



Dispersion model evaluation of PM_{2.5}, NO_x and SO₂ from point and major line sources in Nova Scotia, Canada using AERMOD Gaussian plume air dispersion model

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ABSTRACT

AERMOD was used to model the air dispersion of point and major line emissions of PM_{2.5} in Halifax and Pictou, NO_x in Halifax and SO₂ in Halifax, Sydney and Port Hawkesbury, Nova Scotia, Canada. Emission inventory data for 2004 were used in simulations within four, 50 km x 50 km, domains over annual, monthly and 1-hour averaging periods. Annual averaged surface concentration maps are reported. Modeled versus observed comparisons were made within each domain at the Government, National Air Pollution Surveillance (NAPS) monitoring sites (discrete receptors). Evaluation of the model was conducted on the annual, monthly and hourly results using a number of statistical methods that included R^2 , fractional bias, normalized mean square error and the fraction of predictions within a factor of two of the observations. The AERMOD model evaluation showed that there was good agreement between the modeled and observed SO₂ concentration for the annual and monthly comparison but less skill at estimating the hourly comparisons for SO₂ in Halifax and Sydney. AERMOD showed poor model skill at predicting SO₂ in Port Hawkesbury over the same averaging periods. The model evaluation for PM_{2.5} in Halifax, PM_{2.5} in Pictou and NO_x in Halifax showed poor agreements and model skill. The surface concentrations from the point and major lines sources in all domains from all metrics were found to be well below the National Air Quality Standards. AERMOD has shown its utility as a suitable model for conducting dispersion modeling from point and line sources in Nova Scotia with good model skill for estimating annual and monthly SO₂ concentrations in Halifax and Sydney. The study highlights the validity of using emission inventory data to estimate the surface impact of major point and line sources within domains containing complex terrain, differing land use types and with large variability within the annual meteorology.

Keywords: PM_{2.5}, NO_x, SO₂, AERMOD, Gaussian Dispersion Model

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1. Introduction

Many studies have shown that acute and chronic exposure to fine atmospheric particles with a median aerodynamic diameter equal to, or less than, 2.5 microns (PM_{2.5}), nitrogen oxides (NO_x) and sulfur dioxide (SO₂) are positively and significantly associated with increases in mortality and morbidity (Krewski et al., 2005; Stieb et al., 2008; Neupane et al., 2010; Backes et al., 2013). Sources of PM_{2.5}, NO_x and SO₂ include biogenic, geogenic and anthropogenic local and long-range emissions to, and secondary formations within the atmosphere (Harrison et al., 1997; de Gouw et al., 2008; Gibson et al., 2009a; La Spina et al., 2010; Gibson et al., 2013a; Gibson et al., 2013b). Ambient concentrations of PM_{2.5}, NO_x and SO₂ exhibit diurnal and seasonal variability, influenced by land-use, topography, energy demand for power, space heating and transport and meteorological factors (Riga-Karandinos and Saitanis, 2005; Monks et al., 2009; Wagstrom and Pandis, 2011; Gibson et al., 2013a; Gibson et al., 2013b).

The main sources of PM_{2.5}, NO_x and SO₂ in Nova Scotia, Canada are power generation, domestic and industrial space heating via fossil and biomass fuels, construction activity, ship emissions (Hingston, 2005), vehicle emissions, re-suspended dust with the majority (75%) being long-range transport (LRT) originating from the NE US, Interstate 95 corridor and the Canadian Windsor – Quebec corridor (Gibson et al., 2009b; Dabek-

Zlotorzynska et al., 2011; Jeong et al., 2011). Typical average concentrations of PM_{2.5}, NO₂ and SO₂ in rural Nova Scotia are 0.1 µg m⁻³, 0.1 µg m⁻³ and 0.16 µg m⁻³ (Wheeler et al., 2011) and in urban Halifax 2.5 µg m⁻³, 4.0 µg m⁻³, 1.0 µg m⁻³ respectively, concentrations that can be considered as being low when compared to other Canadian cities (Stieb et al., 2002; Brook et al., 2007; Atari et al., 2008; Jeong et al., 2011).

Due to fiscal and practical constraints, continuous air pollution surveillance cannot be offered for all receptors in Nova Scotia. Dispersion modeling offers a solution by being able to estimate the impact of point, line, volume and area sources to surface air quality in any given airshed, given accurate emission source characteristics, land use, terrain, meteorological data and a measure of the total atmospheric concentration of the metrics in the model domain (Johnson et al., 2010).

A commonly used regulatory air pollution dispersion model is the American Meteorological Society and U.S. Environmental Protection Agency Regulatory Model (AERMOD) (Perry et al., 2005). AERMOD is a steady-state Gaussian plume dispersion model aimed at short-range (<50 km) air pollution dispersion from point, line area and volume sources (Cimorelli et al., 2003; Perry et al., 2005). AERMOD (Lakes Environmental™, Ontario, Canada) incorporates meteorological data pre-processing (AERMET) and uses modern knowledge on planetary boundary layer theory,

which serves as a replacement to Pasquill–Gifford stability class-based plume dispersion models such as ISC–PRIME and ISCST3 (Peters et al., 2003). AERMOD has been promulgated by the USEPA as a preferred air dispersion model to replace the ISCST3 (Lee and Keener, 2008). AERMOD's concentration algorithm considers the effects of vertical variation of wind, temperature and turbulence profiles. These profiles are represented by equivalent values constructed by averaging over the planetary boundary layer (PBL) through which plume material travels directly from the source to the receptor (Cimorelli et al., 2003). The model uses the boundary layer parameters in conjunction with meteorological measurements to characterize the vertical structure profiles as above. In mountainous terrain, AERMOD, divides and streamlines plume flow over and around hills, which greatly increases its accuracy to model in complex terrain (Langner and Klemm, 2011). In addition, Perry et al. (2005) states that AERMOD's good performance in mountainous terrain is also due to the detailed inclusion of boundary layer vertical structure information. AERMOD contains building downwash, plume rise and terrain treatment algorithms (Lakes Environmental, 2010). AERMOD does not take into account chemical reactions. In reality, concentrations of SO_2 and NO_2 would be reduced due to gas-to-particle conversion, with an associated increase in $\text{PM}_{2.5}$ concentration (Gibson et al., 2013b). While dry and wet deposition would decrease ambient concentrations of $\text{PM}_{2.5}$ (Gibson et al., 2009b). It is accepted that the model is not equipped to account for the chemical reactivity of emissions. The reason for this is that within a 50 km x 50 km domain, only ~2% of SO_2 would be converted to sulfate in the gas-phase per hundred km's, therefore even though SO_2 does oxidize and condense onto new and existing particles the losses are minor within a 50 km x 50 km domain (Stevens et al., 2012). This is one of the reasons AERMOD is not recommended to be used in model domains larger than 50 km x 50 km (Stevens et al., 2012).

AERMOD has been used to study PM_{10} dispersion over the city of Pune, India (Kesarkar et al., 2007); to study emissions from roadways for several pollutants including $\text{PM}_{2.5}$ and SO_2 (Cook et al., 2008); to generate artificial $\text{PM}_{2.5}$, NO_x and benzene data sets for use in an exposure study in New Haven (Johnson et al., 2010); to evaluate against similar Gaussian plume models (Perry et al., 2005); and to investigate spatial exposure patterns of SO_2 in Dallas county (Zou et al., 2009).

