensive evaluation of cumulative impacts from many sources at various distances (Scire et al., 2003). Other CALPUFF evaluation studies include Bennett et al. (2002), Levy et al. (2002) and Zhou et al. (2003). The algorithms in CALPUFF for line source dispersion are based on the BLP dispersion model which have been evaluated at aluminum plants in Arkansas and Tennessee (Scire and Schulman, 1981). The CALPUFF modeling system is used extensively throughout the world with users in 101 countries. It has undergone extensive peer review and testing through numerous applications throughout the United States and internationally.

The CALMET/CALPUFF modeling system for the proposed Alcoa facility was selected for the following reasons:

- the presence of complex terrain in the immediate vicinity of the facility, and its importance in producing spatially varying wind fields;
- the presence of a body of water near the facility introducing spatial inhomogeneities in the meteorological fields and the importance of sea breeze circulations;
- the significant anthropogenic heat fluxes associated with the aluminum reduction facility producing local spatial variability in the dispersion characteristics;
- the potential importance of light wind speed and calm wind effects at this site; and
- the potential importance of stagnation, plume recirculation, and plume fumigation.

The CALMET meteorological model uses available sources of meteorological and geophysical information to produce a spatially-varying wind field that is consistent with the local terrain features and atmospheric stability conditions at the site. In this application, a full three-dimensional wind field with a grid spacing of 0.3 km is used to provide appropriate resolution of terrain effects.

There are several limitations and gaps in the air quality models (CONDEP, MATHEW and INPUFF) used in previous studies at this site that are relevant. None of the previous models adequately treat all of the processes and effects that are important for the Alcoa facility. For example,

- CONDEP is a point source model and has no buoyant line source capabilities. The Alcoa potrooms are considered line sources because the emissions are released through roof-top vents running along the length of the potroom buildings. Because line source plume rise has a different functional relationship with buoyancy and distance than point source plume rise, a point source model cannot properly reproduce line source buoyant rise. Estimating line source plume rise with a point source equation may produce large discrepancies in the plume height and potentially large under- or over-estimation of impacts, depending on the number of point sources used to represent each line.

- CONDEP is a straight-line model and computes long-term average concentrations based on single meteorological station observations. It does not treat causality effects.

- CONDEP uses steady-state meteorological and dispersion conditions. Therefore, it does not include the effects of stagnation, flow reversals, or fumigation.

- MATHEW is a diagnostic wind model used in modeling certain episodes together with INPUFF, which is a point source puff model. In this approach, the potrooms are treated as non-buoyant volume sources and so their impact can be significantly overestimated due to the lack of consideration of buoyancy effects.

In Section 2, descriptions of the source configuration and emissions data are provided. The modeling domain, the geophysical data and the meteorological data used in the analysis are described in Section 3. Section 4 contains a description of the MM5 modeling. Section 5 includes an overview of the CALMET and CALPUFF models, and the importance of evaluating non-steady-state effects in this application and describes the CALMET/CALPUFF model configuration. In Section 6, the MM5 and CALMET outputs are analyzed and compared to observations, while in Section 7, the meteorological conditions for the year modeled are compared to other years. Finally, Section 8 presents the modeling results of predicted pollutant concentrations. A comparison of the predicted concentrations due to the proposed facility against the relevant air quality standards is provided.

2. SOURCE DESCRIPTION

2.1 Source Data

The proposed Alcoa aluminum plant is to be located at an industrial site in Fjardabyggd, approximately 5 km east of the Reydarfjordur village in Iceland. The proposed plant will have an annual production capacity of 346,000 metric tons of aluminum per year (TPY). Four source configuration scenarios are examined in this study. First are Scenarios A and B, where the plant will consist of two potrooms with one associated dry scrubber, applied with minimum 99.5% efficiency to remove fluorides, and a cast house with three casting furnaces. Second, are Scenarios C and D, where the plant will consist of two potrooms with an associated dry scrubber and four seawater scrubber towers, and a cast house with three casting furnaces. All four scenarios also include a tall anode cooling stack with a height of 78 meters. In Scenarios A and B, this stack also vents the dry scrubber emissions. In Scenarios C and D, the scrubber emissions are vented through four separate 40-m stacks.

The four sea water scrubber towers are used only in Scenarios C and D. The casthouse furnaces will use electric heating. The smelting operation will use 1.8% sulfur coke in Scenarios A and B, and 3.0% sulfur coke in Scenarios C and D. Scenarios A and C are applied for all pollutants and averaging periods required for comparison with air quality standard guidelines and for risk assessment applications. Scenarios B and D are applied for HF only for the growing season averaging period (April 1st to September 30th). The scenario summary is:

Scenario A: Dry scrubber, single tall stack venting anode cooling and scrubber emissions, 1.8% S coke, annual average fluoride emissions.

Scenario B: Same as Scenario A except fluoride emissions are growing season average values.

Scenario C: Dry scrubber followed by sea water scrubbers, four 40-m scrubber stacks, tall stack for anode cooling emissions only, 3.0% S coke, annual average fluoride emissions.

Scenario D: Same as Scenario C, except fluoride emissions are growing season average values.

Figure 2-1 shows a plot plan of the facility for all four scenarios, with the emission sources and buildings important for building downwash indicated. The point sources information for Scenarios A and B are listed in Table 2-1. The line sources information is listed in Table 2-2 for Scenario A and in Table 2-3 for Scenario B. The point sources information for Scenarios C and D are listed in Table 2-4, and the information for the line sources is listed in Table 2-5 for Scenario C and Table 2-6 for Scenario D. The source information tables include emission rates for SO_2, PM_{10}, HF, PF, BaP and PAH. The proposed facility will be based on technology in use at the existing Alcoa facility in Deschambault, Quebec, Canada. The line source parameters used to compute the average buoyancy parameter (F') were provided by Alcoa from measurements made at the Deschambault facility. The average temperature differences between the rooftop emissions and the ambient air for the calculation of the line source F' was computed using a full year of measurements made during the year 2001 at the Deschambault facility (see Appendix A). The annual average temperature difference was computed to be 19.2º Celsius (C). This temperature difference is applied at Fjardabyggd facility. The average potroom exit temperature is used in the calculation of the buoyancy parameter is 23º Celsius (296.15 Kelvin), which produces a value for the line source buoyancy parameter (F') of 1813 m^4/s^3.

PAH emitted at the Deschambault facility, from both the roof top vents (lines) and the wet or dry scrubber stacks (point sources) was measured and speciated. It is partly gas and partly particulate matter, the proportion of gas and particles being different for the lines and the point source stacks as described in Appendix B. For the roof top vents (line sources), a total PAH emission of 34.14µg has 33.13µg of gas and 1.01µg of particles, which gives an estimate of 97% gas and 3% particles for this application. For the wet and dry scrubber stacks (point sources), a total of 0.0075mg PAH is emitted, and 0.0035mg (46.7%) is gas and 0.0040mg (53.3%) is particles. This PAH gas/particles partitioning for the roof top vents and stacks measured at Deschambault facility will be used for the PAH gas/particles partitioning in the present application.

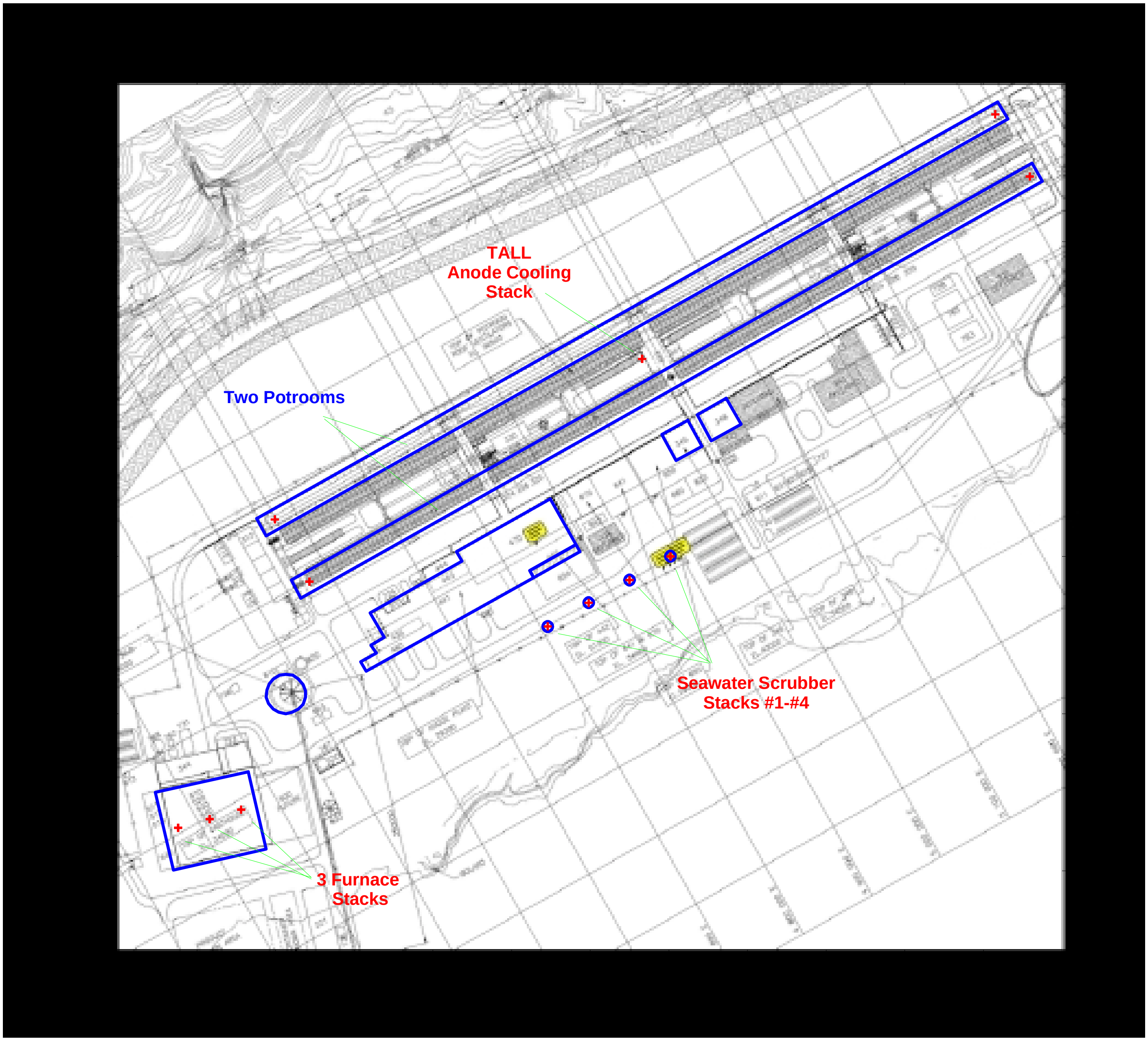


Figure 2-1. Plan of the Alcoa facility showing building locations and the emission sources. Note that the location of the potrooms was extracted from a separate more detailed map.

Table 2-1. Point Source Parameters and Emission Rates for Scenarios A and B

Source Description	UTM-28 X-Coord. (km)	UTM-28 Y-Coord. (km)	Stack Height (m)	Base Elev. (m)	Stack Diameter (m)	Exit Veloc. (m/s)	Exit Temp. (K)	HF Emission Rate (g/s)	PF Emission Rate (g/s)	SO_2 Emission Rate (g/s)	PM_{10} Emission Rate (g/s)	PAH Emission Rate (g/s)	BaP[(2)] Emission Rate (g/s)
Fume Stack 1	542.366	7212.451	78	14	9.45[(3)]	19.0	362.15	0.94	0.086	142.8 [(1)]	2.16	1.41E-03	2.81E-05
Furnace 1	541.776	7211.855	29.5	12	0.8	12.0	553.15	0	0	0[(4)]	0.05		0
Furnace 2	541.816	7211.866	29.5	12	0.8	12.0	553.15	0	0	0[(4)]	0.05		0
Furnace 3	541.856	7211.878	29.5	12	0.8	12.0	553.15	0	0	0[(4)]	0.05		0

(1) SO_2 emission rate is based on 1.8% sulfur coke.

(2) The BaP emission rate for the Fume Stack is 2% of the PAH emission rate.

(3) Gives a normal volume flow of 3,883,249 Nm^3/hr.

(4) SO_2 emission rate for the three Furnaces is set to 0g/s, electric heating will be used.

Table 2-2. Line Source (Potroom) Emissions Data for Scenario A

Source Description	Line No.	UTM-28 Coord. Beg. X (km)	UTM-28 Coord. Beg. Y (km)	UTM-28 Coord. End X (km)	UTM-28 Coord. End Y (km)	Release Height (m)	Base Elevation (m)	HF Emission Rate (g/s)	PF Emission Rate (g/s)	SO_2 Emission Rate (g/s)	PM_{10} Emission Rate (g/s)	PAH Emission Rate (g/s)	BaP(1) Emission Rate (g/s)
LINE 1	1	541.899	7212.247	542.815	7212.762	22.5	14	0.59	0.395	1.46 (2)	0.29	2.14E-03	2.14E-05
LINE 2	2	541.943	7212.168	542.859	7212.683	22.5	14	0.59	0.395	1.46 (2)	0.29	2.14E-03	2.14E-05

(1) The BaP emission rate for the potrooms is 1% of the PAH emission rate.

(2) SO_2 emission rate is based on 1.8% sulfur coke.

Table 2-3. Line Source (Potroom) Emissions Data for Scenario B

Source Description	Line No.	UTM-28 Coord. Beg. X (km)	UTM-28 Coord. Beg. Y (km)	UTM-28 Coord. End X (km)	UTM-28 Coord. End Y (km)	Release Height (m)	Base Elevation (m)	HF Emission Rate (g/s)	PF Emission Rate (g/s)	SO_2 Emission Rate (g/s)	PM_{10} Emission Rate (g/s)	PAH Emission Rate (g/s)	BaP(1) Emission Rate (g/s)
LINE 1	1	541.899	7212.247	542.815	7212.762	22.5	14	0.76	0.505	1.46 (2)	0.29	2.14E-03	2.14E-05
LINE 2	2	541.943	7212.168	542.859	7212.683	22.5	14	0.76	0.505	1.46 (2)	0.29	2.14E-03	2.14E-05

(1) The BaP emission rate for the potrooms is 1% of the PAH emission rate.

(2) SO_2 emission rate is based on 1.8% sulfur coke.

