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Air Quality and Acid Deposition Simulation of South Athabasca Oil Sands Area Applying WRF, CMAQ and CALPUFF Models, and Model Performance Evaluations of WRF and CMAQ Models

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1. INTRODUCTION

In situ oil sands development is expected to dominate bitumen production in the coming decades and much of it will be located in the south Athabasca oil sands area (SAOS). The Weather Research and Forecasting (WRF) model is run for SAOS in 2010 to provide meteorological input for the air quality models, improve model performance and reduce model biases. The SAOS WRF modelling uses a fine temporal input resolution (i.e., 3-hourly interval NARR) and local observation data for nudging to generate WRF meteorological fields for use in CMAQ and CALPUFF modelling. Based on developed emission inventories and modelling inputs for 2010 (Environ and Novus, 2014), this study applies the CMAQ model to simulate the ground level concentrations of ozone, $PM_{2.5}$, PM_{10}, NO_2, SO_2, CO, and acid deposition in SAOS in 2010. CALMET and CALPUFF models are also applied to a relatively smaller domain, to compare CALPUFF modelling results of 2010 acid deposition in SAOS with the CMAQ modelling output.

The CMAQ modelling results for 2010 are evaluated against observations from 10 ambient monitoring stations. The model overestimates ground level ozone concentrations by 0 to 10 ppb monthly, but is robust enough to capture monthly patterns and high percentile values from observed ozone concentrations. It also illustrates a larger underestimation of $PM_{2.5}$ concentrations during summer months mainly due to counting out wild fire events during wildfire season in 2010. Furthermore, the model overall underestimates NO and NO_2 concentrations, except in some summer time overestimations. Nevertheless, the model captures the monthly patterns of NO and NO_2 concentrations in the observations throughout the year.

The WRF model full-year simulation is also evaluated for application in the SAOS area for 2010. Weather parameters, including temperature, wind speed and direction, etc., are compared and evaluated with observations from 9 surface weather stations in the SAOS modelling domain. The evaluation indicates the model performs reasonably well and that the WRF model is sufficient to support CMAQ and CALPUFF modelling in this study.

The study focuses on air modeling for year 2010, the baseline case. Baseline modelling provides a benchmark, to which observations are compared to evaluate the simulation, to which predictions for future scenarios can be compared to assess future development impacts. Therefore this study lays the foundation for the next research work – the future development predictions.

2. WRF MODELLING

WRF ARW V3.4.1 was used in the SAOS WRF run. The NARR (North America Regional Reanalysis) 3-hourly data, together with upper and surface observation data were used to prepare WRF initial and boundary conditions as well as Four-Dimensional Data Assimilation (FDDA) and observation nudging inputs. The 36/12/4 km WRF modelling domains are much larger than CMAQ modelling domain so as to create sufficient boundary relaxation zone for SMOKE and CMAQ modelling. Main model physics options in this WRF simulation include Turbulent Kinetic Energy (TKE) boundary layer scheme, WSM6 microphysics scheme, and Noah Land surface process. The modified Kain-Fritcsh cumulus scheme was used for both 36 and 12 km domain

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and no cumulus scheme was used in the 4 km domain under the assumption that the 4 km resolution was sufficiently fine to explicitly resolve the convective activity. Model restarts every 84 hours with 12-hour spin-up. Data outputs are hourly for the 72 hour after the spin-up period.

3. WRF MODELLING EVALUATION

Model evaluation was performed for the WRF 2010 full-year annual simulation for the 4 km SAOS WRF modelling domain.

Table1 lists the stations included in this analysis. These stations are all within the SAOS 4 km WRF modelling domain.