Detailed descriptions of the principles and formulations of AERMOD are described in Perry et al. (1994) and Cimorelli et al. (2003, 2005). Lee and Keener (2008) suggest that AERMOD has a tendency to under predict the ground level concentrations in both stable and convective cases. Dresser and Huizer (2011) showed that the Lagrangian model CALPUFF consistently agreed with predictions of high concentrations with no obvious tendency to under–or over predict. Dresser and Huizer (2011) also found that, although AERMOD's predictions are relatively close to observed concentrations, the model had a tendency to under predict the highest 3-hr and 24-hr monitored concentrations. AERMOD's moderate over prediction during neutral and stable conditions contrasted with its severe underprediction during unstable conditions for complex terrain (Dresser and Huizer, 2011). Langner and Klemm (2011) found that AERMOD's predictions were closer to field observations than those of the German Lagrangian dispersion model AUSTAL2000, especially in urban and complex terrain.

A number of studies have evaluated and compared AERMOD's performance to other air dispersion models (Hanna et al., 2001; Chang and Hanna, 2004; Barton et al., 2010; Dresser and Huizer, 2011; Langner and Klemm, 2011). A number of statistical tests can be applied to AERMOD estimated average surface concentrations and observed concentrations at discrete receptors within the model domain (Hanna et al., 1991a; Hanna et al., 1991b; Hanna et al., 1993; Hanna et al., 2001; Chang and Hanna, 2004; Lee and Keener, 2008). These include, fractional bias (FB), fraction of data that satisfy (FAC2), normalized mean square error (NMSE) and R^2

(Hanna et al., 2001; Chang and Hanna, 2004; Barton et al., 2010). A perfect model would have an $\text{FAC2}=1.0$; and FB and $\text{NMSE}=0.0$. A negative FB value implies an AERMOD model over–prediction with a positive value implying an under–prediction (Chang and Hanna, 2004). The equations that were used to calculate the FB, FAC2 and NMSE are provided in Chang and Hanna (2004).

This paper presents annual mean (based upon 2004 emissions inventory data) spatial concentration maps of surface NO_x in one, $\text{PM}_{2.5}$ in two and SO_2 in three model domains that capture the cities of Halifax, Pictou, Port Hawkesbury and Sydney, Nova Scotia, Canada. A comparison and model evaluation was made between the annual, monthly and hourly mean modeled values with observed $\text{PM}_{2.5}$, NO_x , and SO_2 at Federal Government, NAPS monitoring sites (discrete receptors) in the model domains. The FAC2, FB, NMSE and R^2 were calculated for annual, monthly and hourly average concentrations of each metric at the discrete receptors within each domain.

2. Materials and Methods

2.1. Air quality dispersion modeling in Nova Scotia using AERMOD View v6.2

The following paragraphs describe the characteristics of the four modeling domains, provide detail of the Lakes Environmental AERMOD View v6.2 model input parameters and the NAPS data sets used for comparing the calculated with the observed $\text{PM}_{2.5}$, NO_x and SO_2 data for 2004.

2.2. Modeling domains and description of emission sources

Figure 1 shows the location of the Halifax (HFX), Sydney (SYD), Port Hawkesbury (PRTHWKS) and Pictou (PIC) modeling domains.

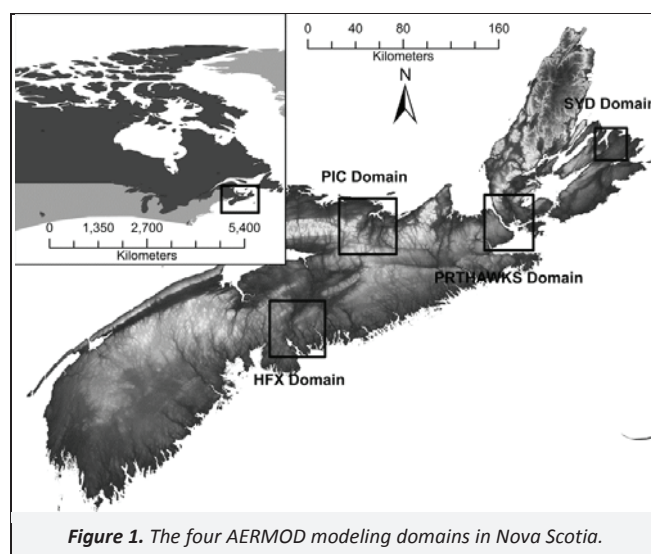


Figure 1. The four AERMOD modeling domains in Nova Scotia.

Table 1 provides the detailed characteristics of each model domain.

The HFX domain contains Halifax Regional Municipality, Halifax harbor, a complex coastline and significant rural areas. The SYD domain includes the city of Sydney, a portion of rural Cape Breton county (chiefly grassland) and the Lingan Power Station located on the Atlantic coast. The Port Hawkesbury (PRTHWKS) domain includes the town of Port Hawkesbury and New Page Paper Mill located on the Atlantic Coast, surrounded by cultivated agricultural land and water bodies. The PIC domain includes the city of New Glasgow and the Neenah Paper Mill located on the Atlantic Coast. The PIC domain contains considerable cultivated agricultural land, water bodies and the town of Pictou.

The running times were unavailable and therefore it was assumed that the stacks were running 24-hr a day throughout the year, which, according to the facility operators, is a fair reflection of the reality of these point sources. A constant emission factor of

1 was therefore chosen for the point sources in all four domains. The stack emission characteristics, PM_{2.5}, NO_x and SO₂ emissions found within the HFX, SYD, PRTHWKS and PIC modeling domains are provided in Table 2.

Table 1. Model domain characteristics

Domain	South-West Corner UTM Coordinates (x:y) (m)	North-East Corner UTM Coordinates (x:y) (m)	Length (East:West) (m)	Length (North:South) (m)	Maximum Elevation from the Mean Sea Level (m)	Highway: Length (km)	Main Road: Length (km)	Total Length (km)
Halifax (HFX)	432 907.86: 4 940 306.88	482 351.56: 4 991 354.16	50 585	48 550	185	101:56.7 102:57.8 103: 12.8	107:36.8 111:9.0 118:32.6	205.8
Sydney (SYD)	707 486.23: 5 104 407.14	728 994.84: 5 125 770.9	21 250	21 250	179.6	105:4.36	125:17.9	22.3
Pictou (PIC)	492 097.16: 5 022 396.44	539 644.44: 5 065 136.59	47 013	42 654	320.4	104:44.5 106:19.4		63.9
Porthawksbury (PRTHWKS)	609 805.32: 5 024 268.03	657 403.62: 5 073 720.92	49 000	47 308	283.1	104:35.5 105:17.9		35.54
Pictou (PIC)	492 097.16: 5 022 396.44	539 644.44: 5 065 136.59	47 013	42 654	320.4	104:44.5 106:19.4		63.9