Potroom dimensions: Building length = 1081.2m

Building height = 22.5m

Building width = 25.8m

Line source width = 2.9m

Average separation between building = 64.36m

Exit velocity = 1m/s

Total vent length = 984m

Average buoyancy parameter = 1813 m^4/s^3; ΔT = 19.2º C, average exit temperature = 23º C

Table 2-4. Point Source Parameters and Emission Rates for Scenarios C and D

Source Description	UTM-28 X-Coord. (km)	UTM-28 Y-Coord. (km)	Stack Height (m)	Base Elev. (m)	Stack Diameter (m)	Exit Veloc. (m/s)	Exit Temp. (K)	HF Emission Rate (g/s)	PF Emission Rate (g/s)	SO_2 Emission Rate (g/s)	PM_{10} Emission Rate (g/s)	PAH Emission Rate (g/s)	BaP[(2)] Emission Rate (g/s)
Fume Stack 1	542.366	7212.451	78	14	9.45[(3)]	3.17	288.15	0.33	0.018	0	0.45	0	0
Furnace 1	541.776	7211.855	29.5	12	0.8	12.0	553.15	0	0	0	0.05	0	0
Furnace 2	541.816	7211.866	29.5	12	0.8	12.0	553.15	0	0	0	0.05	0	0
Furnace 3	541.856	7211.878	29.5	12	0.8	12.0	553.15	0	0	0	0.05	0	0
Seawater Scrubber 1	542.246	7212.111	40.0	12	4.38	14.0	288.15	0.02	0.012	1.2[(1)]	0.30	1.77E-04	3.54E-06
Seawater Scrubber 2	542.298	7212.141	40.0	12	4.38	14.0	288.15	0.02	0.012	1.2[(1)]	0.30	1.77E-04	3.54E-06
Seawater Scrubber 3	542.350	7212.170	40.0	12	4.38	14.0	288.15	0.02	0.012	1.2[(1)]	0.30	1.77E-04	3.54E-06
Seawater Scrubber 4	542.402	7212.200	40.0	12	4.38	14.0	288.15	0.02	0.012	1.2[(1)]	0.30	1.77E-04	3.54E-06

(1) SO_2 emission rate is based on 3.0% sulfur coke.

(2) The BaP emission rate for the scrubber stacks is 2% of the PAH emission rate.

(3) Gives a normal volume flow of 3,883,249 Nm^3/hr.

Table 2-5. Line Source (Potroom) Emissions Data for Scenario C

Source Descriptio n	Line No.	UTM-28 Coord. Beg. X (km)	UTM-28 Coord. Beg. Y (km)	UTM-28 Coord. End X (km)	UTM-28 Coord. End Y (km)	Release Height (m)	Base Elevation (m)	HF Emission Rate (g/s)	PF Emission Rate (g/s)	SO_2 Emission Rate (g/s)	PM_{10} Emission Rate (g/s)	PAH Emission Rate (g/s)	BaP(1) Emission Rate (g/s)
LINE 1	1	541.899	7212.247	542.815	7212.762	22.5	14	0.59	0.395	2.43 (2)	0.29	2.14E-03	2.14E-05
LINE 2	2	541.943	7212.168	542.859	7212.683	22.5	14	0.59	0.395	2.43 (2)	0.29	2.14E-03	2.14E-05

(1) The BaP emission rate for the potrooms is 1% of the PAH emission rate.

(2) SO_2 emission rate is based on 3% sulfur coke.

Table 2-6. Line Source (Potroom) Emissions Data for Scenario D

Source Descriptio n	Line No.	UTM-28 Coord. Beg. X (km)	UTM-28 Coord. Beg. Y (km)	UTM-28 Coord. End X (km)	UTM-28 Coord. End Y (km)	Release Height (m)	Base Elevation (m)	HF Emission Rate (g/s)	PF Emission Rate (g/s)	SO_2 Emission Rate (g/s)	PM_{10} Emission Rate (g/s)	PAH Emission Rate (g/s)	BaP(1) Emission Rate (g/s)
LINE 1	1	541.899	7212.247	542.815	7212.762	22.5	14	0.76	0.505	2.43 (2)	0.29	2.14E-03	2.14E-05
LINE 2	2	541.943	7212.168	542.859	7212.683	22.5	14	0.76	0.505	2.43 (2)	0.29	2.14E-03	2.14E-05

(1) The BaP emission rate for the potrooms is 1% of the PAH emission rate.

(2) SO_2 emission rate is based on 3% sulfur coke.

<u>Potroom dimensions</u>: Building length = 1081.2m

Building height = 22.5m

Building width = 25.8m

Line source width = 2.9m

Average separation between building = 64.36m

Exit velocity = 1m/s

Total vent length = 984m

Average buoyancy parameter = 1813 m^4/s^3; ΔT = 19.2º C, average exit temperature = 23º C

2.2 Building Downwash Analysis

Because some of the stacks are short and relatively close to buildings or other structures, some building downwash effects will occur. Building downwash will also be a factor for the rooftop vent (line source) emissions. A complete building downwash analysis was conducted to develop wind-direction-specific effective building dimensions for use in the modeling analysis. Results of this analysis are shown in Appendix C.

The building downwash analysis was produced using the Environmental Protection Agency's Building Profile Input Program (BPIP, dated 95086). The program incorporates Good Engineering Practice (GEP) guidance and building downwash guidance to produce the building heights and projected building widths that affect the dispersion of pollutants from the source in question. It has been determined that a building's wake has a direct effect on the dispersion of a pollutant. For every wind direction, this area of influence extends five times L (5L) directly downwind from the trailing edge of the structure, where L is the lesser of the building's height or direction specific projected building width. The area of influence extends 0.5L in the crosswind direction and 2L in the upwind direction. A building's wake effect height is determined by adding 1.5L to the building's height. The building with the largest wake effect height, whose area of influence encompasses a stack, is the dominant influential building for that stack. Wakes from two structures, that are closer than the greater of either structure's L, are considered "sufficiently close" to one another that their wakes effectively act as one. If the projected widths of the structures do not overlap, then the structures are combined and the gap between the two structures is treated as if the gap had been filled with a structure equal in height to the lower structure.

The buildings and emission sources are shown in Figure 2-1. A description of the eight structures tall enough to be included in the building downwash analysis is summarized in Table 2-7.

Table 2-7. Building Dimensions

	Building Length (m)	Building Width (m)	Building Height Above Ground (m)	Base Elevation (m)	Height Above Sea Level (m)
2 potrooms	1081.2	25.8	22.5	14	36.5
Cast House	120	100	22	12	34
Building 345	37.5	37.5	23	17	40
Building 346	43	37.5	17.5	17	34.5
Building 442	67.5	9.375	34	17	51
Anode Plant	More than 4 sides building (see Figure 2-1)		12.3	17	29.3
Silo	Diameter: 25m		55	14	69
4 Sea Water Scrubber Towers Separated by 60m	Radius: 6.2m		25	12	37

3. GEOPHYSICAL AND METEOROLOGICAL DATA

3.1 Modeling Domain and Terrain

The CALMET modeling domain consists of 170 x 170 grid cells centered on the Alcoa facility with a grid size of 0.3 km. The southwest corner of the domain has a UTM Coordinate of 521 km East, 7192 km North in UTM Zone 28, datum NWS-84 (NWS 6370 Radius, Sphere). The size of the domain is 51 km x 51 km.

Gridded terrain elevations are derived from digitized terrain data. In this data set, elevations are in meters relative to mean sea level, and the spacing of the elevations along each profile is approximately 0.092 km. Figure 3-1 shows a contour plot of terrain elevations within the CALMET modeling domain.

3.2 Land Use

The USGS Global Land Use data in the vicinity of the facility has been used to produce a gridded field of dominant land use categories. The land use data were obtained from the USGS FTP site, with a resolution of 0.9 km.

Land use data were processed to produce a 0.3 km resolution gridded field of fractional land use categories. As the USGS Global Land Use dataset has a resolution of 900 meters, in order to map this data onto the 300 meter resolution grid of the modeling domain the gaps were filled with the closest available land use, while accounting for the known coastline boundary. The 38 USGS land use categories were then mapped into 14 CALMET land use categories. Surface properties such as albedo, Bowen ratio, roughness length, and leaf area index were computed proportionally to the fractional land use. The USGS land use categories are described in Table 3-1. Table 3-2 displays the 14 CALMET land use categories and their associated geophysical parameters. Figure 3-2 shows the dominant land use category for each CALMET grid cell in the modeling domain. These land use categories were used for the summer months (beginning of May to the end of October).

Using snow observations recorded at four on-shore stations located within the CALMET domain, a period with total snow cover was determined. This period begins at the end of October and ends at the end of April (not shown). A snow month period is then selected, October 29 through April 26. During the snow month period, all land use categories are set to ice or perennial snow (land use category 90) except for water, forest and urban areas (not shown).

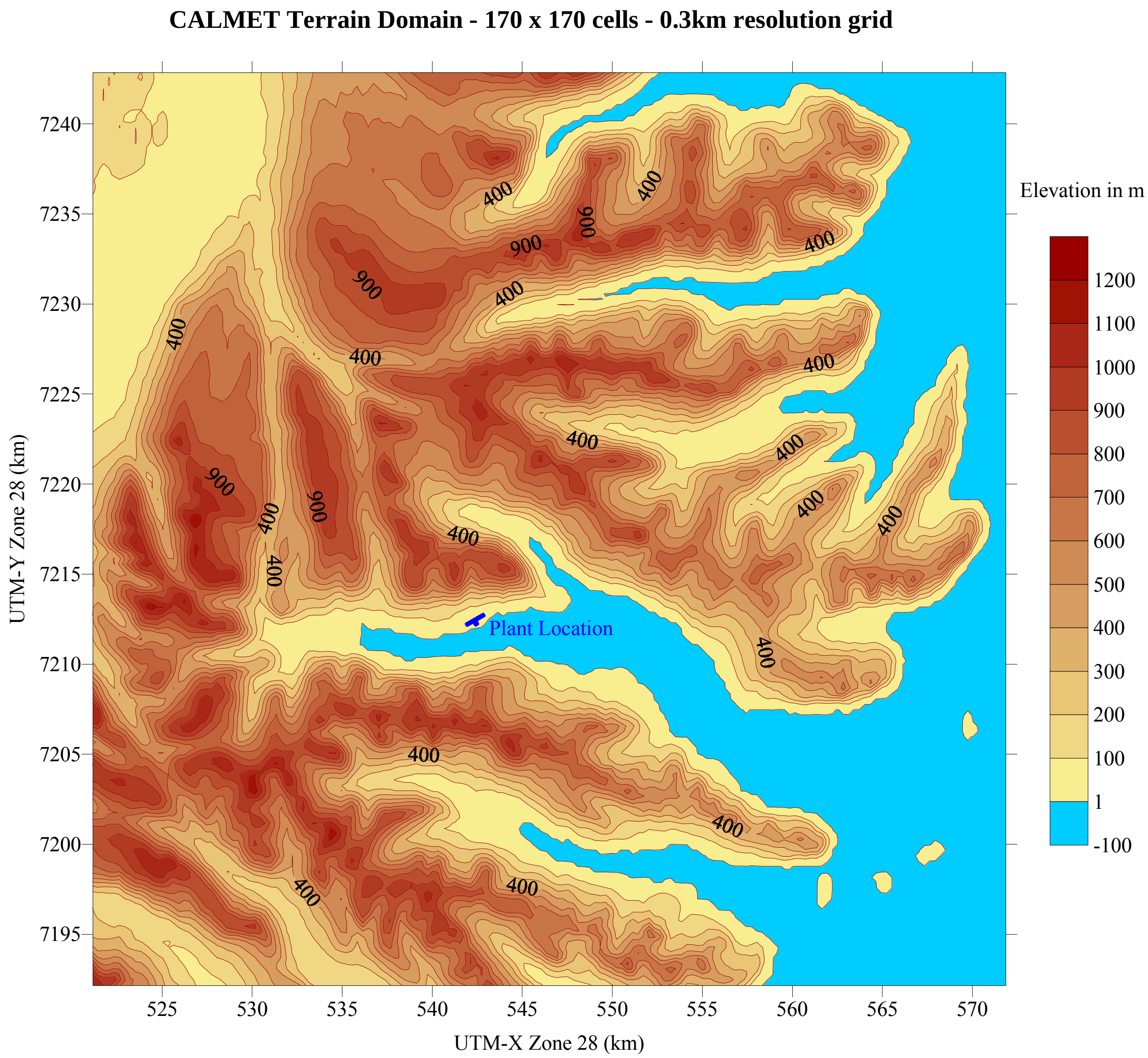


Figure 3-1. Terrain elevations for the CALMET computational domain. The facility is shown by the blue lines.

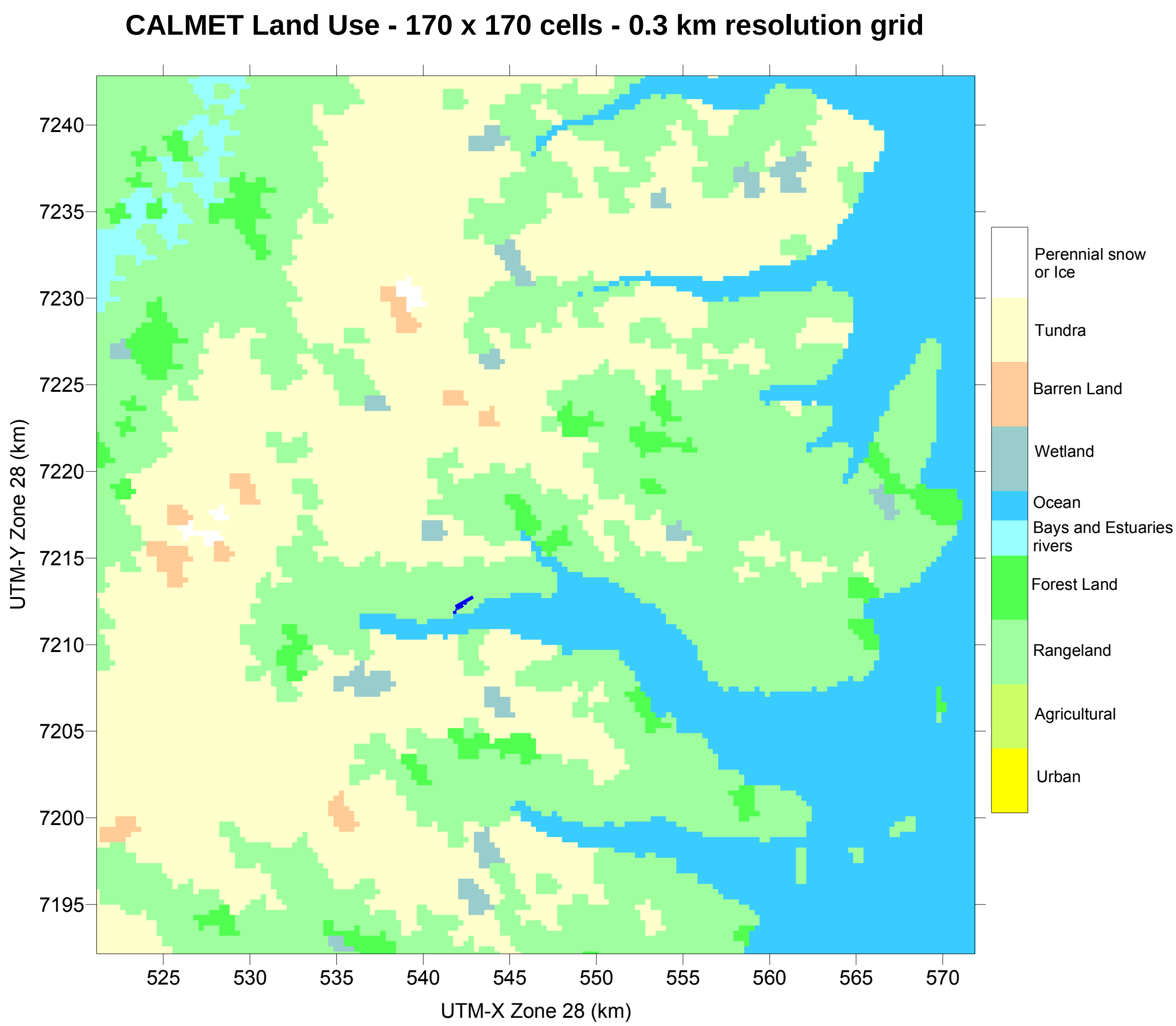


Figure 3-2. Dominant land use categories for the 0.3 kilometer grid resolution for the CALMET computational domain (summer months). The Alcoa facility is shown by the blue lines.