Table1. List of stations used in SAOS WRF model performance evaluation.

id	name	county	province	latitude	longititude	altitude (m)
CWLB	LAC-LA-BICHE-(MARS)	CA	AB	54.767	-112.017	567
CWRD	RED-EARTH	CA	AB	56.533	-115.267	546
CXBD	BARRHEAD CS	CA	AB	54.0947	-114.4475	646
CWVI	VEGREVILLE	CA	AB	53.517	-112.1	639
CXZU	WHITECOURT	CA	AB	54.15	-115.783	785
CYED	EDMONTON-NAMAO-ALTA	CA	AB	53.667	-113.467	688
CYMM	FORT-MCMURRAY-ARPT	CA	AB	56.65	-111.217	369
CYZH	SLAVE-LAKE-AIRPORT	CA	AB	55.283	-114.783	581
CYZU	WHITECOURT APT	CA	AB	54.133	-115.783	802

To quantify model performance, several statistical measures were calculated and evaluated for the monitoring stations.

Table1 illustrates the statistics of 2-meter temperature, among which Mean Correlation Coefficient is 0.99, Gross Mean Error is -0.34 ℃, and Mean RMSE is 1.8 ℃.

Table2. WRF modelling performance of Temperature in 4km SAOS domain (at 2-meter height; unit = ℃).

STATION ID	CORR	Mean Error	RMSE
CWLB	0.988	-0.673	2.034
CWRD	0.990	-0.332	1.927
CWVI	0.992	-0.439	1.716
CXBD	0.988	-0.463	2.025
CXZU	0.990	-0.384	1.694
CYED	0.990	-0.121	1.725
CYMM	0.991	-0.184	1.766
CYZH	0.992	-0.126	1.579
CYZU	0.988	-0.338	1.853
Gross Mean	0.990	-0.34	1.813

As to 10-meter wind speed, Table 3 indicates that the SAOS WRF simulation has a correlation coefficient ranging between 0.6-0.7. Meanwhile, for 10-meter wind direction, Table 4 shows that the SAOS WRF modelling exhibits a 25 degree Mean Error for mean direction (Mean_DIR) and 16 degree Mean error for Aggregated Mean Direction (AGGR_DIR). For 2-meter humidity mixing ratio, Table 5 shows the simulation statistics with Correlation Coefficient as 0.943, Gross Mean Error as 0.15g/kg, and Mean RMSE as 0.97g/kg.

Table3. WRF modelling performance of Wind Speed in 4km SAOS domain (at 10-meter height; unit = m/s).

STATION ID	CORR	Mean error	RMSE
	SAOS	SAOS	SAOS
CWLB	0.648	1.030	1.864
CWRD	0.635	1.402	2.170
CWVI	0.706	0.389	1.858
CXBD	0.641	1.297	2.292
CXZU	0.637	0.989	2.143
CYED	0.657	0.634	2.026
CYMM	0.625	0.299	1.717
CYZH	0.635	1.022	2.397
CYZU	0.606	0.563	2.419
Gross Mean	0.644		2.098

Table4. WRF modelling performance of Wind Direction in 4km SAOS domain (at 10-meter height; unit = degree).

	Mean_DIR[1]	AGGR_DIR[2]
STATION	Mean Error	Mean Error
	SAOS	SAOS
CWLB	2.9	-8.9
CWRD	0.4	5.0
CWVI	26.7	12.8
CXBD	-21.6	-0.9
CXZU	-46.5	-40.4
CYED	6.9	-1.3
CYMM	19.6	-31.1
CYZH	-96.4	38.1
CYZU	-9.1	-8.2
Gross Mean	25.6	16.3

4. CMAQ MODELLING

4.1 Methodology

[1] "MEAN_DIR": Each of the speed $(U^2+V^2)^{1/2}$ is treated separately and given equal weight. The mean forecast wind direction, mean observation wind direction, and the associated error are computed for each model-observation pair. Then the means are computed across all of these modelling wind directions, observation wind directions, and their errors.

[2] "AGGR_DIR": The wind speed values are taken into account to calculate aggregated wind direction, i.e., a higher wind speed will gain more direction statistic weight than a lower wind speed record. .

There are 3 tiers of modelling domain in this study: 36 km resolution domain -western US and Canada, 12 km resolution domain -provincial scale and 4 km resolution domain –SAOS, the research area (Figure 1). Simulation for each coarser domain generates boundary condition and initial condition for the finer domain.