Table 2. Halifax, Pictou, Port Hawkesbury and Sydney Stack Characteristics

Domain	Stack Location	Stack Characteristics	UTM (x:y) Coordinate (m)	Height: Diameter (m)	Exit Velocity (m sec ⁻¹)	Exit Temp. (°K)	NO _x Emission Rate (tons yr ⁻¹)	SO ₂ Emission Rate (tons yr ⁻¹)	PM _{2.5} Emission Rate (tons yr ⁻¹)
Halifax	Dartmouth Refinery	Vacuum Furnace Stack	457 301.70: 4 943 212.30	51 1.72	10	573	602.01	1 112.06	20.1
	Dartmouth Refinery	Feed Preheat Furnace Stacks	457 799.02: 4 943 127.40	59.5 1.3	1.3	590	593.18	992.75	61.05
	Dartmouth Refinery	Atmospheric Furnace Stack	458 045.61: 4 944 442.52	61.9 1.31	8.7	646	596.48	1 000.5	35
	Dartmouth Refinery	Furnace Stacks	459 114.14: 4 943 620.57	50.9 1.37	6.4	503	565.27	1 070.01	9.89
	Dartmouth Refinery	Incinerator Stack	458 127.80: 4 946 086.00	61 0.79	15	788	558.12	1 045.5	53.63
	Dartmouth Refinery	Flare Stack	459 977.17: 4 942 387.65	56.4 0.61	30.8	1 273	560.1	1 123.98	70.37
	Capital Health	Steel stack	456 494.00: 4 944 584.00	53.33 1.22	20	563	35.11	110.24	4.776
	Capital Health	Brick stack	447 087.29: 4 951 404.04	200 6	5.6	563	78.124	267.612	11.37
	Capital Health	Steel Stack	453 561.80: 4 943 704.60	56.08 1.22	20	563	43.945	150.531	6.395
	Dalhousie University	Central Services Building Stack	453 380.50: 4 942 761.70	50 1.17	8.5	478	85.902	259.923	11.358
	Tufts Cove Power Station	Tufts Cove Unit 5 Stack	452 754.59: 4 947 176.40	24.38 2.9	40.43	727	1 463.46	5 019.87	95.91
	Tufts Cove Power Station	Tufts Cove Unit 2 Stack	452 538.54: 4 949 045.45	152 2.44	12	448	1 422.71	4 890.24	155.01
	Tufts Cove Power Station	Tufts Cove Unit 3 Stack	452 620.73: 4 948 141.30	152 3	29	453	1 505.62	4 758.16	125.21
Pictou	Neenah Paper industry	Recovery Boiler/Modo Scrubber	521 948.50: 5 055 566.50	80.77 3.05	13.5	342	NA	NA	216.1
	Neenah Paper industry	Power Boiler/Venturi Scrubber	522 921.77: 5 051 901.82	62.18 1.52	23	341	NA	NA	210.28
	Neenah Paper industry	Dissolving Tank vent Combined	520 312.25: 5 049 636.13	62.18 1.22	9.3	356	NA	NA	186.4
	Neenah Paper industry	High Level Roof Vent	521 725.35: 5 050 396.17	76.99 1.83	20.7	321	NA	NA	230.5
Port Hawkesbury Sydney	New page Paper industry	Power Boiler stack	626 196.73: 5 052 845.18	51.8 3.02	20.7	460	NA	1 164.6	NA
	Lingan Power Station	Lingan Units Stack	728 296.90: 5 124 509.20	152 4.7	30	443	NA	56 755.7	NA

In all model domains the highways were divided into a number of segments of different lengths base upon protocols followed in the National Pollution Release Inventory for vehicle counts (NPRI, 2010). Each road segment was converted into a volume source with distinct emission rates to fulfill the model input requirement. The mathematical details of the vehicle emission rate calculation is presented in Cook et al. (2008). Highways and main road lengths are given in Table 1. An emission factor of 1 for the vehicle sources was used between 07:00 and 19:00 due to high traffic density during daytime. Outside of 07:00 and 19:00 an emission factor of 0.1 was used. Based upon traffic data obtained from Nova Scotia Environment, four vehicle categories were used and included light duty passenger vehicle, light duty commercial vehicle, medium duty commercial vehicle and buses (Transport Canada, 2011).

A number of trials were conducted to optimize the domain grid size that had the maximum number of receptors and within a reasonable model run time. From a series of iterative trial simulations of increasing mesh size, it was found that there was no change in model efficiency with mesh spacing up to 2.5 km × 2.5 km. The Cartesian grid mesh spacing for each domain were as follows: HFX 2.48 km × 2.52 km; SYD 1.25 km × 1.25 km; PRTHWKS 2.36 km × 2.45 km and PIC 2.47 km × 2.51 km. A 1 km resolution Digital Elevation Maps (DEM) of Nova Scotia was used to calculate the elevation of each receptor grid from mean sea level in the model domains. A number of Geotiff files were used to manipulate the DEM to produce the desirable input data for AERMOD's AERMAP utility tool.

2.3. Meteorological observations

Hourly surface air observations from Halifax International Airport (UTM x 459 196.21 m: y 4 970 120.17 m) and Sydney Meteorological Station (UTM x 716 155.19 m: y 5 116 377.04 m) were used in model simulations. The Halifax meteorological observations were used in the HFX and PIC domains while the Sydney meteorological observations were used in the PRTHWKS

and SYD domains respectively. Balloon sonde upper air observations from Yarmouth station (UTM x 250 899.37 m: y 4 861 736.2 m) were used in model simulations for all four domains. Following Environment Canada's advice we acquired the upper air data from the University of Wyoming, College of Engineering, Department of Atmospheric Science web portal (<http://weather.uwyo.edu/upperair/sounding.html>) (Oolman, 2012). The AERMET function in AERMOD was used to preprocess all meteorological observations prior to model simulations. Table 3 provides detail of the meteorological observations at two surface air stations.

The values of the land use parameters albedo, Bowen ratio, surface roughness, water bodies and grassland are provided in Table 4. These values were used during AERMET meteorological data processing.

Wind roses were generated using the WRPLOT feature within the AERMET module of AERMOD. The meteorological data used in WRPLOT was obtained from the Halifax and Sydney weather stations. The wind roses are presented in Figure 2.

2.4. Monitoring of NO_x, PM_{2.5} and SO₂ at different NAPS stations

AERMOD estimated concentrations at the NAPS site discrete receptor on the roof of the Roy Building in downtown Halifax (UTM x 454 489.11 m: y 4 943 814.66 m, elevation 18 m) were used to compare with NO_x and SO₂ observations. AERMOD estimated PM_{2.5} were compared with the Lake Major NAPS site discrete receptor located within the HFX domain (UTM x 461 857.05 m: y 4 951 925.57 m, elevation 67 m) and a NAPS site discrete receptor in the PIC domain (UTM x 523 624.29 m: y 5 058 724.52 m, elevation 13.2 m). Likewise, SO₂ was compared at Welton Street NAPS site discrete receptor in SYD (UTM x 718 370.52 m: y 5 113 736.26 m, elevation 40 m), a coastal site in PRTHWKS NAPS site discrete receptor (UTM x 627 685.26 m: y 5 052 459.15 m, elevation 14.8 m).