Table 3-1. U.S. Geological Survey Land Use and Land Cover Classification System

Level I		Level II	
10	Urban or Built-up Land	11	Residential
		12	Commercial and Services
		13	Industrial
		14	Transportation, Communications and Utilities
		15	Industrial and Commercial Complexes
		16	Mixed Urban or Built-up Land
		17	Other Urban or Built-up Land
20	Agricultural Land	21	Cropland and Pasture
		22	Orchards, Groves, Vineyards, Nurseries, and Ornamental Horticultural Areas
		23	Confined Feeding Operations
		24	Other Agricultural Land
30	Rangeland	31	Herbaceous Rangeland
		32	Shrub and Brush Rangeland
		33	Mixed Rangeland
40	Forest Land	41	Deciduous Forest Land
		42	Evergreen Forest Land
		43	Mixed Forest Land
50	Water	51	Streams and Canals
		52	Lakes
		53	Reservoirs
		54	Bays and Estuaries
		55	Oceans and Seas
60	Wetland	61	Forested Wetland
		62	Nonforested Wetland
70	Barren Land	71	Dry Salt Flats
		72	Beaches
		73	Sandy Areas Other than Beaches
		74	Bare Exposed Rock
		75	Strip Mines, Quarries, and Gravel Pits
		76	Transitional Areas
		77	Mixed Barren Land
80	Tundra	81	Shrub and Brush Tundra
		82	Herbaceous Tundra
		83	Bare Ground
		84	Wet Tundra
		85	Mixed Tundra
90	Perennial Snow or Ice	91	Perennial Snowfields
		92	Glaciers

Table 3-2. Default CALMET Land Use Categories and Associated Geophysical Parameters Based on the U.S. Geological Survey Land Use Classification System (14-Category System)

Land Use Type	Description	Surface Roughness (m)	Albedo	Bowen Ratio	Soil Heat Flux Parameter	Anthropogenic Heat Flux (W/m^2)	Leaf Area Index
10	Urban or Built-up Land	1.0	0.18	1.5	.25	0.0	0.2
20	Agricultural Land - Unirrigated	0.25	0.15	1.0	.15	0.0	3.0
-20*	Agricultural Land - Irrigated	0.25	0.15	0.5	.15	0.0	3.0
30	Rangeland	0.05	0.25	1.0	.15	0.0	0.5
40	Forest Land	1.0	0.10	1.0	.15	0.0	7.0
50	Water	0.001	0.10	0.0	1.0	0.0	0.0
54	Small Water Body	0.001	0.10	0.0	1.0	0.0	0.0
55	Large Water Body	0.001	0.10	0.0	1.0	0.0	0.0
60	Wetland	1.0	0.10	0.5	.25	0.0	2.0
61	Forested Wetland	1.0	0.1	0.5	0.25	0.0	2.0
62	Nonforested Wetland	0.2	0.1	0.1	0.25	0.0	1.0
70	Barren Land	0.05	0.30	1.0	.15	0.0	0.05
80	Tundra	.20	0.30	0.5	.15	0.0	0.0
90	Perennial Snow or Ice	.05	0.70	0.5	.15	0.0	0.0

* Negative values indicate "irrigated" land use

3.3 Meteorological Data Base

3.3.1 Meteorological stations

The CALMET diagnostic model requires hourly surface observations of wind speed, wind direction, temperature, cloud cover, ceiling height, surface pressure and relative humidity. It also requires an hourly precipitation rate when wet deposition is modeled. In Iceland, these variables are routinely measured by various organizations, including the Icelandic Meteorological Office, Public Roads Administration, National Power Company and Marine Authority. CALMET allows observational data to be supplemented by three dimensional gridded data sets from a prognostic numerical model such as MM5. Table 3-3 lists the types of observational and modeled data available for the modeling including available parameters.

In this study, the CALMET simulations use three dimensional gridded data from the Fifth Generation Penn State/NCAR Mesoscale Model Version 3 (MM5) along with available surface observations. The MM5 data set consists of hourly values of wind speed, wind direction, temperature, and pressure on a grid with a horizontal grid cell size of 1 km and 24 vertical half-sigma levels. The MM5 simulations were conducted by Earth Tech specifically for this application (see Section 4).

Table 3-4 lists the surface stations and precipitation stations included in the CALMET simulations and Figure 3-4 shows a plot of the surface stations and precipitation stations along with the MM5 grid points used in the CALMET computational domain. The surface stations include 17 stations from the Icelandic Meteorological Office, Public Roads Administration, National Power Company and Marine Authority. Four have hourly measurements of precipitation rate. These data were provided to Earth Tech by the Icelandic Meteorological Office.

Three of the meteorological stations were installed in Reydarfjordur in connection with plans for the new aluminum plant. Three meteorological towers are located in the fjord less than 10 km from the project facility and are key data for the CALMET/CALPUFF modeling.

First, at Somastadagerdi on the industrial site, a 38-meter observation mast is located on a low gravel platform. The elevation of the platform is 32 meters above mean sea level. Observations exist from the beginning of May 1998 through to the present, with the same original set of instruments used throughout. Platinum resistance thermometers Logan 100PRT have been used for air temperature observations at 3 meters, 10.5 meters and 36.5 meters above the platform. For observations of wind direction and wind velocity a Wind Monitor-MA 05106, Marine Model, from R.M. Young has been used at a height of 10.3 meters. Two Gill UVW anemometers have also been installed in the mast at 10.8 meters and 36.6 meters, and a Vaisala temperature and relative humidity sensor HMP-35D located at a height of 3 meters is also recording data at this site (Sigurdsson F. H. et al., 2000a).

The two other key meteorological stations included in the modeling are Ljosa and Kollaleira 2. They were installed in June 2000 (Sigurdsson F. H. et al., 2000b). Ljosa is an automatic station located on a promontory named Slaegjubryr, in the hillside above and north of Framnes and approximately 1.5 km northwest of Somastadagerdi. The ground elevation is 280 meters above mean sea level. For observations of wind direction and wind speed, a R.M. Young propeller anemometer of the same type as used at Somastadagerdi was installed at 9.9 meters above the ground. For temperature observations, a platinum resistance thermometer Logan 100PRT with a 6-plate Gill radiation shield is used at 2 meters above the ground. Observations started in the afternoon of June 2, 2000. An automatic station Kollaleira 2, located approximately 5 km west of Somastadagerdi, measuring wind direction, wind speed, temperature and humidity was installed at the manned station of the same name and became operational in the evening of June 3, 2000. Wind and temperature measurements are the same as at Ljosa. The ground elevation is 43.5 meters above mean sea level. The height of the anemometer above ground is 9.5 meters and 2 meters for the thermometer.

Four other meteorological stations located in the Reydarfjordur area have important measurements which are used in the CALMET/CALPUFF modeling (Sigurdsson F. H. et al., 2000b).

- The automatic station Vattarnes was also installed in June 2000 in connection with plans to build the aluminum plant site. It is located on a small peninsula extending northward into the mouth of Reydarfjordur. The ground elevation is 6 meters above mean sea level. Wind and temperature measurements are the same as at Ljosa. The height of the anemometer above the ground is 11.2 meters and 2 meters for the thermometer.

- The automatic station Eskifjordur is located at the end of the fjord Eskifjordur a short way west of the small town with the same name. The ground elevation is approximately 2 meters above mean sea level. Wind and temperature were measured the same way as at Ljosa. Humidity and precipitation are also measured at the station. The height of instruments above ground is 10 meters for the anemometer and 2 meters for the thermometer.

- The automatic weather and road station Oddskard is located at 520 meters height in the hillside of Eskifjordur at the road pass Oddskard. The station is owned by the Public Road Administration.

- The automatic weather station Seley is located on an island approximately 5 km off Krossanes on the north side of the mouth of Reydarfjordur. The station is owned by the Icelandic Maritime Administration. The station ground elevation is 18 meters above mean sea level. The instruments at Seley are the same type as at Ljosa.

The locations of these seven stations are shown in Figure 3-5.

In addition, winds at Fagridalur (34073, Figure 3-4) were rotated by 25 degrees counter-clockwise (recommended by Pordur Arason, personal communication). For the stations Kollaleira, Egilsstadir, Dalatangi and Neskaupstadur all parameters are from the automated stations except for the cloud cover and ceiling height which were measured at the manned (climatic) station of the same name. Hourly precipitation rates were recorded at four of the automatic stations, Egilsstadir, Seydisfjordur, Neskaupstadur and Eskifjordur (Figure 3-6). These four stations were used to create a precipitation data file.

Measurements made at Somastadagerdi were available from June 1998 to May 2002. However, at other stations, including Vattarnes, Ljosa and Kollaleira, data are available only since June 2000 (starting around June 5) up to May 2002. In order to have a complete year with data from several stations, we chose to start the CALMET simulation on July 1, 2000. Thus, the CALMET/CALPUFF modeling is for the period July 1, 2000 through June 30, 2001. Meteorological conditions during the modeled time period is compared with other years in Section 7.

3.3.2 Sea data

As the domain includes both land and water, CALMET requires a SEA.DAT file for the overwater boundary layer model. The SEA.DAT file contains air-sea temperature difference data used with a profile technique to compute the micrometeorological parameters in the marine boundary layer. To create this file, the large-scale analysis data from the National Centers for Environmental Prediction (NCEP) called the NCEP final analysis (FNL), was used with a spatial resolution of 1 degree x 1 degree and a time step of 6 hours. The sea surface temperature (SST) and air temperature at 2 m were extracted at the grid point closest to the shore, east of the fjord (13W, 65N). Figure 3-6 shows a plot of air temperature and SST at this grid point, averaged daily for the modeling period July 1, 2000 to June 30, 2001. The FNL data SST are compared to observations of SST in Mjoifjordur (Figure 3-7), located north of Reydarfjordur measured by the Iceland Marine Research Institute at 1 meter below mean low spring tide and daily averaged, but the air temperature was not measured at the same time. These observations were provided by Gunnar G. Tomasson. The annual cycle is well represented in both dataset, while the observed SSTs are about 2.5 degrees smaller than FNL data during winter months (October to April). Considering the difference in location, FNL SSTs are a good representation of sea temperature offshore of Reydarfjordur. In addition, since the FNL data set is available at a higher resolution time step than observations and give air temperature at the same location as the sea temperature, it was used to create the SEA.DAT file used in CALMET.

Table 3-3. Meteorological Data Sources and Parameters Available

Type of Dataset	Frequency	Source	Parameters
Surface	Hourly	Various sources	- Wind speed, wind direction, - air temperature, - ceiling height, cloud cover, - relative humidity, - surface pressure, - precipitation rate
Modeled Profiles	Hourly	Produced by MM5	- Gridded fields of winds, - temperature, - pressure, - relative humidity

Table 3-4. Summary of Surface Meteorological Stations Near or Within the CALMET Modeling Domain

Station Name	Source	Station Identifier	Parameters Available	Latitude (° N)	Longitude (° W)	UTM East (km)	UTM North (km)	Elevation (m)
Seley	MA	5993	W,T,Rh,P	64.983	13.517	569.976	7207.188	18
Kollaleira	IMO	5975	W,T,Rh,Cld	65.037	14.240	535.790	7212.601	43.5
Ljosa	IMO	5977	W,T,Rh	65.043	14.162	539.440	7213.348	280
Vattarnes	IMO	5988	W,T,Rh	64.937	13.685	562.175	7201.886	6
Somastadagerdi	IMO	7078	W,T,Rh	65.033	14.111	541.871	7212.234	32
Egilsstadir	IMO	4271	W,T,Rh,P,Cld,Prc	65.276	14.405	527.769	7239.153	24
Dalatangi	IMO	4193	W,T,Rh,P,Cld	65.268	13.575	566.523	7238.882	10
Seydisfjordur (3m)	IMO	615	W,T,Rh,P,Cld	65.262	14.009	546.274	7237.826	3
Seydisfjordur (93m)	IMO	4180	W,T,Rh,Prc	65.281	14.000	546.661	7239.950	93
Neskaupstadur	IMO	5990	W,T,Rh,Prc	65.150	13.669	562.412	7225.637	50
Eskifjordur	IMO	5981	W,T,Rh,Prc	65.076	14.037	545.283	7217.077	2
Oddskard	PRA	34087	W,T,Rh	65.064	13.919	550.855	7215.830	520
Fagridalur	PRA	34073	W,T,Rh	65.126	14.333	531.306	7222.470	333
Hallormsstadahls	NPC	5960	W,T,Rh	65.080	14.675	515.281	7217.161	573
Kambanes	IMO	5885	W,T,Rh	64.801	13.842	555.013	7186.586	30
Fjardarheidi	PRA	34175	W,T,Rh	65.266	14.259	534.596	7238.111	600
Gagnheidi	IMO	4275	W,T,Rh	65.223	14.259	65.223	14.259	949

W=wind speed + wind direction; T=air temperature; Rh= relative humidity; P=pressure; Cld= Cloud cover or/and ceiling height; Prc=hourly precipitation rate.