Table5. WRF modelling performance of Humidity Mixing Ratio in 4km SAOS domain (at 2-meter height; unit = g/kg).

STATION	CORR	Mean Error	RMSE
CWLB	0.957	0.10	0.84
CWRD	0.923	0.35	1.09
CWVI	0.938	0.15	1.03
CXBD	0.943	0.19	0.96
CXZU	0.935	0.03	0.97
CYED	0.948	0.05	0.97
CYMM	0.958	0.24	0.91
CYZH	0.956	-0.10	0.89
CYZU	0.926	0.36	1.08
Gross Mean	0.943	0.15	0.97

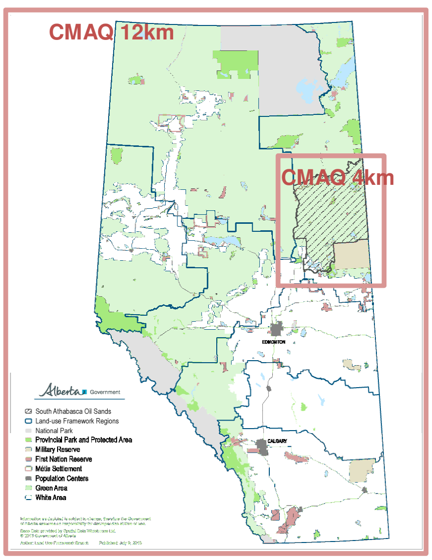

Figure1. Provincial and Research Modelling Domain

4.2 Hourly Average Modelling Results

Predicted 1-hr average ground level concentrations (Figure 2) illustrate larger regional effect of ozone and $PM_{2.5}$ formed as secondary pollutants, combined regional and local effect of NO_2, SO_2 and CO, and also local effect caused significantly by nitrogen titration and primary $PM_{2.5}$.

4.3 8-Hour and 24-Hour Average Modelling Results

The result for 8-hr average ozone modelling is consistent in spatial pattern with 1-hr average ozone simulation. The highest value occurs outside SAOS boundary. Worthy of note is the remarkable nitrogen titration effect clearly demonstrated in Fort McKay to Fort McMurray corridor (Figure 2).

Likewise, 24-hour average NO_2 simulation depicts similar spatial pattern to 1-hr average NO_2 modelling result. Maximum 24-hour average $PM_{2.5}$ concentrations for the major part of SAOS area are below 30 µg/m^3. A few hot spots are nearby larger industrial and transportation sources and in the area north of SAOS. The other $PM_{2.5}$ hot spots are located in the southern portion of SAOS with values lower than 50 µg/m^3 and they are associated with community and industrial area within and in the vicinity of SAOS.