Table 3. Meteorological parameters

Location	Values	Wind Speed (m sec ⁻¹)	Ambient Temp. (°K)	Sensible Heat Flux (Wm ⁻²)	Surface Friction Velocity (m sec ⁻¹)
Halifax Airport Met Station	Range	0-20.1	247.5-304.9	1.9-364.8	0.0-3.49
Sydney Met Station	Range	0-19.0	250.0-310.0	0.033-353.8	0.0-2.5

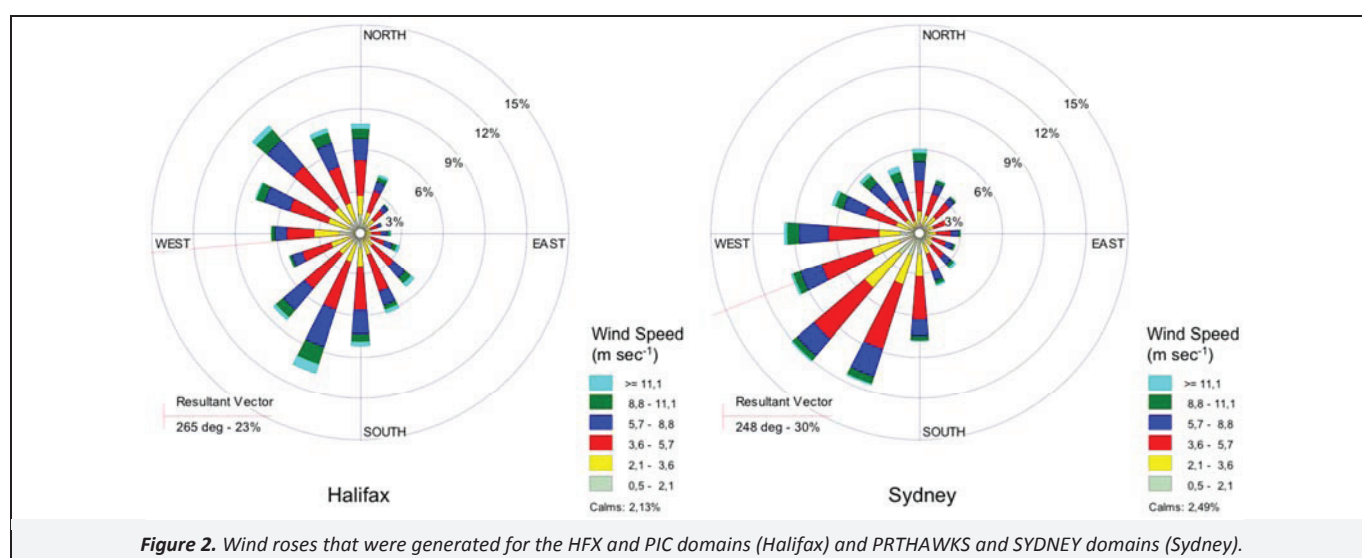


Table 4. Land use parameters

Land Cover Type	Values	Albedo	Bowen Ratio	Surface Roughness Length (m)
Urban areas	Range	0.14-0.35	1-1.5	1
Water bodies	Range	0.1-0.2	0.1-1.5	0.0001
Grassland	Range	0.4-1.5	0.18-0.6	0.001-0.1
Cultivated Land	Range	0.14-0.6	0.3-1.5	0.01-0.2

3. Results and Discussion

3.1. Meteorological observations

The wind speed at the HFX weather station for 2004 ranged from 0.0 m sec^{-1} to 20.1 m sec^{-1} with an annual average wind speed of 4.7 m sec^{-1} . It can be observed in Figure 2 that the prevailing wind direction was 265° (WSW) and was observed for 23% of the time in the HFX. For 33.8% of the time, wind speed varied between 3.6 m sec^{-1} and 5.7 m sec^{-1} at the HFX weather station with ambient temperature ranging from 247.5°K to 304.9°K .

Surface air observations from the SYD weather station showed that the annual wind speed varied between 0.0 to 19.0 m sec^{-1} with an average of 8.6 m sec^{-1} . It can be seen from Figure 2 that the prevailing wind in the SYD was from 248° (SW) for 30% of the time. Wind speed within the SYD varied between 3.6 m sec^{-1} and 5.7 m sec^{-1} for 36.6% of the time. The ambient temperature in the SYD ranged from 250°K to 301°K . The annual prevailing wind direction for Nova Scotia in 2004 can be considered as being from the WSW ($\sim 255^\circ$), which aligns with known up wind sources in the NE US, e.g. Ohio Valley and the Interstate 95 corridor (Gibson et al., 2009b; Gibson et al., 2013b).

3.2. AERMOD dispersion modeling results

Table 5 contains the results of the AERMOD modeling simulations in the four domains.

It includes the annual, monthly and hourly AERMOD estimated and observed concentrations for each metric at the NAPS sites discrete receptors. In addition, Table 5 contains the R^2 , FB, NMSE and FAC2 for each metric at the NAPS sites discrete receptors within each domain.

3.3. Halifax

Annual average spatial concentration maps of surface $\text{PM}_{2.5}$, NO_x and SO_2 concentrations in the HFX domain are presented in Figures 3 through 5.

From Figure 3 it can be seen that the highest NO_x concentrations ($7.97 \mu\text{g m}^{-3}$) were found directly to the East of the Dartmouth Refinery. From Figure 3, the highest SO_2 concentration ($15.9 \mu\text{g m}^{-3}$) was found directly to the East of the Dartmouth Refinery at the same coordinates as for the highest NO_x concentration. Although this spatial pattern is still evident in Figure 4 for $\text{PM}_{2.5}$, the highest $\text{PM}_{2.5}$ concentrations ($2.69 \mu\text{g m}^{-3}$) was found at the intersection of highways 102 and 118; the latter likely due traffic emissions. After re-running the simulations without the point source it was found that the estimated vehicle impact at this location was $1.82 \mu\text{g m}^{-3}$, which equates to 67% of the total for both the point and major line sources at this location.

The reason for the increased concentration gradients observed for $\text{PM}_{2.5}$, NO_x and SO_2 to the East of the refinery in Figures 3 through 5 is due to the Westerly prevailing wind which is advecting the point and line emissions immediately to the East of their source.

From Figure 5 it can be observed that SO_2 does not show a strong association with major line sources. This can be explained by SO_2 being more strongly associated with point source power generation: the hospitals and Universities in Halifax in 2004 that used high sulfur fuel compared to line sources that use low sulfur fuel (Hingston, 2005; Phinney et al., 2006).

The AERMOD estimated annual, monthly and hourly mean $\text{PM}_{2.5}$ concentrations are shown in Table 5. The R^2 for the modeled versus observed annual, monthly and hourly $\text{PM}_{2.5}$ concentrations were poor ($R^2=0.053$, 0.043 and 0.002 respectively). The annual, monthly and hourly FB showed a model under-prediction of 0.96 , 0.88 and 0.89 respectively. The annual, monthly and hourly NMSE was found to be 25.53 , 6.39 and 7.14 respectively which is far from a perfect model ($\text{NMSE}=1.0$). The annual, monthly and hourly FAC2 was found to be 0.04 , 0.12 and 0.11 respectively; a perfect model $\text{FAC2}=1.0$. These results were anticipated as the typical $\text{PM}_{2.5}$ composition in Halifax is comprised of $\sim 75\%$ long-range transport (LRT), with the remaining local sources estimated to be Refinery ($0.081 \mu\text{g m}^{-3}$), Ships ($0.13 \mu\text{g m}^{-3}$), Vehicles ($0.49 \mu\text{g m}^{-3}$) and Fugitive Dust ($0.23 \mu\text{g m}^{-3}$) (Gibson et al., 2013b).