MA = Marine Authority; PRA = Public Roads Administration; IMO = Icelandic Meteorological Office; NPC = National Power Company

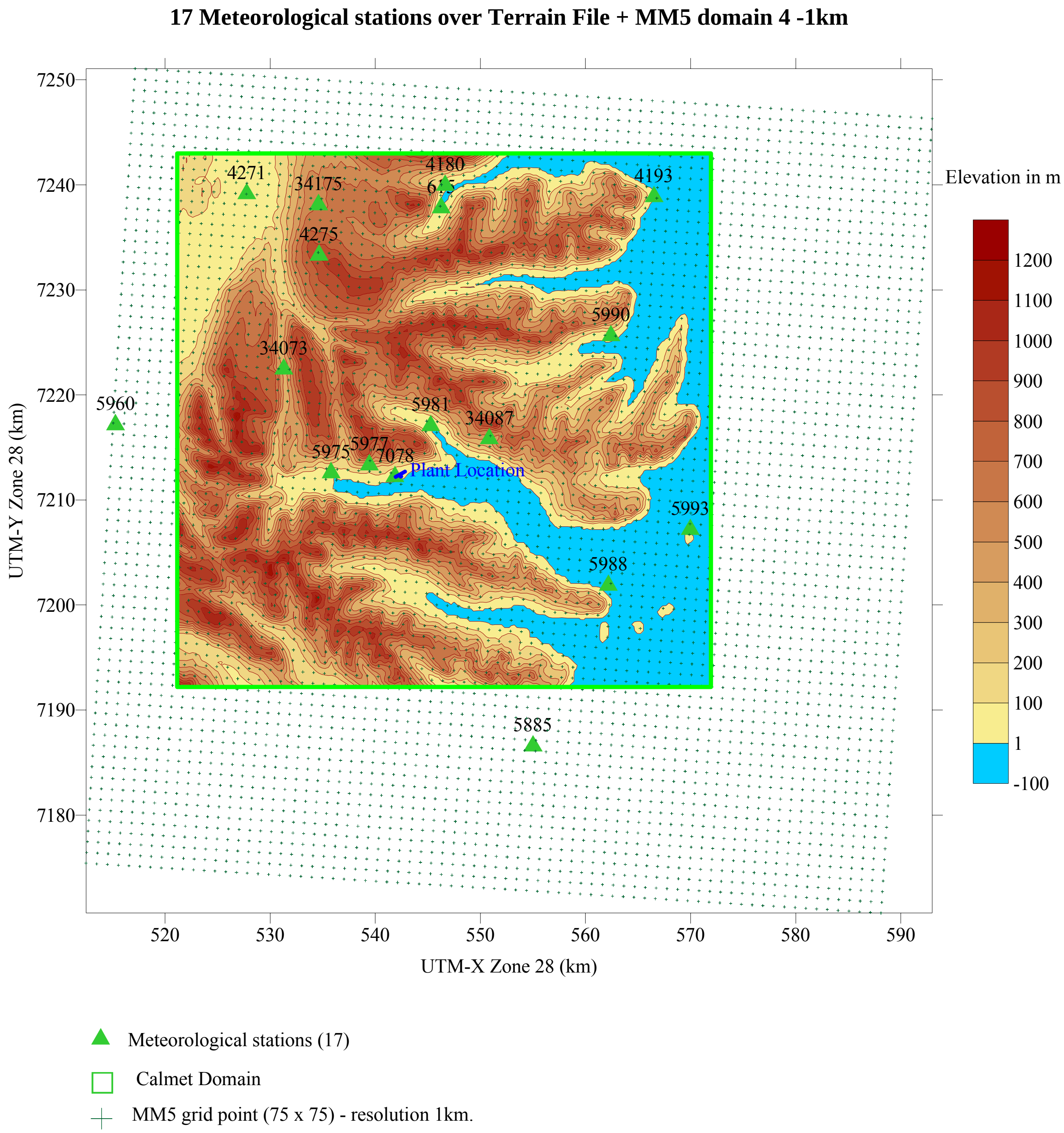


Figure 3-4. Locations of meteorological observations sites used in the CALMET modeling. The dark green crosses are the MM5 grid points and the blue line is the industrial site. The light green square is the CALMET computational domain. The meteorological stations are represented by green triangles.

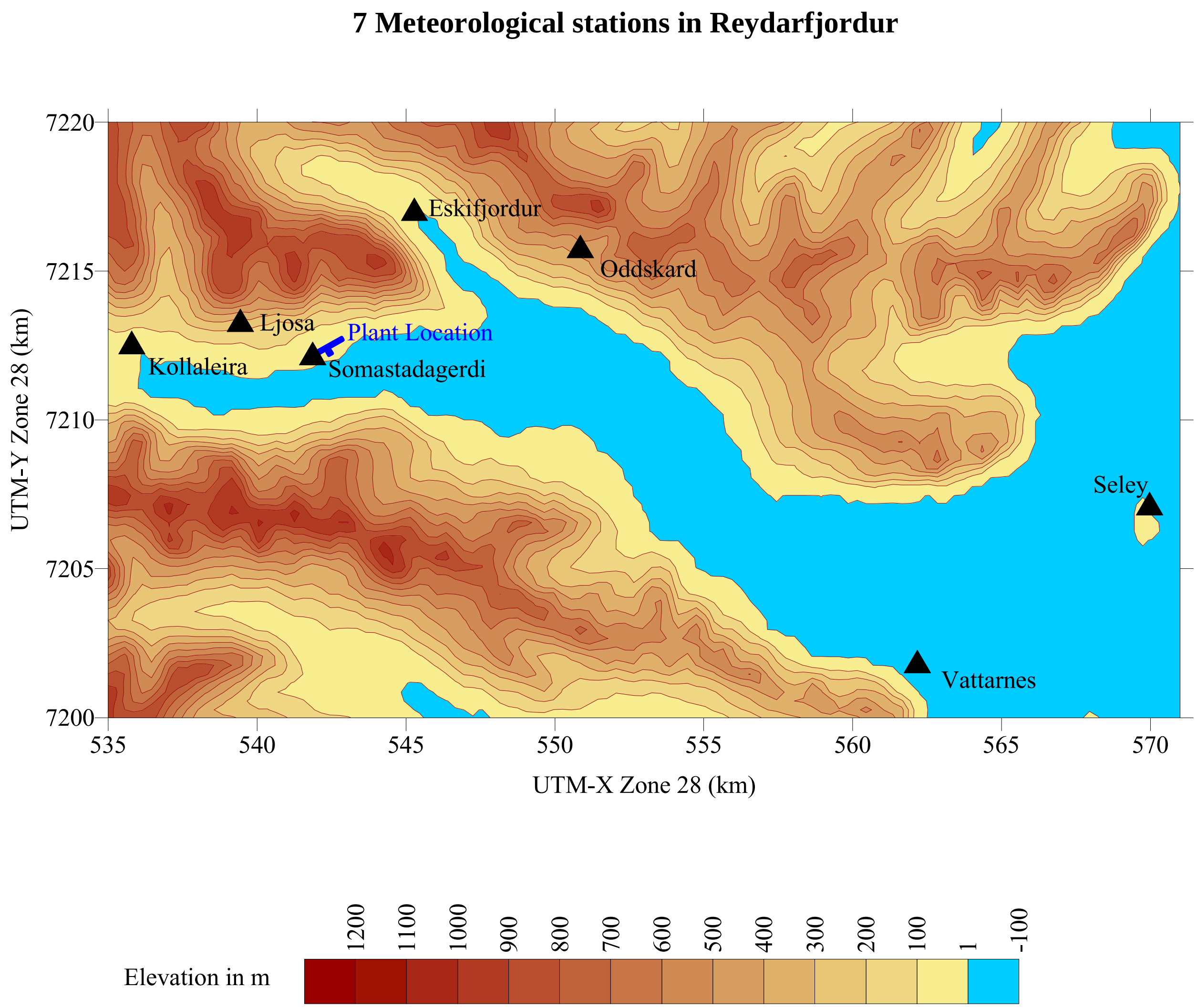


Figure 3-5. Locations of 7 meteorological observations sites used in the CALMET modeling located in Reydarfjordur. The blue line is the industrial site.

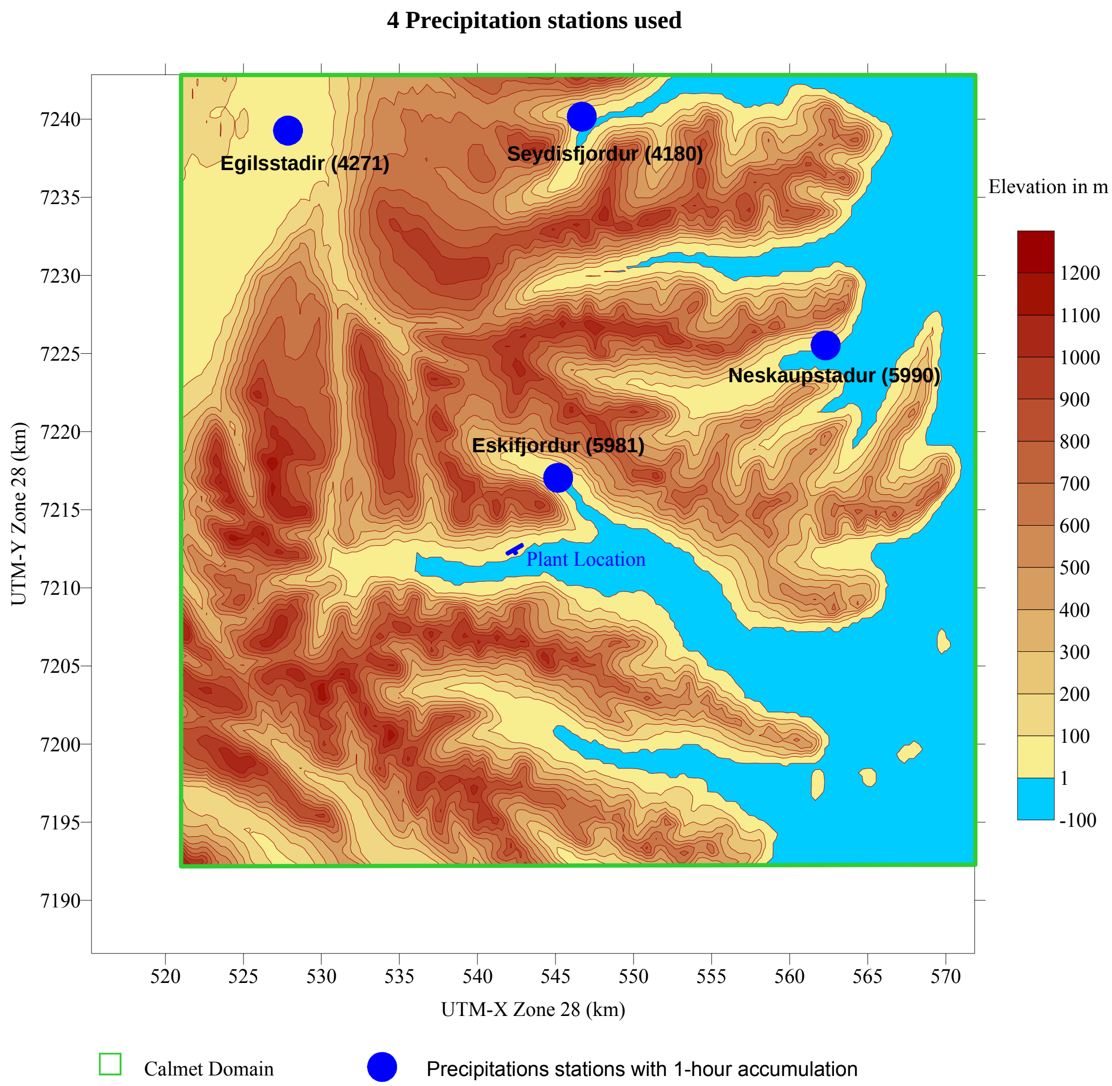


Figure 3-6. Locations of the 4 meteorological observations sites used in the CALMET modeling as precipitation stations. The blue line is the industrial site.

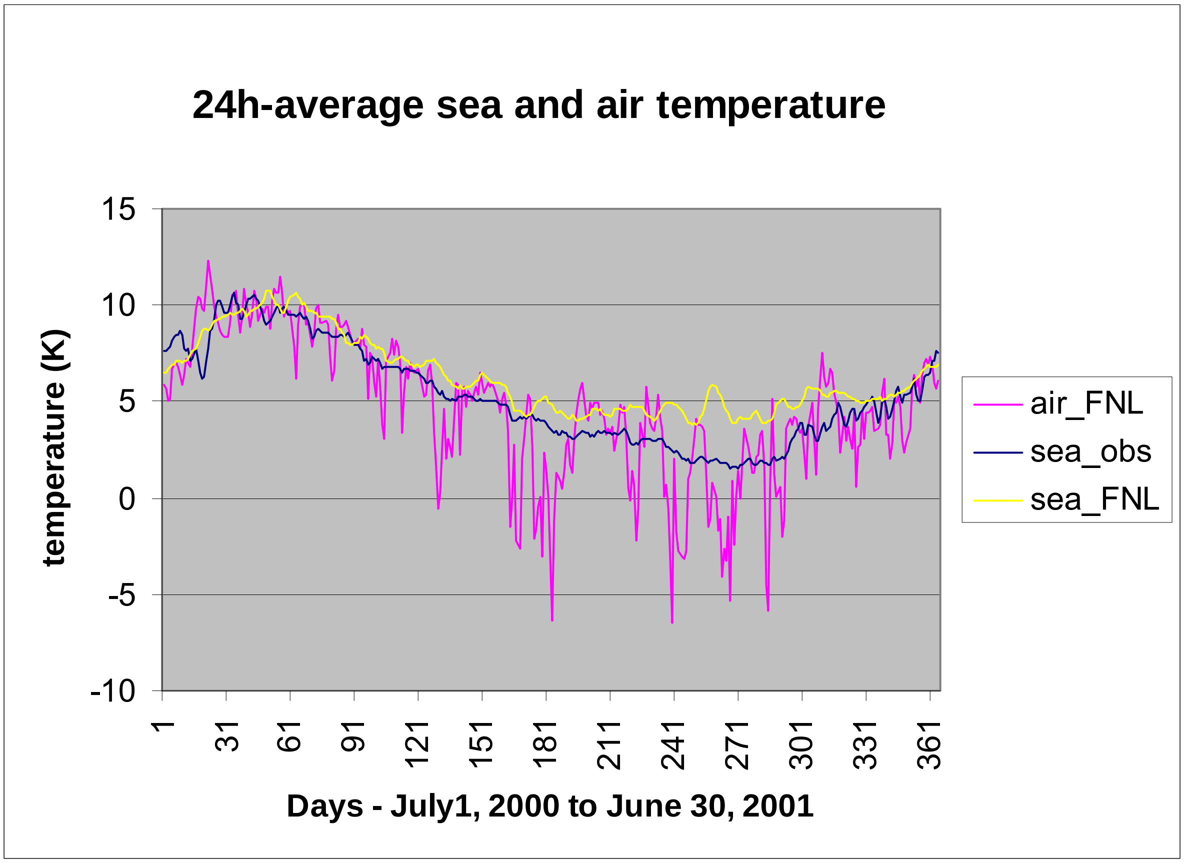


Figure 3-7. 24h-averages of Sea Surface Temperature (SST) and air temperature for the FNL grid point offshore of Reydarfjordur (13W, 65N) plotted with 24h-averages of SST observations in Mjoifjordur.