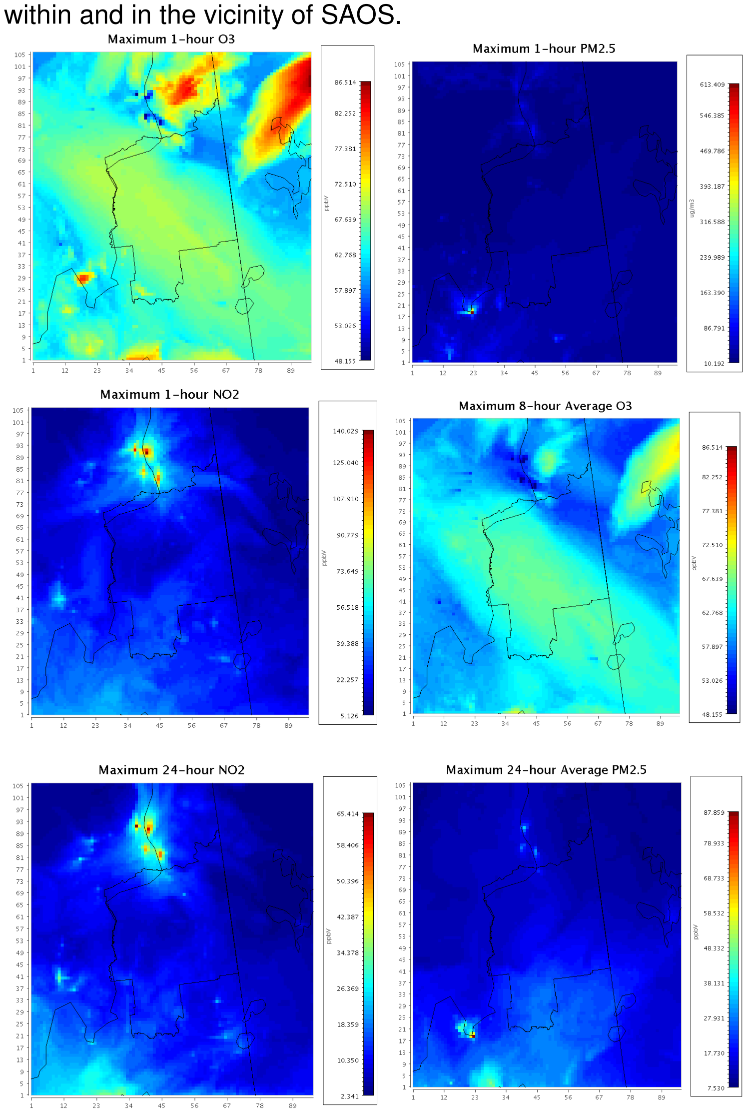

Figure2. Modelling Results for Short-term Averages

4.4 Annual Average Modelling Results

Plots of annual average $PM_{2.5}$ and PM_{10} (Figure 3) show clearly the relatively higher $PM_{2.5}$ and PM_{10} concentrations occur at the locations adjacent to pollutant emitting sources.

Within SAOS boundary, the predicted annual $PM_{2.5}$ and PM_{10} are very low and the relatively higher concentrations nearby sources can be more attributable to direct emissions of PM_{10} and primary $PM_{2.5}$ from the larger emission sources; And the contributive sources outside SAOS boundary locate at Fort McKay to Fort McMurray corridor in the north, and the industry, transportation and community areas in the south. The figures also show the complementarity in spatial distribution pattern between NO_2 concentration and ozone concentration, due to nitrogen titration effect.