Table 5. Dispersion model results and model performance evaluation for annual, monthly and hourly averages for each metric at each discrete receptor within each domain

Model Domain	Metric	Modeled Annual Monthly Hourly Averages ($\mu\text{g m}^{-3}$)	Observed Annual Monthly Hourly Averages ($\mu\text{g m}^{-3}$)	Modeled v Observed R^2 Annual Monthly Hourly	Annual FB Monthly FB Hourly FB	Annual NMSE Monthly NMSE Hourly NMSE	Annual FAC2 Monthly FAC2 Hourly FAC2
Halifax	$\text{PM}_{2.5}$	0.16	4.08	0.053	0.96	23.53	0.04
		0.63	5.21	0.043	0.88	6.39	0.12
		0.92	8.31	0.002	0.89	7.14	0.11
	NO_x	1.86	38.83	0.001	0.95	18.92	0.048
		2.32	42.1	0.003	0.94	16.2	0.055
		5.26	43.5	0.002	0.88	6.39	0.12
	SO_2	4.92	7.3	0.77	0.33	0.15	0.67
		5.24	8.72	0.63	0.4	0.26	0.6
		6.24	10.4	0.46	0.4	0.27	0.6
	SO_2	2.33	2.08	0.68	-0.12	0.013	1.12
		2.41	2.24	0.57	-0.08	0.005	1.08
		3.51	3.16	0.34	-0.11	0.011	1.11
Port Hawkes'	SO_2	1.68	2.2	0.18	0.24	0.073	0.76
		1.95	2.75	0.045	0.29	0.12	0.71
		2.83	3.94	0.021	0.28	0.11	0.72
Pictou	$\text{PM}_{2.5}$	0.26	7.2	0.65	0.96	25.73	0.036
		0.38	8.2	0.043	0.95	19.62	0.046
		0.92	9.42	0.029	0.9	8.34	0.098

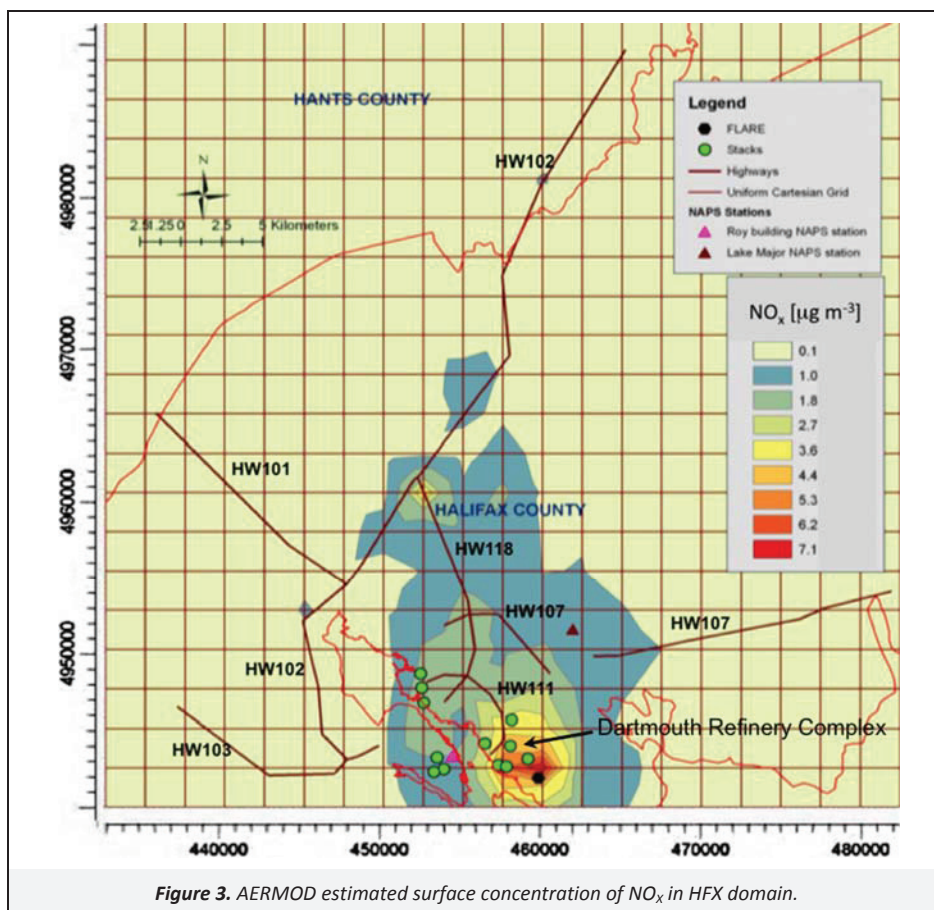


Figure 3. AERMOD estimated surface concentration of NO_x in HFX domain.

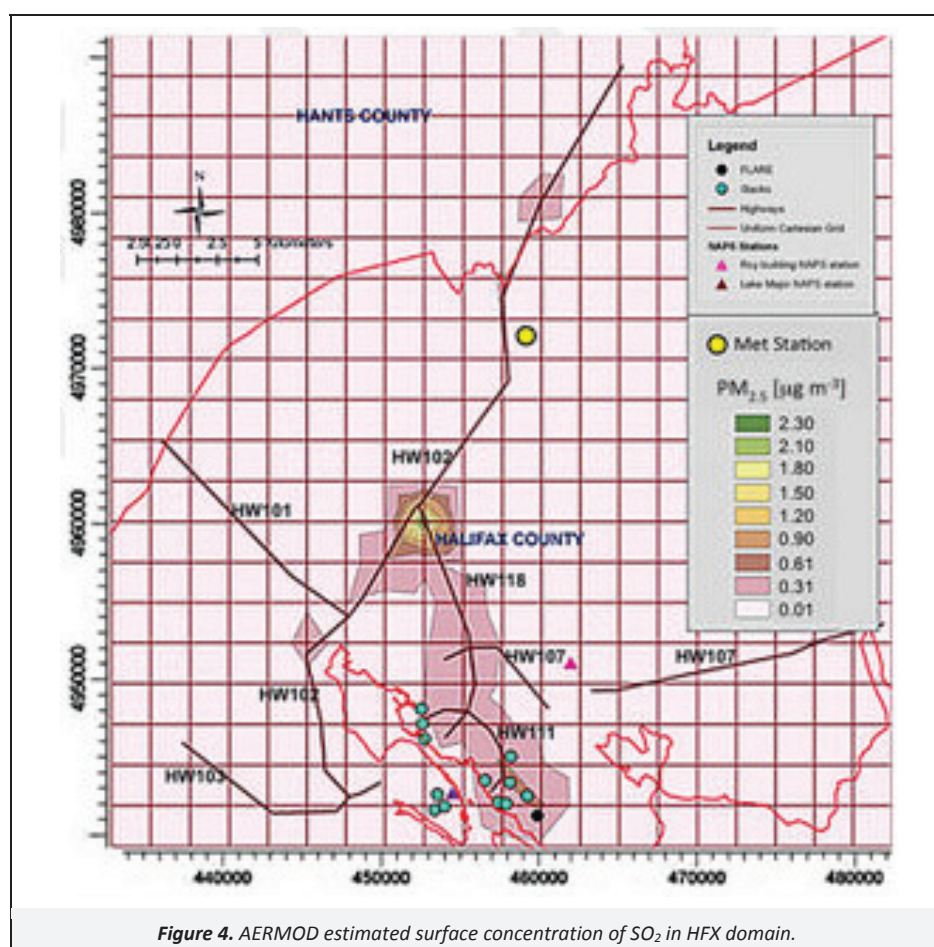


Figure 4. AERMOD estimated surface concentration of SO_2 in HFX domain.