4. MM5 SIMULATIONS

4.1 MM5 Description

The Fifth Generation Penn State/NCAR Mesoscale Model (MM5) is a three-dimensional numerical weather prediction model maintained at the National Center for Atmospheric Research (NCAR). MM5 can be run with multiple nested grids. It contains non-hydrostatic dynamics, a variety of physics options and the capability to perform Four Dimensional Data Assimilation (FDDA). MM5 is capable of simulating a variety of meteorological phenomena such as tropical cyclones, severe convective storms, sea-land breezes, and terrain forced flows such as mountain valley wind systems.

MM5 was used in this analysis to develop high-resolution three-dimensional meteorological fields through FDDA simulations to serve as an initial guess field for the CALMET Diagnostic Meteorological Model. The FDDA simulations involved running MM5 for the one-year period used in this study (July 2000 - June 2001) and then nudging the model solutions (i.e. predictions) toward a gridded analysis at regular intervals. This gridded analysis places a constraint on the model predictions so that the resulting meteorological fields are consistent with observational data for a given time interval and at the same time are dynamically balanced. This gridded analysis is developed using surface and upper air observations over the MM5 modeling domain and consists of both a full three dimensional meteorological analysis and a surface analysis. The result of the MM5 simulations with FDDA is a high resolution three dimensional gridded data set of meteorological fields (i.e. wind, temperature, pressure etc).

Figure 4-1 shows an example of the MM5 model's multi-nested horizontal grid configuration. A staggered grid cell configuration known as the Arakawa-Lamb B staggered grid is used by MM5. In this grid configuration scalars such as temperature or moisture variables are defined at the center of a grid cell known as the cross points. The vector quantities (e.g., u and v wind components) are defined at the corners of each grid cell known as the dot points.

Typically, meteorological analysis is performed on constant pressure levels instead of height. MM5 uses a terrain following vertical coordinate where the model vertical levels are defined by a dimensionless quantity σ. The σ coordinate is defined as:

$$\sigma = \frac{(P - P_t)}{(P_s - P_t)}$$

Where P = Pressure
P_t = Constant top pressure
P_s = Surface pressure

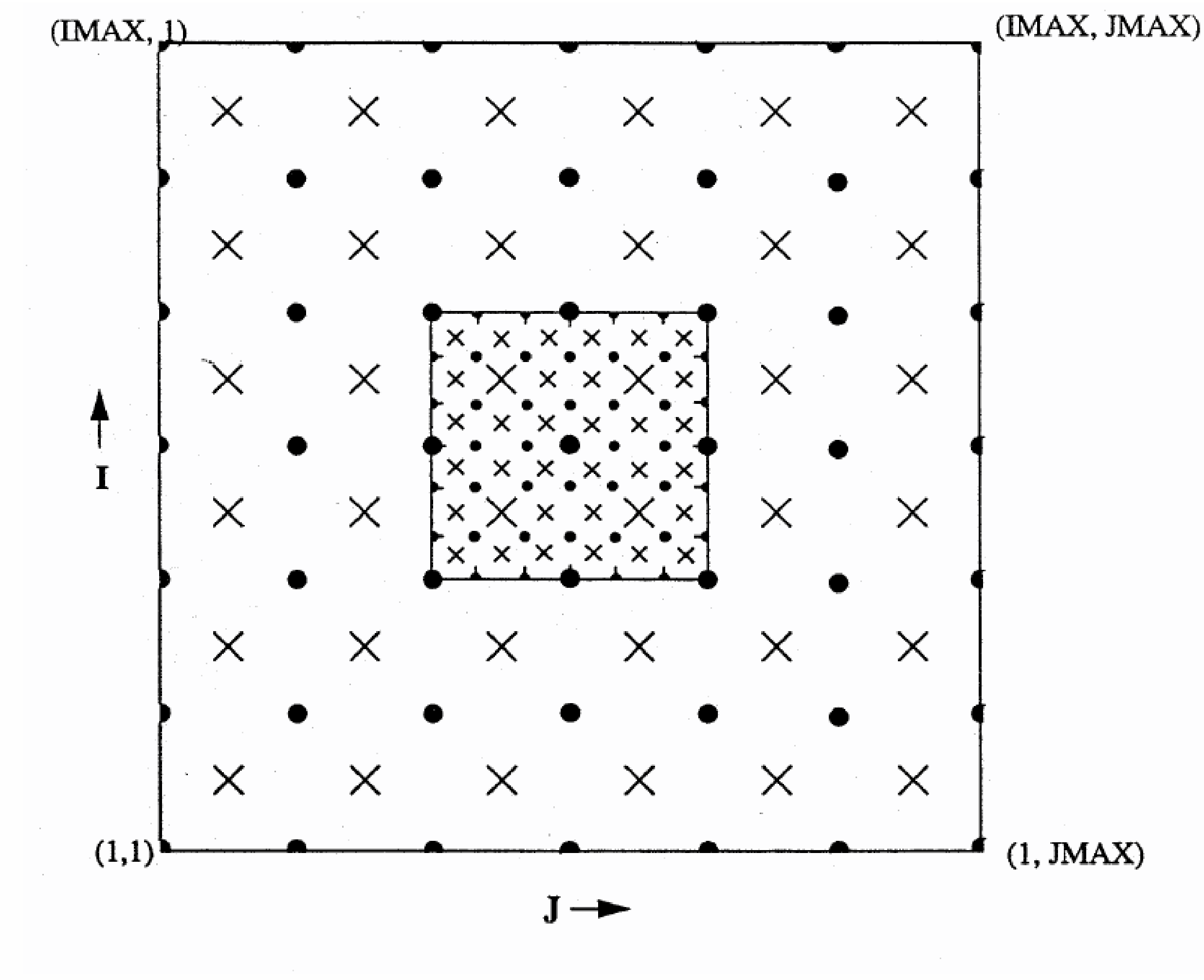


Figure 4-1. MM5 horizontal grid (Arakawa B-grid) showing the staggering of the dot (.) and cross (X) grid points. The smaller inner box is a representative mesh staggering for a 3:1 coarse-grid distance to fine-grid distance ratio (from Dudhia et al., 2000).

The σ coordinate has a value of zero at the top of the model and a value of 1 at the surface. Figure 4-2 shows a schematic of the σ layer vertical structure used by MM5.

The MM5 modeling system uses several preprocessor programs to prepare input data for the model simulations. Figure 4-3 shows a flow chart of the MM5 modeling system showing how the various support programs interface with MM5. The terrain preprocessor is used to interpolate gridded terrain elevations and land use data onto the MM5 modeling grid. The REGRID preprocessor interpolates meteorological analysis data sets from some native grid to the MM5 grids while the RAWINS preprocessor improves the REGRID derived analysis by performing an objective analysis using surface and upper air observations. The RAWINS preprocessor will provide three dimensional meteorological fields used for initial and lateral boundary conditions, provide three dimensional fields for analysis nudging, and surface fields used for surface nudging during the FDDA process.

The INTERPF program takes the various analysis fields generated by REGRID and RAWINS and prepares the data for input to the MM5 Model. INTERPF performs vertical interpolation of the analysis fields to the model σ levels and generates the boundary condition files used by MM5.

4.2 MM5 Configuration

MM5 data to drive the CALMET model was obtained from simulations that are described below. Initial simulations were carried out to test the sensitivity of model output to the domain grid sizes. Two main types of simulations were performed that involved the exclusion and inclusion of Greenland in the modeling domain. Prior studies have shown the presence of a dominant wintertime surface low-pressure system between Greenland and Iceland – the so-called 'Icelandic Low'. The wintertime area of this Icelandic low is a preferred spot for creation of mesocyclones of which many do not travel far. Thus it is essential to have a proper reproduction of the system in the model runs. In order to minimize any boundary effects and to let the model generate its own 'Icelandic Low', we expanded the initial domain (without Greenland) to include the whole of Greenland and also parts of Northern Canada.

The MM5 modeling in this study includes in total four domains. Domains 1 and 2 were one-way nested whereas Domains 2, 3 and 4 were two-ways nested. Geographical locations of the domains are presented in Figure 4-4. The center of the coarse domain (Domain 1) was located at 67.1°N, 18.5°W. Since the MM5 modeling is over a region close to the North Pole, the Polar Stereographic (PS) map projection was used in the model coordinates. The standard latitude of the projection was 60°N. This domain covers almost the entire North Atlantic Ocean and includes besides

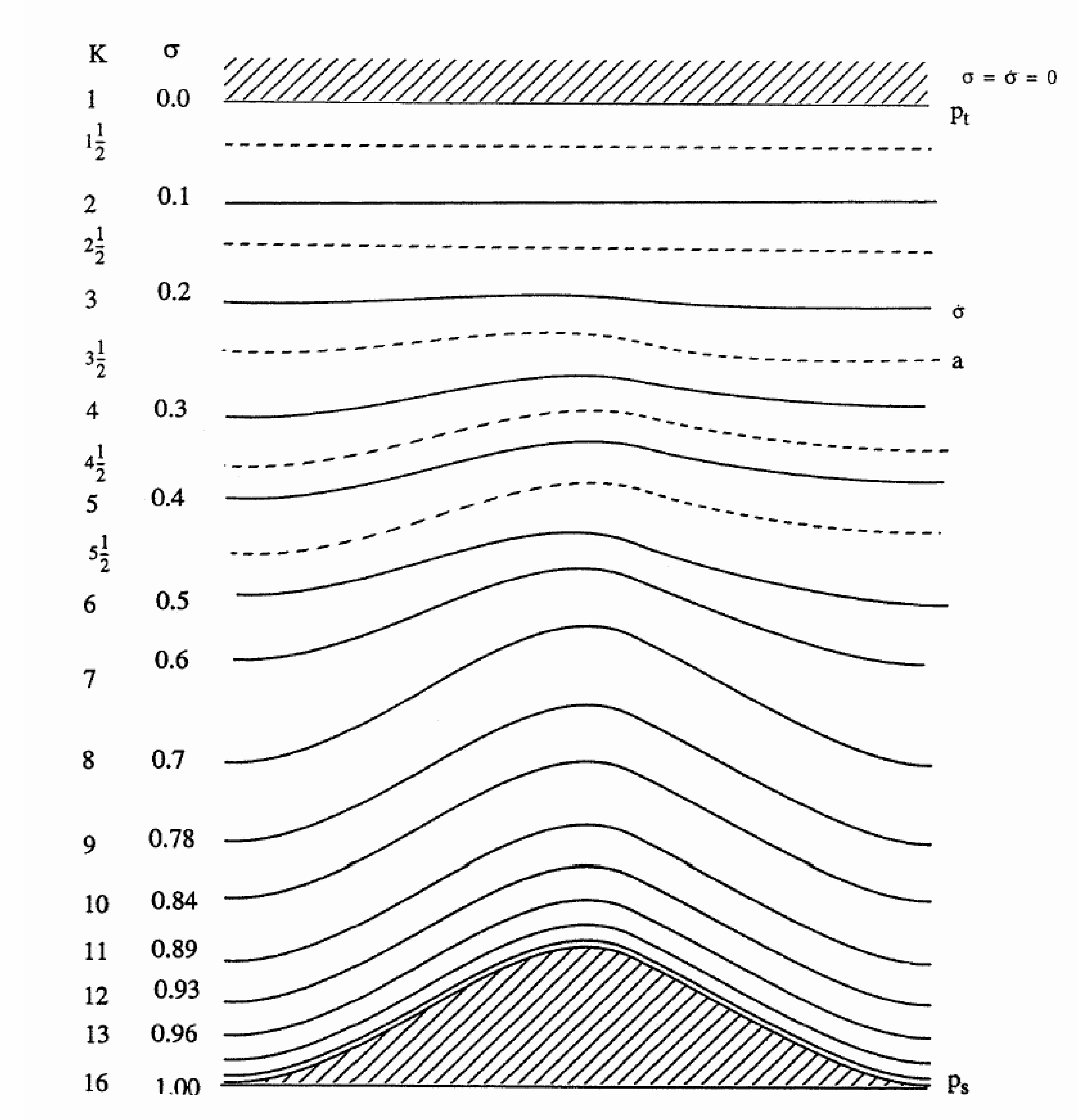


Figure 4-2. Schematic representation of the vertical structure used in MM5. The example is for 15 vertical layers. Dashed lines denote half-sigma levels, solid lines denote full-sigma levels (from Dudhia et al., 2000).