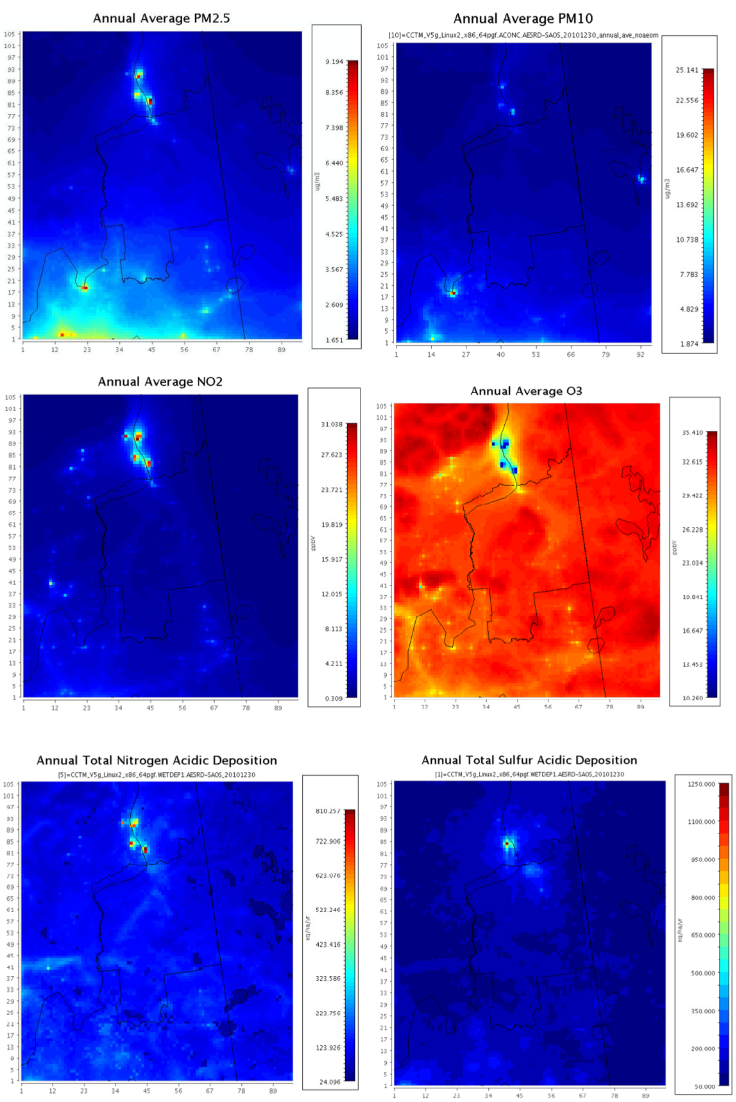

Figure3. Modelling Results for Annual Averages

4.5 Modelling Results of Acid Deposition

The annual total nitrogen deposition and sulphur deposition depict clearly the impact of the sources scattering intensively along the two highways and other individual emission sources. The figures also illustrate the spatial consistency between NO_2 concentrations and nitrogen depositions with similar spatial patterns. The highest nitrogen deposition occurs in the corridor between Fort McKay and Fort McMurray, which is outside SAOS boundary. Within SAOS area, the relatively higher values occur nearby the larger air pollutant emitters and the sources near the two highways. The lake areas have relatively lower nitrogen deposition. This is due to higher water surface resistance and consequently lower solubility of nitrogen compounds, compared to the absorption capacity of floras surrounding the lakes (AENV, 2008).

With the same conditions as SO_2, because of stringent regulation on sulphur emission, less sulphur sources with significant emissions exist. The highest sulphur deposition occurs close to the major sulphur emission plant site. Within SAOS, the relatively higher sulphur depositions occur close to the sulphur emission source sites.

5. CMAQ MODELLING EVALUATION

5.1 Evaluation Approach for CMAQ Modelling Performance

The modelling results are evaluated against observations at 10 air monitoring stations (Figure 4) in this study. Various types of bias and error metrics are examined to evaluate the simulation. AMET tool is applied to the model performance evaluation.

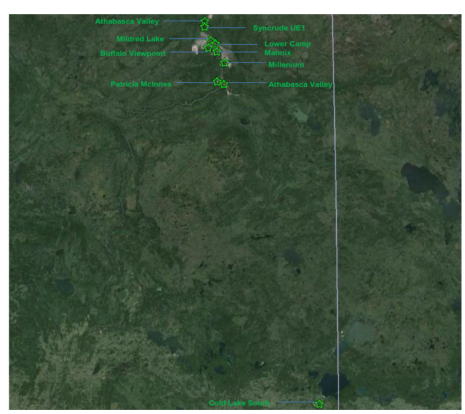

Figure4. Ambient Air Monitoring Stations Applied for Modelling Results Evaluation

5.2 Ozone Modelling Result Evaluation

Figure 5 demonstrates various graphic statistics for evaluating ozone simulation. The first figure shows the scatter plot of ozone concentrations, comparing simulation and observation; the second shows monthly bias and error, which are in general higher than the USEPA model performance goal. However, the third figure demonstrates that simulations are close to observations for high percentile values, indicating the model is robust to capture the peak values in observations.

As shown in the time series plot of simulated and observed ozone concentrations (Figure 5), simulation during winter matches the real fluctuation better than summer time. Considering together with the monthly comparison plot (Figure 5), the model overall overestimates the reality by monthly 0 to 10 ppb but is robust to capture the temporal patterns and peak values.