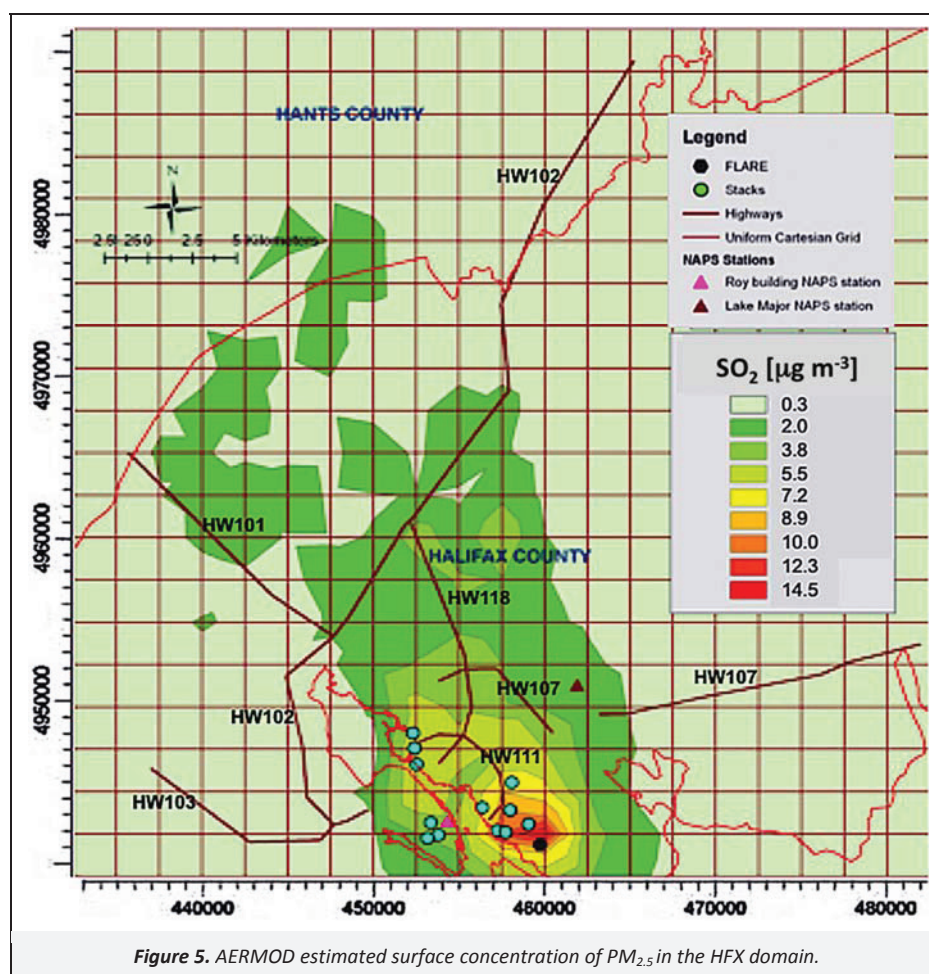


Figure 5. AERMOD estimated surface concentration of PM_{2.5} in the HFX domain.

Table 5 contains the estimated AERMOD results for the PM_{2.5} concentrations. The annual, monthly and hourly results and model evaluation are characterized by poor R^2 's large model under-prediction, e.g. the estimated annual mean NO_x of 1.86 µg m⁻³ is a factor of 21 lower than the annual mean observed NO_x of 38.8 µg m⁻³ from the Halifax downtown NAPS site, with no correlation between the monthly mean model and observations ($R^2=0.001$). The reason for the large difference between the annual, monthly and hourly calculated and observed is likely due to AERMOD only modeling a small portion of the total NO_x emissions in Halifax, the remainder being from vehicle emissions from the other minor roads and ship emissions are the other known large NO_x emitters in Halifax (Phinney et al., 2006). This helps to explain the large difference between the AERMOD surface estimate at the NAPS site and the observed NO_x concentrations. Therefore, one can conclude that the model estimates that NO_x emissions from the point and major lines sources have little impact on surface NO_x concentrations in the HFX domain.

Table 5 contains the estimated AERMOD results pertaining to SO₂ in the Halifax domain. The annual, monthly and hourly results and model evaluation are characterized by reasonable R^2 's for the annual and monthly model versus observed comparison (0.77, 0.63 and 0.43 respectively). There was reasonable model agreement ($0.5 \leq \text{FAC2} \leq 2$), e.g. the estimated AERMOD annual mean concentration estimated SO₂ of 4.9 µg m⁻³ is <2 agreement with the NAPS measured annual mean concentration of 7.3 µg m⁻³. The explanation for the relatively small difference (<2) between the calculated and observed SO₂ concentrations is probably due to the fact that the large emitters were included in the model (Phinney et al., 2006). The NMSE annual, monthly and hourly=0.15, 0.26 and 0.27 respectively which is not perfect but far closer to ideal when compared to PM_{2.5} and NO_x in Halifax.

3.4. Sydney

Annual average spatial concentration map of surface SO₂ concentrations in the SYD domain are presented in Figure 6.

It can be seen from Figure 6 that enhanced SO₂ concentration gradients are observed to the North East (NE) of the Lignan Power Station, directly downwind of the power station. The highest SO₂ concentration (8.7 µg m⁻³) was found directly to the NE of the Lignan Power Station, being advected out to sea and away from receiving communities, which was the intended outcome of placing the power station at this location. Table 5 contains the estimated AERMOD results and model evaluation for SO₂ in SYD. The annual, monthly and hourly results and model evaluation are characterized by reasonable agreement between the annual and monthly modeled vs. observed ($R^2=0.68$ and 0.57 respectively). However, the R^2 drops to 0.34 for the hourly comparison. The good agreement between the modeled and observed SO₂ in the SYD domain is probably due to the fact that the Lignan Power Station is the dominant SO₂ emitter in the domain by virtue of the fact that it uses coal with 1–2% sulfur content (Gibson et al., 2013a). The reduction in R^2 for the hourly modeled versus observed is probably a result from using meteorology that differs from the precise conditions at the measurement and source emission site. The FB is within a factor of 2, FAC2 is almost 1.0 and the NMSE approaches 1 for annual, monthly and hourly comparison results showing good model skill for SO₂ in SYD.

3.5. Port Hawkesbury

It can be seen from Figure 7 that the highest SO₂ concentrations (1.62 µg m⁻³) were found directly downwind of the New Page Paper Mill to the NE.