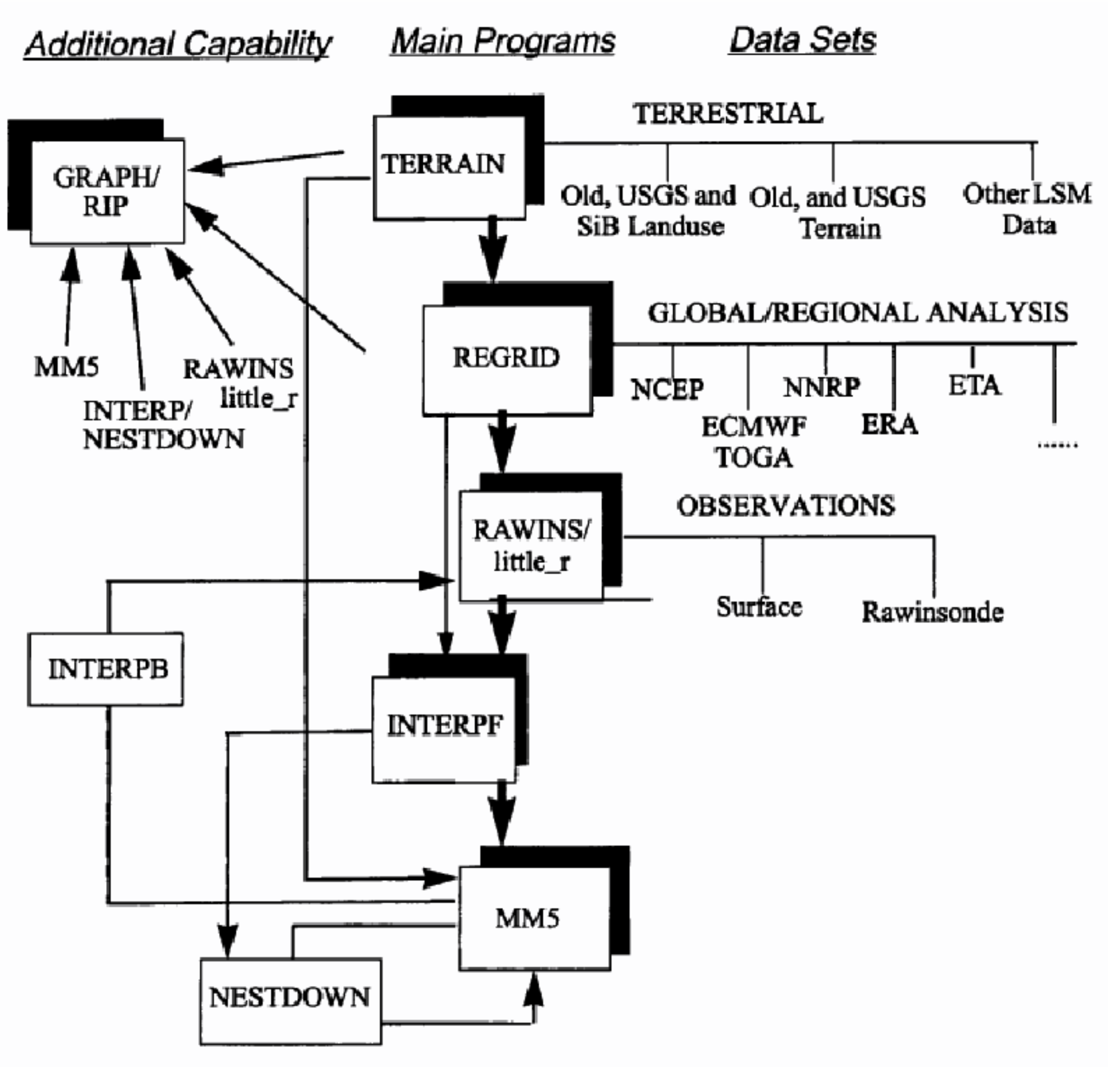
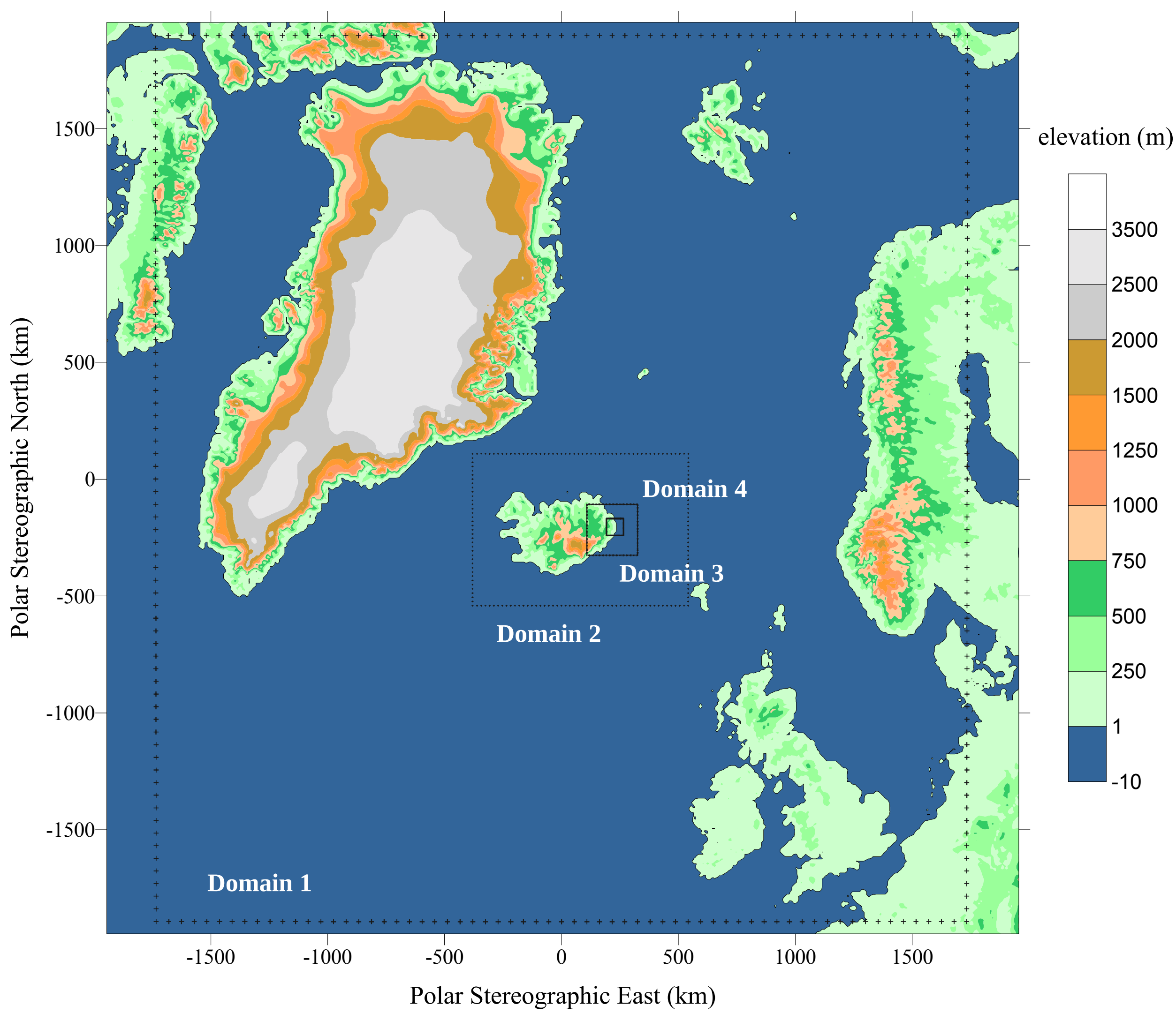


Figure 4-3. Flow chart of MM5 modeling system (Dudhia et al., 2000).

MM5 Domains over Iceland
Polar Stereographic Center: 67.1 N, 18.5 W
True Latitude: 60 N



Domain 1: 3870 km X 3600 km (87 X 81 - DX = 45 km)
Domain 2: 810 km X 540 km (91 X 61 - DX = 9 km)
Domain 3: 144 km X 144 km (49 X 49 - DX = 3 km)
Domain 4: 75 km X 75 km (76 X 76 - DX = 1 km)

Figure 4-4. Plot of MM5 modeling domains with terrain elevations.

Iceland, the whole of Greenland, Norway, United Kingdom and parts of Western Europe and northern parts of Canada with a total area of about 14×10^6 km^2. The grid spacing was 45 km. The second-nesting domain (Domain 2) covers all of Iceland with a grid size of 9 km. The third and the fourth nesting domains (Domains 3 and 4) were selected based on the needs of CALMET modeling and were more or less centered on the location of the facility (Figure 4-5). The grid spacing of these domains were 3 km and 1 km, respectively. Table 4-1 lists the details of configurations for the four domains. In the vertical direction, there were 25 sigma levels (24 half sigma levels) from the surface to 100 hPa, located at the sigma values of 1.00, 0.996, 0.992, 0.983, 0.973, 0.961, 0.948, 0.933, 0.916, 0.897, 0.875, 0.851, 0.823, 0.792, 0.756, 0.716, 0.670, 0.618, 0.559, 0.493, 0.418, 0.333, 0.236, 0.128, 0.0. More details of vertical levels are presented in Table 4-2.

The terrain elevation and land use category were from the 5-min, 2-min, 30-sec (~9 km, ~4 km, ~0.9 km, 0.9 km, respectively) global data set for Domains 1 through 4. The terrain elevations of all domains are shown in Figure 4-4.

The MM5 model was run in the non-hydrostatic mode. Two-way nesting was used between Domains 2 to 4. Extensive research has been done in mesoscale modeling in the polar regions with the development of the polar version of MM5 – the Polar MM5 (Bromwich et al., 2001; Cassano et al., 2001). Our model settings were based on the options recommended from the work of the Polar MM5 research team. The mixed phase explicit moisture scheme that represents microphysics parameterizations (Reisner et. al., 1998) was used in all domains. The Grell cumulus parameterization scheme (Grell et. al., 1994) was used for convections in Domains 1, 2 and 3, while explicit convection was carried out for Domain 4. The Grell scheme uses the updraft and downdraft fluxes and the compensating flow to determine the heating and moisture vertical profiles. The planetary boundary layer module is from the NCEP Eta Model. Turbulent fluxes in the atmosphere and the turbulent fluxes between the atmosphere and the surface are parameterized using the 1.5 order turbulence closure parameterization. The region of our modeling experiences long periods of darkness and light. For this we used a sophisticated radiation scheme based on the NCAR community climate model (CCM2) (Hack et. al. 1993). The scheme accounts for the long wave and short wave interactions with cloud and clear air. The cloud cover is predicted as a simple function of the grid box relative humidity, with the cloud liquid water path determined from the grid box temperature. The five-layer soil model was used to predict soil temperatures at about 1, 2, 4, 8, and 16 cm. The vertical resolved soil temperature profile allows rapid response to surface temperature changes. The SOILFAC parameter in the MM5 deck was increased to 1.5 in order to reduce the timestep in the soil model calculations. With larger timesteps, instability in numerical calculations significantly deteriorates the integration results. Physics options employed in the MM5 simulations are shown in Table 4-3.

MM5 was initialized using the large-scale analysis data from NCEP at NCAR. The NCEP Final Analysis (FNL) (http://dss.ucar.edu/datasets/ds083.2) data archived at NCAR exists every 6 hours at a spatial resolution of 1^o x 1^o at 21 standard pressure levels under 100 hPa: the surface, 1000, 975, 950, 925, 900, 850, 800, 750, 700, 650, 600, 550, 500, 450, 400, 350, 300, 250, 200, 150, and 100 hPa. The data include two-dimensional variables of snow cover, sea surface temperature, and sea level pressure, and three-dimensional variables of temperature, geopotential height, U and V components, and relative humidity. Sea surface temperature (SST) data was available from two other sources – Real Time Global SST (RTG SST) analysis from NOAA (0.5^ox0.5^o resolution) and MODIS (Moderate Resolution Imaging Spectroradiometer) from NASA (4-km resolution). However, model calculations from the FNL SST data were the most encouraging. MM5 now has an option to vary the lower boundary condition with respect to time. Hence we employed this option to provide a realistic representation of the time variation of the lower boundary condition. For the FNL dataset, the temporal resolution of the data being 6 hours, the lower boundary conditions were updated every 6 hours. Moreover, the SST data was interpolated to the four domain grids prior to the start of the simulation. This assures that the spatial lower boundary condition comes from the original FNL dataset. Alternatively, MM5 interpolates the lower boundary on the fly. In this case, the lower boundary values for domains 2 through 4 come from those integrated in domain 1 and may not be the original FNL values.

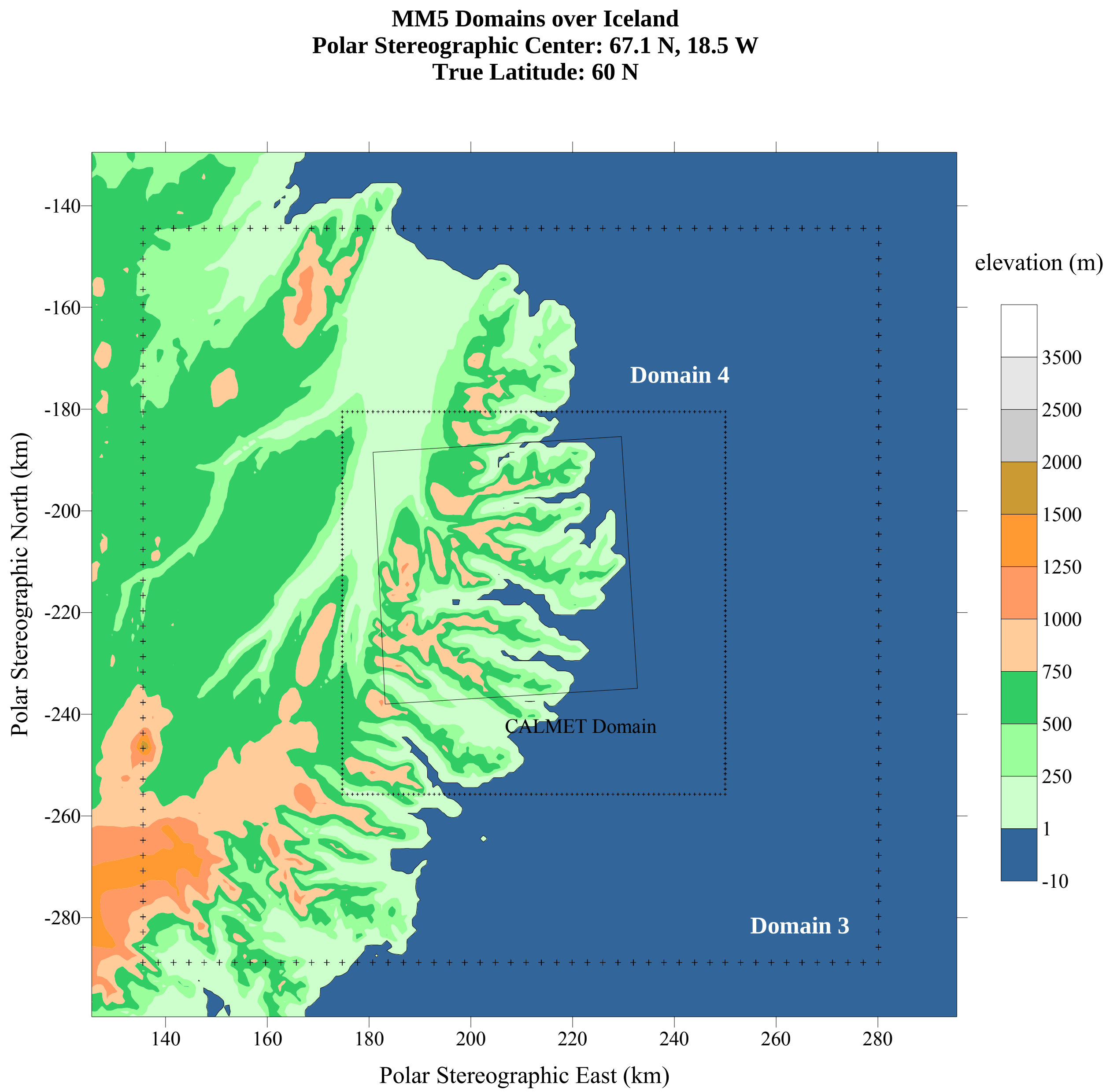
Four dimensional data assimilation (FDDA) was used to force the model integration to the fields from the FNL data. Only three-dimensional FDDA was carried out since the surface observations were with a time resolution of 6 hours. In the FDDA, only Domain 1 (D1) was nudged toward the observations while the model integrated Domains 2, 3 and 4. Winds, temperature and moisture were nudged to the observed values every 6 hours. Further details about the runtime options and the nudging coefficients are given in Table 4-4.

The MM5 simulations were carried out on a 17-node, 34-processor Bewoulf Cluster running Linux. A parallel version of MM5 – the MM5 MPP was used for this purpose. The underlying model development of this version is the same as the original MM5, but provides additional capabilities for the model to be run on distributed memory machines. However, while analyzing the results from the MM5 MPP version of the model in memory distributed mode, we discovered at the end of December, 2002 that the radiation scheme (CCM2) was not working properly due to a bug in the NCAR parallel code.