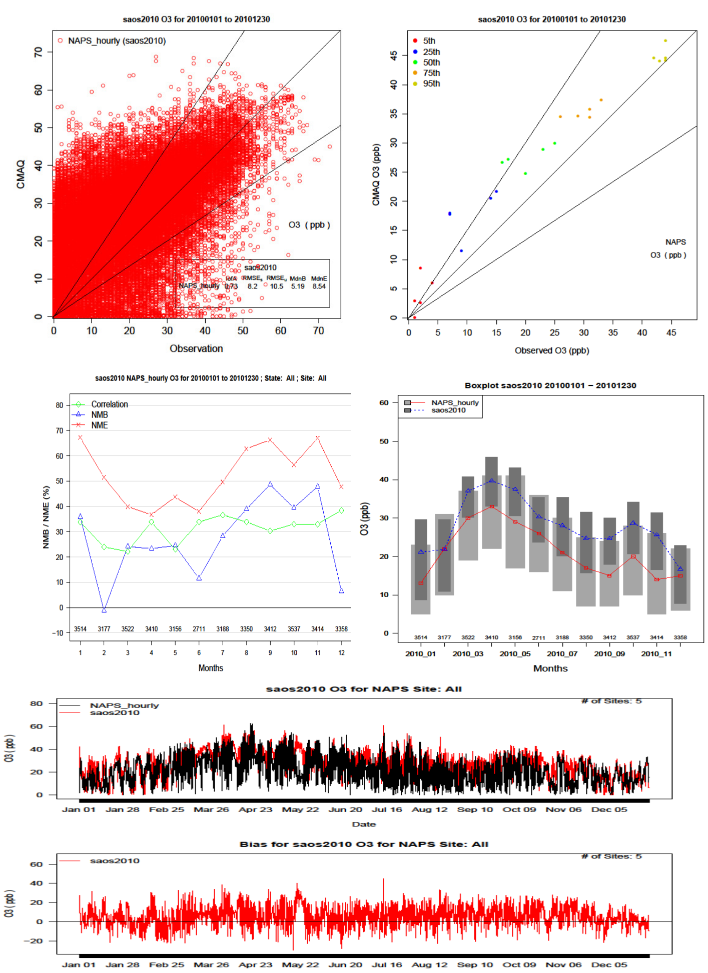

Figure5. Modelling Evaluation for Ozone

Table 6 contains ozone modelling performance metrics that compare the spatially paired predicted and observed peak values, including hourly ozone peaks and 8-hour ozone peaks, at available monitoring stations in the 4 km modelling domain. Overall, the predicted hourly ozone peaks near the monitoring stations are meeting the USEPA's model performance goal, and the predicted 8-hour ozone peaks are matching the observations quite well.

Table6. Summary of model performance statistics for maximum 1-hour and 8-hour average ozone concentrations for the 2010 CMAQ 4 km simulation

Site	Peak Hourly Ozone			Maximum 8-hour Average			Number of data points
	Max Obs (ppb)	Max Prd (ppb)	Paired A_P (%)	Avg Obs (ppb)	Avg Prd (ppb)	Bias (ppb)	
All sites in 4km domain	66	64.292	-2.98%	63	58.222	-5	82884
Athabasca Valley	66	68.409	3.65%	61	57.944	-3	8315
Patricia McInnes	73	64.970	-11.00%	68	58.991	-9	8323
Fort McKay	66	60.904	-7.72%	64	55.432	-9	8348
Fort McKay South	62	60.826	-1.89%	58	55.068	-3	8350
Cold Lake South	65	66.351	2.08%	63	63.676	1	8336

5.3 $PM_{2.5}$ Modelling Result Evaluation

As shown in Figure 6, the monthly comparison between $PM_{2.5}$ simulation and observation demonstrates larger underestimation during summer time, while simulation matches observation quite well for the other months. The time series plot of predicted and observed $PM_{2.5}$ concentrations depicts that the reason is wild fire events. For example, the highest peak $PM_{2.5}$ on Aug.19, 2010 was blown in by the prevailing winds from the British Columbia forest fire. Furthermore, during 2010 fire season that started on April 1 and ended on October 31, Alberta recorded over 1800 wildfires in the Forest Protection Area.

In addition, some of the forest fires were lit up by a string of lightning strikes. While lightning strikes are taken into account for reckoning in lightning NO_x generation and its effect added in nitrogen deposition, wild fires are not, in order to make consistency between baseline case and the to-be-modelled future scenarios in which exists wildfire uncertainty.