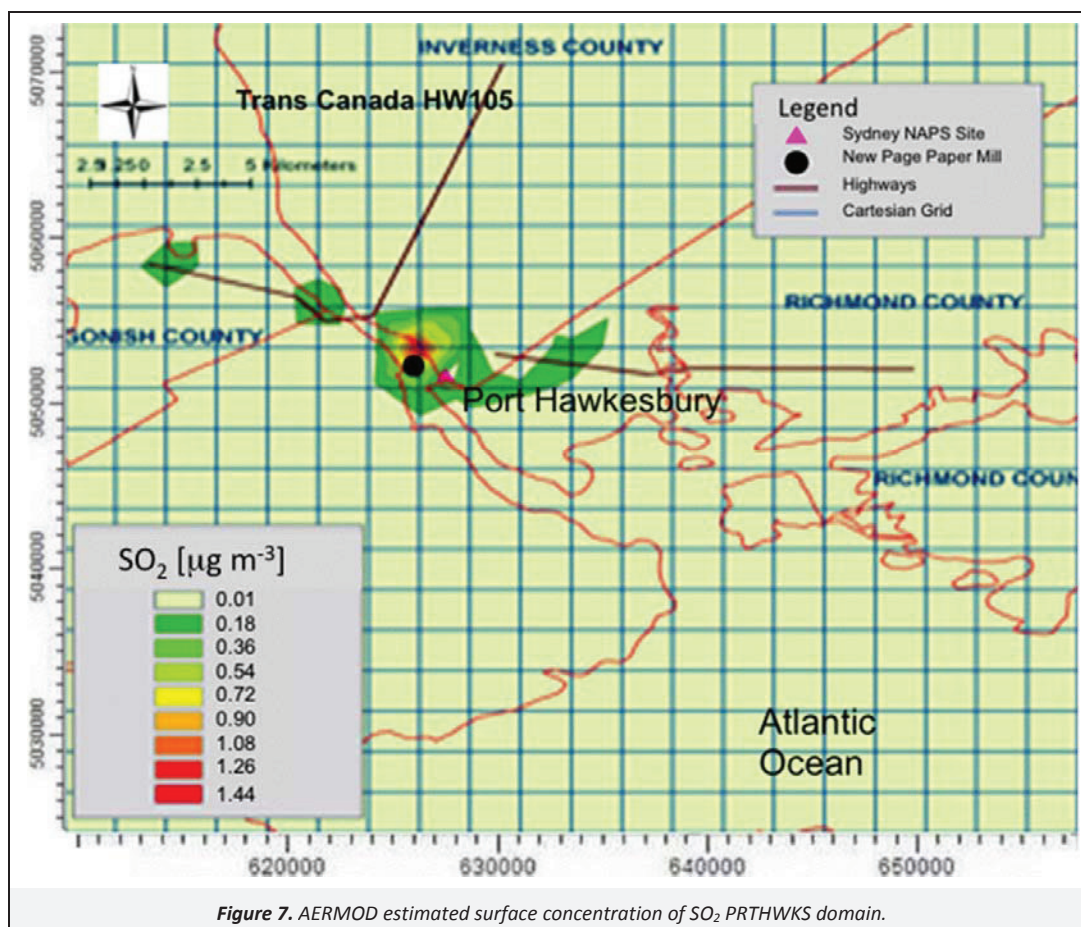
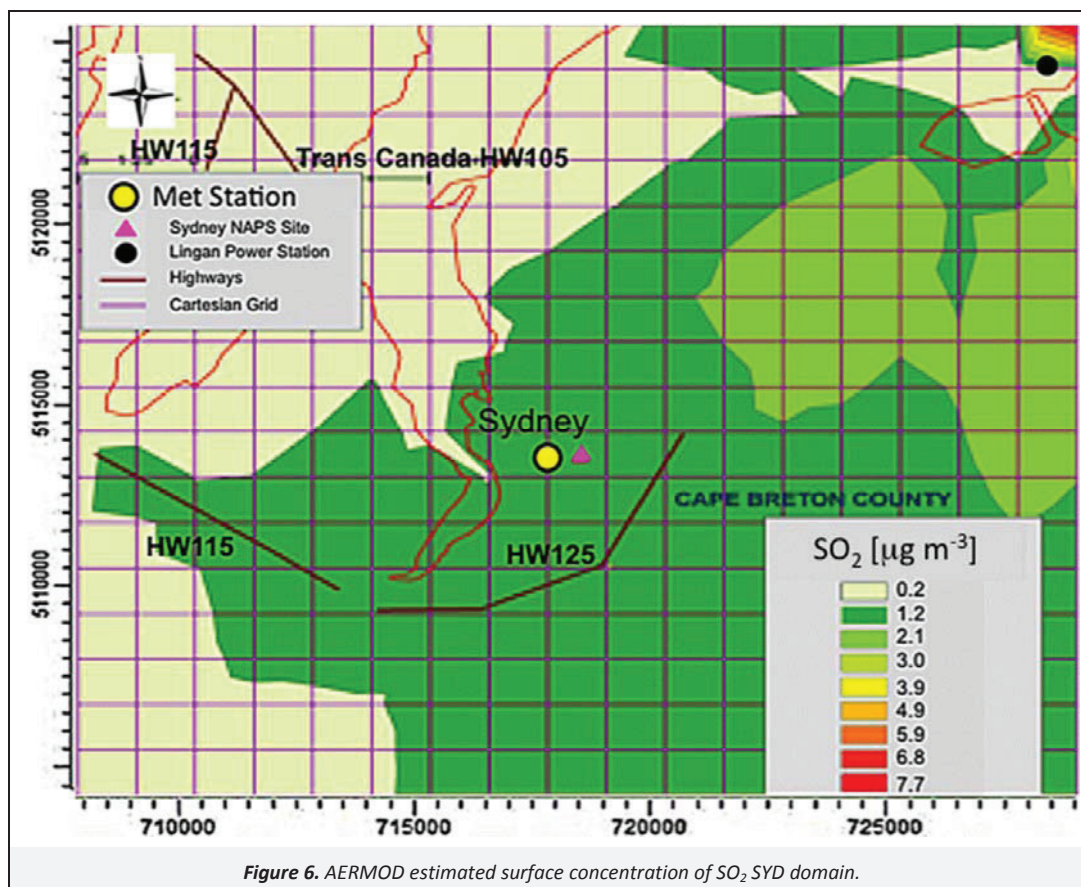


Table 5 contains the estimated AERMOD results and model evaluation for SO₂ in PRTHWKS. The annual, monthly and hourly results and model evaluation are characterized by extremely weak correlation between the annual, monthly and hourly model v observed ($R^2=0.18$, 0.045 and 0.021 respectively). The chief emission sources in the PRTHWKS domain are New Page, Exxon Mobil Inc. and highways, all of which were included in the model simulations. This likely explains why the estimated and observed annual mean SO₂ concentrations in PRTHWKS are of a similar magnitude. The remaining SO₂ emissions in this model domain are likely to have a contribution from ship emissions (Hingston, 2005; Phinney et al., 2006; Gibson et al., 2013b). The FB is within a factor of 2 for the annual, monthly and hourly SO₂ comparison results with the associated FAC2 0.5≤2≤2.0 and the NMSE=0.073, 0.12 and 0.11 respectively. AERMOD performed reasonably well in PRTHWKS, especially when compared to PM_{2.5} (HFX and PIC) and NO_x (HFX) in the other domains for annual, monthly and hourly comparison results showing good model skill for SO₂ in SYD.

3.6. Pictou

It can be seen from Figure 8 that the highest PM_{2.5} concentration (0.88 µg m⁻³) was found centered downwind of the four Neenah Paper Mill stacks.