At this point, additional test simulations were conducted. In early January 2003, it was determined that the option to run MM5 MPP in single processor mode did not contain the coding error in the radiation flux calculation. Because the CCM2 radiation scheme worked properly when run in single processor mode, the MM5 simulations were re-run in this mode, using each processor of the Beowulf cluster to simulate a different time period. In early February, NCAR confirmed the code error, and has provided a code fix to eliminate the problem in parallel mode runs (see Appendix D).

A second change made in the re-runs of MM5 included a higher spatial resolution for the inner domains. Testing performed as part of the diagnostic analysis of the radiation problem showed improved results with a higher resolution inner domain. In the final runs, the Domain 4 resolution was increased from 2 km to 1 km. Hence, the 4 Domains described above, were selected based on these criteria.

The model was run in single processor mode. Each MM5 simulation was 6-day long with one day of overlap between simulations. The first day of each run was discarded as an initialization spin-up period, and the final 5 days of each run were appended to other runs to form a complete and continuous full year dataset. Up to 32 MM5 simulations were run at the same time, one on each slave processor (the 2 master processors were reserved for other system functions).



Domain 3: 144 km X 144 km (49 X 49 - DX = 3 km)
Domain 4: 75 km X 75 km (76 X 76 - DX = 1 km)

Figure 4-5. MM5 Domain 3 and MM5 Domain 4 along with the CALMET domain.

Table 4-1. Configuration of MM5 domains

Domain #	Dimensions (kmxkm)	Map Projection	Grid size (km)	Vertical Levels	Grid Numbers	Mother Domain	Mother Domain (i, j)	Terrain Resolution (km)
Domain 1	3870x3600	PS	45	24	87x87			9
Domain 2	810x540	PS	9	24	91x61	1	36,30	4
Domain 3	144x144	PS	3	24	49x49	2	56,24	0.9
Domain 4	75x75	PS	1	24	76x76	3	14,12	0.9

Table 4-2. Vertical Wind Levels in the MM5 Modeling

Level No.	½ sigma lev	Ref P (mb)	Height (m)
1	0.998	1008.18	14.51
2	0.994	1004.54	43.59
3	0.988	998.63	91.03
4	0.978	989.98	160.78
5	0.967	979.97	242.17
6	0.955	968.60	335.49
7	0.941	955.86	441.07
8	0.925	941.30	563.16
9	0.907	924.94	702.36
10	0.886	906.26	863.36
11	0.863	885.33	1047.24
12	0.837	861.67	1259.42
13	0.807	834.37	1510.20
14	0.774	803.89	1798.24
15	0.736	769.76	2131.37
16	0.693	730.63	2528.39
17	0.644	686.04	3002.29
18	0.589	635.54	3569.97
19	0.526	578.66	4254.28
20	0.456	514.51	5093.85
21	0.376	441.71	6153.72
22	0.285	359.35	7533.06
23	0.183	266.08	9430.51
24	0.064	158.24	12399.89

Table 4-3. Physics Options Used in the MM5 Modeling

Domain #	Explicit Moisture Schemes (IMPHYS)	Cumulus Schemes (ICUPA)	PBL Scheme (IBLTYP)	Radiation Cooling of Atmosphere (FRAD)	Shallow Convection (ISHALLO)	Multi Layer Soil Model (ISOIL)
Domain 1	Mixed Phase	Grell	ETA-Yamada-Mellor	CCM2	None	Yes
Domain 2	Mixed Phase	Grell	ETA-Yamada-Mellor	CCM2	None	Yes
Domain 3	Mixed Phase	Grell	ETA-Yamada-Mellor	CCM2	None	Yes
Domain 4	Mixed Phase	None	ETA-Yamada-Mellor	CCM2	None	Yes

Table 4-4. Runtime Options Used in the MM5 modeling

3D Data	SST Data	Time-varying SST	Update Frequency of SST	Space-varying SST	Runtime	Integration Timestep
FNL	FNL	Yes	24 hours	Yes	6 days with 1day overlap	108 sec

FDDA	Domains Nudged	Fields Nudged	Frequency of Nudging	Nudging Coefficients		
				Wind	Temperature	Moisture
3D (analysis)	D1	Winds, temperature, moisture	6 hours	2.5E-04	2.5E-04	1.0E-05

5. AIR QUALITY MODELING METHODOLOGY

5.1 Model Selection

Principal factors in the selection of a modeling approach included the complex terrain of the region, the importance of light wind and calm wind conditions and flow reversals, the need to handle both buoyant line and point sources, the importance of building downwash effects, the importance of spatial inhomogeneities in the meteorological fields due to terrain features and a nearby water body and significant anthropogenic heat fluxes. The complex terrain considerations include the need to incorporate terrain channeling effects on the flow field, diurnally varying slope flows (downslope at night, upslope during the day), and representing the strong spatial variability of the wind fields over relative short distances. The ability to treat plume interactions and plume impingement on terrain above stack height are also important.

The CALMET/CALPUFF modeling system (Scire et al., 2000a,b) was used in the modeling of the Somastadagerdi facility. CALPUFF, and its meteorological model CALMET, were designed to handle the complexities posed by the complex terrain location and the other issues listed above. CALMET is a diagnostic meteorological model that produces three-dimensional wind and temperature fields and two-dimensional fields such as mixing heights and stability class. It contains slope flow effects, terrain channeling, and kinematic effects of terrain. CALPUFF is a non-steady-state Gaussian puff model. It includes algorithms for building downwash effects of both point sources and buoyant line sources. One capability of CALPUFF not found in CONDEP or MATHEW/INPUFF is the ability to treat the combined effects of multiple processes (e.g., building downwash effects in complex terrain; dry deposition and overwater dispersion, etc.). A complete summary of the capabilities and features of CALMET and CALPUFF is provided in Sections 5.1.1 and 5.1.2. CALMET Version 5.542 and CALPUFF Version 5.714 were used for the current analysis.

Models used in the previous studies of the area of interest such as CONDEP or MATHEW/INPUFF model have several important limitations. One important limitation is that CONDEP is a steady-state, straight line plume model that cannot respond to the spatial variability to the wind fields. CONDEP uses spatially-invariant wind fields based on single-station wind observations, which are not allowed to vary in space. Another factor is CONDEP does not account for dispersion during low wind speed and calm wind events. Calm hours are excluded from the analysis by CONDEP. Also, CONDEP accounts for only point sources and not line sources. In MATHEW/INPUFF, while line sources are accounted for, they are treated as non-buoyant volume sources which can result in a significant overestimation of impacts due to the lack of consideration of buoyancy effects. CONDEP does not account for spatial inhomogeneities in the meteorological fields due to the presence of water bodies, anthropogenic heating, or terrain. In addition, these steady-state models do not account for causality effects or pollutant build-up during stagnation, plume recirculation, or plume fumigation.

5.1.1 Major Features of CALMET

The CALMET meteorological model consists of a diagnostic wind field module and micrometeorological modules for overwater and overland boundary layers. When using large domains, the user has the option to adjust input winds to a Lambert Conformal Projection coordinate system to account for the curvature of the Earth. The diagnostic wind field module uses a two step approach in the computation of the wind fields (Douglas and Kessler, 1988). In the first step, an initial-guess wind field is adjusted for kinematic effects of terrain, slope flows, and terrain blocking effects to produce a Step 1 wind field. The second step consists of an objective analysis procedure to introduce observational data into the Step 1 wind field to produce a final wind field.

The major features and options of the meteorological model are summarized in Table 5-1. The techniques used in the CALMET model are briefly described below.

Step 1 Wind Field:

Kinematic Effects of Terrain: The approach of Liu and Yocke (1980) is used to evaluate kinematic terrain effects. The domain-scale winds are used to compute a terrain-forced vertical velocity, subject to an exponential, stability-dependent decay function. The kinematic effects of terrain on the horizontal wind components are evaluated by applying a divergence-minimization scheme to the initial guess wind field. The divergence minimization scheme is applied iteratively until the three-dimensional divergence is less than a threshold value.

Slope Flows: The slope flow algorithm in CALMET has recently been upgraded (Scire and Robe, 1997). It is based on the shooting flow algorithm of Mahrt (1982). This scheme includes both advective-gravity and equilibrium flow regimes. At night, the slope flow model parameterizes the flow down the sides of the valley walls into the floor of the valley, and during the day, upslope flows are parameterized. The magnitude of the slope flow depends on the local surface sensible heat flux and local terrain gradients. The slope flow wind components are added to the wind field adjusted for kinematic effects.

Blocking Effects: The thermodynamic blocking effects of terrain on the wind flow are parameterized in terms of the local Froude number (Allwine and Whiteman,

Table 5-1. Major Features of the CALMET Meteorological Model

- **Boundary Layer Modules of CALMET**
  - Overland Boundary Layer - Energy Balance Method
  - Overwater Boundary Layer - Profile Method
  - Produces Gridded Fields of:
    - Surface Friction Velocity
    - Convective Velocity Scale
    - Monin-Obukhov Length
    - Mixing Height
    - PGT Stability Class
    - Air Temperature (3-D)
    - Precipitation Rate

- **Diagnostic Wind Field Module of CALMET**
  - Slope Flows
  - Kinematic Terrain Effects
  - Terrain Blocking Effects
  - Divergence Minimization
  - Produces Gridded Fields of U, V, W Wind Components
  - Inputs Include Domain-Scale Winds, Observations, and (optionally) Coarse-Grid Prognostic Model Winds
  - Lambert Conformal Projection Capability

1985). If the Froude number at a particular grid point is less than a critical value and the wind has an uphill component, the wind direction is adjusted to be tangent to the terrain.

Step 2 Wind Field:

The wind field resulting from the adjustments described above of the initial-guess wind is the Step 1 wind field. The second step of the procedure involves the introduction of observational data into the Step 1 wind field through an objective analysis procedure. An inverse-distance squared interpolation scheme is used which weighs observational data heavily in the vicinity of the observational station, while the Step 1 wind field dominates the interpolated wind field in regions with no observational data. The resulting wind field is subject to smoothing, an optional adjustment of vertical velocities based on the O'Brien (1970) method, and divergence minimization to produce a final Step 2 wind field.

CALMET Boundary Layer Models:

The CALMET model contains two boundary layer models for application to overland and overwater grid cells.

Overland Boundary Layer Model: Over land surfaces, the energy balance method of Holtslag and van Ulden (1983) is used to compute hourly gridded fields of the sensible heat flux, surface friction velocity, Monin-Obukhov length, and convective velocity scale. Mixing heights are determined from the computed hourly surface heat fluxes and observed temperature soundings using a modified Carson (1973) method based on Maul (1980). Gridded fields of PGT stability class and optional hourly precipitation rates are also determined by the model.

Overwater Boundary Layer Model: The aerodynamic and thermal properties of water surfaces suggest that a different method is best suited for calculating the boundary layer parameters in the marine environment. A profile technique, using air-sea temperature differences, is used in CALMET to compute the micrometeorological parameters in the marine boundary layer.

An upwind-looking spatial averaging scheme is optionally applied to the mixing heights and 3-dimensional temperature fields in order to account for important advective effects.

5.1.2 Major Features of CALPUFF

By its puff-based formulation and through the use of three-dimensional meteorological data developed by the CALMET meteorological model, CALPUFF can simulate the effects of time- and space-varying meteorological conditions on pollutant transport from point and line sources in complex terrain. The major

Table 5-2. Major Features of the CALPUFF Model

- **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 (winds, temperature)
  - Spatially-variable fields of mixing height, friction velocity, convective velocity scale, Monin-Obukhov length, precipitation rate
  - Vertically and horizontally-varying turbulence and dispersion rates
  - Time-dependent source and emissions data for point, area, and volume sources
  - Temporal or wind-dependent scaling factors for emission rates, for all source types

- **Interface to the Emissions Production Model (EPM)**
  - Time-varying heat flux and emissions from controlled burns and wildfires

- **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
  - Pasquill-Gifford (PG) dispersion coefficients (rural areas)
  - McElroy-Pooler (MP) dispersion coefficients (urban areas)
  - CTDM dispersion coefficients (neutral/stable)

- **Vertical wind shear**
  - Puff splitting
  - Differential advection and dispersion

- **Plume rise**
  - Buoyant and momentum rise
  - Stack tip effects
  - Building downwash effects
  - Partial penetration
  - Vertical wind shear

- **Building downwash**
  - Huber-Snyder method
  - Schulman-Scire method

- **Complex terrain**
  - Steering effects in CALMET wind field
  - Optional puff height adjustment: ISC3 or "plume path coefficient"
  - Optional enhanced vertical dispersion (neutral/weakly stable flow in CTDMPLUS)

Table 5-2. Major Features of the CALPUFF Model (Cont'd)

- **Subgrid scale complex terrain (CTSG option)**
  - Dividing streamline, H_d, as in CTDMPLUS:
    - Above H_d, material flows over the hill and experiences altered diffusion rates
    - Below H_d, material deflects around the hill, splits, and wraps around the hill

- **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

- **Overwater and coastal interaction effects**
  - Overwater boundary layer parameters
  - Abrupt change in meteorological conditions, plume dispersion at coastal boundary
  - Plume fumigation

- **Chemical transformation options**
  - Pseudo-first-order chemical mechanism for SO_2, $SO_4^{=}$, NO_x, HNO_3, and NO_3^- (MESOPUFF II method)
  - Pseudo-first-order chemical mechanism for SO_2, $SO_4^{=}$, 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 model setup and data input
  - Enhanced error checking of model inputs
  - On-line Help files

- **Interface Utilities**
  - Scan ISCST3 and AUSPLUME meteorological data files for problems
  - Translate ISCST3 and AUSPLUME input files to CALPUFF input format

features and options of the CALPUFF model are summarized in Table 5-2. Some of the technical algorithms are briefly described below.

Complex Terrain: The effects of complex terrain on puff transport are derived from the CALMET winds. In addition, puff-terrain interactions at gridded and discrete receptor locations are simulated using one of two algorithms that modify the puff-height (either that of ISCST3 or a general "plume path coefficient" adjustment), or an algorithm that simulates enhanced vertical dispersion derived from the weakly-stratified flow and dispersion module of the Complex Terrain Dispersion Model (CTDMPLUS) (Perry et al., 1989). The puff-height adjustment algorithms rely on the receptor elevation (relative to the elevation at the source) and the height of the puff above the surface. The enhanced dispersion adjustment relies on the slope of the gridded terrain in the direction of transport during the time step.

Subgrid Scale Complex Terrain (CTSG): An optional module in CALPUFF, CTSG treats terrain features that are not resolved by the gridded terrain field, and is based on the Complex Terrain Dispersion Model (CTDMPLUS) (Perry et al., 1989). Plume impingement on subgrid-scale hills is evaluated at the CTSG subgroup of receptors using a dividing streamline height (H_d) to determine which pollutant material is deflected around the sides of a hill (below H_d) and which material is advected over the hill (above H_d). The local flow (near the feature) used to define H_d is taken from the gridded CALMET fields. As in CTDMPLUS, each feature is modeled in isolation with its own set of receptors.