The estimated annual mean PM_{2.5} (0.26 µg m⁻³) shown in Table 5 is a factor of 25 lower than the NAPS site (7.2 µg m⁻³). Interestingly, there was good agreement ($R^2=0.65$) in the trend in

the monthly mean modeled and observed concentrations, but not the actual concentration at observed at the NAPS site. There was no correlation observed between the hourly comparison ($R^2=0.003$), again likely due to using meteorology that differs from the source and measurement site. The FB, NMSE and FAC2 results provided in Table 5 for the annual, monthly and hourly comparisons are poor and far from a perfect model for PM_{2.5} in PIC.

4. Conclusion

Wind rose analysis showed that the prevailing wind direction in the modeling domains was from the WSW (range 248° to 265°). The AERMOD model evaluation showed that there was good agreement between the modeled and observed SO₂ concentration for the annual and monthly comparison (R^2 HFX=0.77 and 0.63 SYD=0.68 and 0.57). However, the R^2 was seen to drop for hourly comparisons for SO₂ in HFX and SYD (0.46 and 0.34 respectively), probably a result from using meteorology that differs from the precise conditions at both the measurement and emitter. For SYD, AERMOD slightly overpredicted the annual, monthly and hourly SO₂ concentration (−0.12, −0.08 and −0.11). The SO₂ over-prediction in Sydney is likely due to the NAPS site being upwind of the major SO₂ point source and potential modeling issues associated with modeling such low concentrations and discrepancy between the meteorological variables used in the model and the actual values found at the emission site and measurement site (Perry et al., 2005). Although, AERMOD showed reasonable model skill for estimating surface annual and monthly SO₂ concentrations

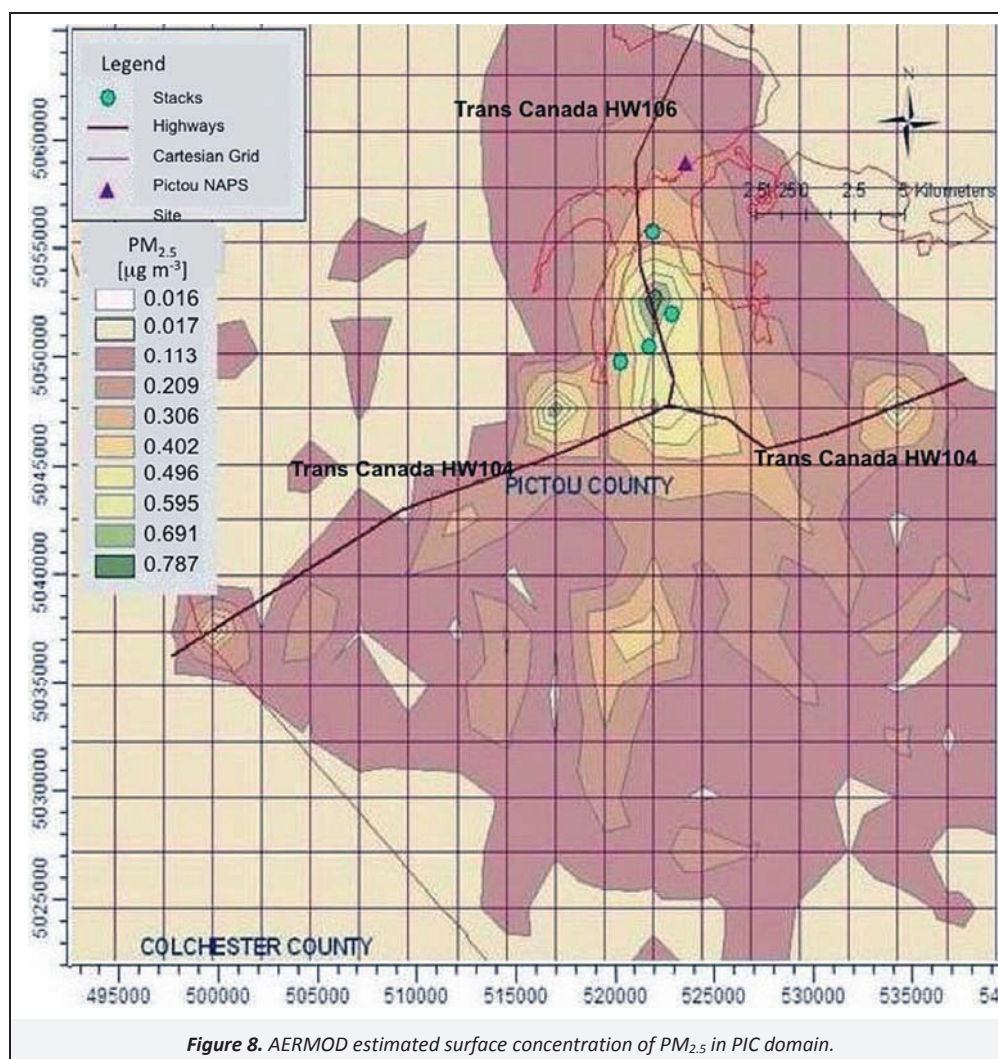


Figure 8. AERMOD estimated surface concentration of PM_{2.5} in PIC domain.

in HFX and SYD, AERMOD showed poor model skill at predicting SO_2 in PRTHAWKS over the same averaging periods. The FAC2 for SO_2 at the NAPS receptors in HFX, SYD and PRTHAWKS were seen to be within a factor of 2 of the observed concentrations, which demonstrates that the major sources influencing these receptors were likely contained in the model simulations. The AERMOD estimated annual mean $\text{PM}_{2.5}$ and NO_x impacting the NAPS site discreet receptor in Halifax was $0.16 \mu\text{g m}^{-3}$ and $1.9 \mu\text{g m}^{-3}$ respectively, demonstrating little surface impact from the point and major line sources for these metrics in the Halifax domain. The AERMOD estimated annual mean $\text{PM}_{2.5}$ concentration at the NAPS receptor in Pictou was $0.02 \mu\text{g m}^{-3}$ demonstrating that the point and major highway vehicle emissions also contributed little to surface $\text{PM}_{2.5}$ concentrations in this domain. The model evaluation of $\text{PM}_{2.5}$ in HFX and PIC show poor agreements and model skill. This result for $\text{PM}_{2.5}$ is likely due to the influence of LRT of aerosols from upwind source regions and also due to the fact that the NAPS site is upwind of the modeled emissions. In addition, the influence of fugitive dust and vehicle emissions from the streets surrounding the NAPS site must also provide source input to the $\text{PM}_{2.5}$ concentrations observed at the NAPS site (Gibson et al., 2013b). The model evaluation for NO_x in HFX also shows poor agreements and poor model skill. Again, mainly due to other large emitters not being present in the model, e.g. other major and minor roads and Halifax harbor ship emissions. The results of the model evaluation showed that AERMOD could estimate surface concentrations of SO_2 with reasonable accuracy in HFX and SYD over annual and monthly averaging periods, with less confidence in the estimates of SO_2 over hourly averaging periods. This study has shown that AERMOD can be used to provide insight into the surface impact of $\text{PM}_{2.5}$, NO_x and SO_2 from point and major line sources at annual, monthly hourly averaging periods in model domains within Nova Scotia, Canada. The study highlights the validity of using emission inventory data to estimate the surface impact of major point and line sources within domains containing complex terrain, differing land use types and with large variability in the annual meteorology.

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