Puff Sampling Functions: A set of accurate and computationally efficient puff sampling routines are included in CALPUFF which solve many of the computational difficulties encountered when applying a puff model to near-field releases. For near-field applications during rapidly-varying meteorological conditions, an elongated puff (slug) sampling function may be used. An integrated puff approach may be used during less demanding conditions. Both techniques reproduce continuous plume results under the appropriate steady state conditions.

Building Downwash: The Huber-Snyder and Schulman-Scire downwash models are both incorporated into CALPUFF. An option is provided to use either model for all stacks, or make the choice on a stack-by-stack and wind sector-by-wind sector basis. Both algorithms have been implemented in such a way as to allow the use of wind direction specific building dimensions.

Dispersion Coefficients: Several options are provided in CALPUFF for the computation of dispersion coefficients, including the use of turbulence measurements (σ_v and σ_w), the use of similarity theory to estimate σ_v and σ_w from modeled surface heat and momentum fluxes, or the use of Pasquill-Gifford (PG) or McElroy-Pooler (MP) dispersion coefficients, or dispersion equations based on the Complex Terrain

Dispersion Model (CTDM). Options are provided to apply an averaging time correction or surface roughness length adjustments to the PG coefficients.

Overwater and Coastal Interaction Effects: Because the CALMET meteorological model contains both overwater and overland boundary layer algorithms, the effects of water bodies on plume transport, dispersion, and deposition can be simulated with CALPUFF. The puff formulation of CALPUFF is designed to handle spatial changes in meteorological and dispersion conditions, including the abrupt changes which occur at the coastline of a major body of water.

Dry Deposition: A full resistance model is provided in CALPUFF for the computation of dry deposition rates of gases and particulate matter as a function of geophysical parameters, meteorological conditions, and pollutant species. Options are provided to allow user-specified, diurnally varying deposition velocities to be used for one or more pollutants instead of the resistance model (e.g., for sensitivity testing) or to by-pass the dry deposition model completely. For particles, source-specific mass distributions may be provided for use in the resistance model.

Wind Shear Effects: CALPUFF contains an optional puff splitting algorithm that allows vertical wind shear effects across individual puffs to be simulated. Differential rates of dispersion and transport among the "new" puffs generated from the original, well-mixed puff can substantially increase the effective rate of horizontal spread of the material.

Wet Deposition: An empirical scavenging coefficient approach is used in CALPUFF to compute the depletion and wet deposition fluxes due to precipitation scavenging. The scavenging coefficients are specified as a function of the pollutant and precipitation type (i.e., frozen vs. liquid precipitation).

Chemical Transformation: CALPUFF includes options for parameterizing chemical transformation effects using the five species scheme (SO_2, $SO_4^{=}$, NO_x, HNO_3, and NO_3^{-}) employed in the MESOPUFF II model, the six species RIVAD scheme (SO_2, $SO_4^{=}$, NO, NO_2, HNO_3, and NO_3^{-}), or a set of user-specified, diurnally-varying transformation rates.

5.2 Modeling Domain Configuration

The CALMET computational domain consists of a uniform horizontal grid with a grid cell size of 0.3 km. It extends out to approximately 20 to 30 km from the facility and consists of 170 x 170 grid cells (51 km x 51 km domain). The southwest corner of the domain has a UTM coordinate of 521 km east, 7192 km north in UTM Zone 28. In the vertical, a stretched grid is used with fine resolution in the lower layers in order to resolve the mixed layer and a somewhat coarser resolution aloft. Ten vertical layers are used that are centered at 10, 30, 60, 120, 240, 460, 800, 1250, 1850, and 2600 meters. This horizontal and vertical grid structure was chosen to provide a detailed fine-scale representation of terrain effects. There are significant topographical features in the area that affect the wind flow and offer the potential for plume-terrain interaction. Peak terrain heights are over 1000 meters in the area surrounding the proposed Alcoa facility. The base elevation of the plant is approximately 14-17 meters and the majority of the emission points have heights between 22.5 and 78.0 meters. Therefore, complex terrain effects, in terms of both low-level wind flow channeling as well as terrain-plume interaction effects, are expected to be important.

5.3 Meteorological Modeling Options

Initial Guess Field

Gridded MM5 meteorological fields produced by Earth Tech were used to define the initial guess fields for the CALMET simulations. The MM5 simulations were made for the period July 2000 to June 2001, the same period selected for the CALMET/CALPUFF runs. The MM5 data were produced at a horizontal resolution of 1 km and at 25 vertical sigma levels (24 half-sigma levels where the winds are defined).

Step 1 Field: Terrain Effects

In developing the Step 1 wind field, CALMET adjusts the initial guess field to reflect slope flows and blocking effects. Slope flows are a function of the local slope and altitude of the nearest crest. The crest is defined as the highest peak within a radius TERRAD around each grid point. A value of TERRAD of 8 km is considered most appropriate for the Reydarfjordur computational domain and was determined based on an analysis of the width size of Reydarfjordur (see Figure 3-2). The Step 1 field produces a flow field consistent with the fine-scale CALMET terrain resolution (0.3 km).

Step 2 Field: Objective Analysis

In Step 2, observations are incorporated into the Step 1 wind field to produce a final wind field. Each observation site influences the final wind field within a radius of influence (parameters RMAX1 at the surface and RMAX2 aloft). Observations and the Step 1 field are weighted by means of parameters R1 at the surface and R2 aloft: at a distance R1 from an observation site, the Step 1 wind field and the surface observations are weighted equally. In complex terrain, channeling (blocking effects) and slope flows contribute significantly to the wind field. Therefore, relatively small values (2 km) of R1 and R2 were selected because the three meteorological stations in the vicinity of the Alcoa facility project are located very close to each other (at a distance of less than 5 km), and each of these stations should have an important weight. Since the initial guess field is driven by the MM5 winds and terrain effects are expected to be important, RMAX1 and RMAX2 were set to 10 km in order to give greater weight to the surface station and RMIN=0.1 km.

5.4 Dispersion Modeling Options

The CALPUFF simulations were conducted for the period July 2000 to June 2001 using the following model options:

-Gaussian near-field distribution

-Transitional plume rise

-Stack tip downwash

-PG dispersion coefficients (rural areas, McElroy-Pooler coefficients (urban areas)

-Transition of σ_y to time-dependent (Heffter) growth rates

-Building downwash effects – (ISCST3 techniques)

-Wet and dry deposition were applied

-Chemical transformation was not considered.

The configuration of the sources is such that building downwash effects will influence dispersion. Wind direction building dimensions were derived from the application of the BPIP building downwash program. The Gaussian vertical distribution option is selected in CALPUFF to provide a better representation of near-field concentrations.

The CALPUFF computational grid consists of a sub-domain within the meteorological grid (i.e., 51 x 51 km with a 0.3 km resolution or 170 x 170 grid cells). This sub-domain (51 x 32 km, 170 x 106 grid cells) is designed to improve the computational efficiency of the CALPUFF simulations and consists of an area that extends the full width of the CALMET domain but starts approximately 7.5 km north of the southern edge of the CALMET domain and stops approximately 12.5 km south of the northern edge of CALMET domain (see Figure 5-1). Two important computational parameters in CALPUFF are XMXLEN (maximum length of an emitted puff, in grid units) and XSAMLEN (maximum travel distance of a puff, in grid units, during one time step). Both of these variables were set to 1.0 grid units in the CALPUFF simulations in order to allow the wind channeling effects to be accounted for in the puff trajectory calculations. The first parameter ensures that the length of an emitted puff does not become so large that it cannot respond to changes in the wind field on the scale of the meteorological grid (0.3 km resolution). The model automatically increases the frequency of puff releases to ensure the length of a single puff is not larger than the grid size. The second parameter decreases the internal time step to ensure the travel distance during one time step does not exceed the grid size.

Deposition effects were modeled using the default dry deposition model and the scavenging coefficient wet removal module. Deposition fluxes are derived from the total (wet + dry) deposition fluxes of the species produced by the CALPUFF model. The SO_2 default values are used for SO_2 and for PM_{10}, which is mostly sub 2.5 microns, the default value of SO_4 or NO_3 can be used both for dry and wet deposition parameters, but these parameters need to be estimated for HF, PF, PAH and BaP. PAH will be modeled partly as gas (PAHGAS) and partly as particles (PAHPM). The gas to particles proportion will be different for the roof top vents (line sources) versus the stacks (point sources) (see Source Description in Section 2). Therefore, HF and PAHGAS need gas dry and wet deposition coefficients, while PF and PAHPM need particle dry and wet deposition coefficient estimates. BaP will then be scaled from PAH.

HNO_3 and HF have similar solubility and reactivity parameters. Therefore, the default HNO_3 chemical parameters are used for the HF dry deposition parameters. For the gas part of PAH, benzene is used as a surrogate. Two of the dry deposition parameters for benzene are computed, using the EPA's On-line Diffusion Coefficient Calculator (http://www.epa.gov/athens/learn2model/part-two/onsite/estdiffusion.htm) at a temperature of 15º C and pressure of 1 atm for diffusivity, and for solubility using the EPA's On-line Estimated Henry's Law Constant Calculator (http://www.epa.gov/athens/learn2model/part-two/onsite/esthenry.htm). Alpha star is set to 1.0. The reactivity is set to half that of SO_2 at 4.0, and the mesophyll resistance is set to 1 s/cm, roughly one-fifth the value for NO_3. For wet deposition, scavenging coefficients need to be defined for both liquid and frozen forms of precipitation. Because both HF and PAHGAS are gases, the frozen precipitation scavenging coefficient is set to 0.0 s^{-1} for both. The liquid precipitation scavenging coefficients are taken from Table 2 of Campbell, 1998: a value of $7.06E^{-05}$ s-^{1} for HF and a value of $3.52E^{-05}$ s^{-1} for PAHGAS (benzene surrogate). PF and PAHPM are assumed to be in the form of particles with an average diameter of less than 1 micron (same as organic condensable). Dry and wet deposition coefficients are similar to what is used for PM_{10}, i.e. the default values for either SO_4 or NO_3.

5.5 Receptor Grid

CALPUFF was run using a UTM-based Cartesian receptor grid that extended 19 km west, 32 km east, 18 km north and 13 km south from the Alcoa facility. The receptor grid consists of two nested grids of discrete receptors with the highest resolution (100 meters) confined to the immediate vicinity of the Alcoa site. The fine resolution 100 meter spaced discrete receptor grid was confined to a 14 x 6 km rectangle around and including the facility. Beyond this area, a receptor spacing of 200 meters was used out to 10 km east and west and 6 km north and south of the facility (see Figure 5-1). This resulted in a total of 10,784 discrete receptors, 6,560 receptors with 100 m spacing and 4,224 receptors with 200 m spacing. Receptor elevations were obtained from the 92 m resolution terrain elevation data.

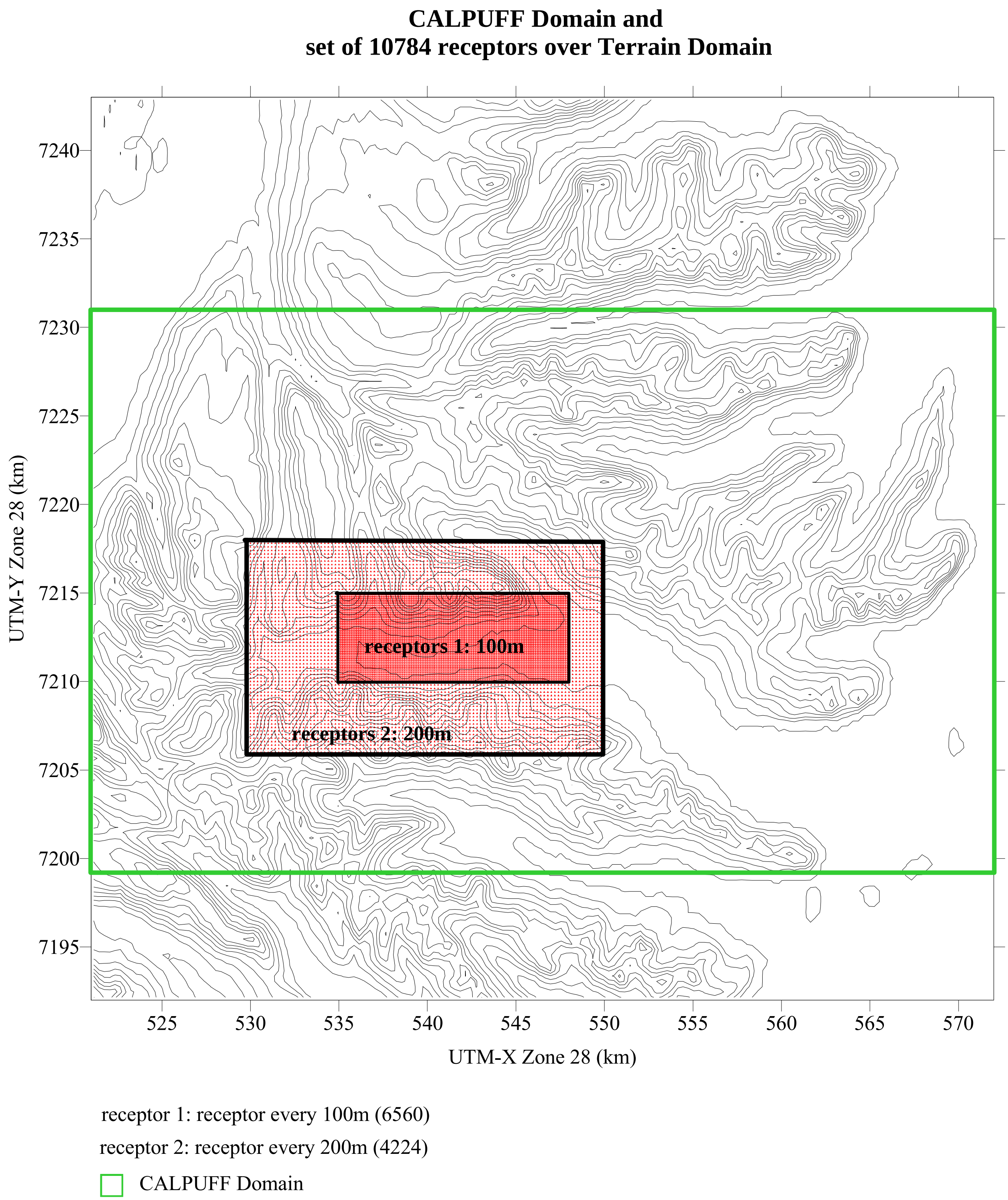


Figure 5-1. Plot of CALPUFF domain and CALPUFF discrete receptors. In Receptors 1, receptors are spaced every 100 meters. In Receptors 2, receptors are spaced every 200 meters.