Overall, counting out wild fire effects, the model performs better at matching $PM_{2.5}$ simulation with observation, particularly for the temporally unpaired peak values, except the extreme peak values caused by forest fires.

5.4 Precursors of Ozone and PM2.5 Modelling Result Evaluation

The monthly comparisons between simulations and measurements of NO, NO_2 and O_3 (Figure 7) show that the model overall underestimates NO and NO_2 concentrations and overestimates ozone, except in some summer time overestimates NO and NO_2. Nevertheless, the model captures the monthly patterns of NO, NO_2 and O_3 throughout the year.

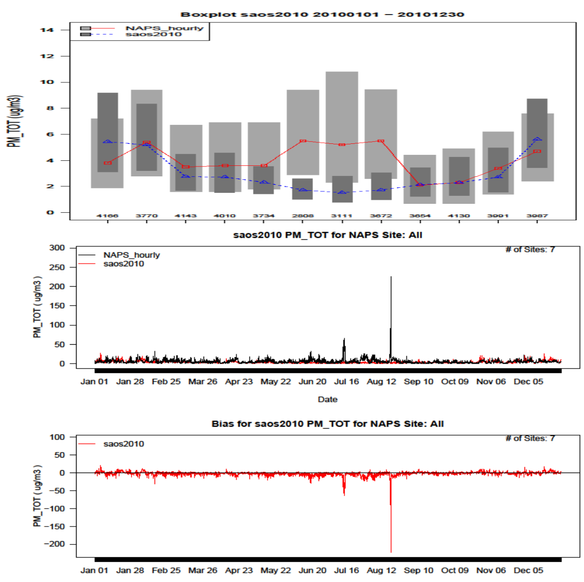

Figure6. Modelling Evaluation for $PM_{2.5}$

Consistently, the predicted time series cycle of NO_2 concentration (Figure 7) depicts higher bias to the observation during summer months with overestimation of the peak values, although the model reproduces the temporal pattern and temporally unpaired peaks throughout the year.

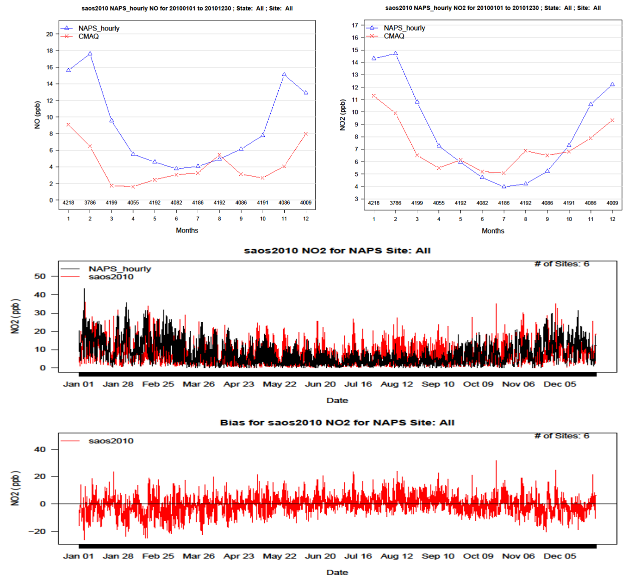

Figure7. Modelling Evaluation for Ozone and $PM_{2.5}$ Precursors

5.5 Modelling Result Evaluation of Nitrogen and Sulphur Wet Depositions

Table7 shows the comparisons between simulations and observations of sulphur and nitrogen wet depositions at the 3 monitoring sites. There are both overestimation and underestimation. One reason for this, particularly for the larger biases observed in Fort McKay station, can be the combination of two factors. On one hand, there are large concentration gradients in the Fort McKay to Fort McMurray corridor due to near-field effect. On the other hand, the 4km modeling has resolution limitation, with which simulated results are averaged over the 4 km by 4 km grid cells, while a monitoring station is about a point spot in the modelling domain.

Table7. Wet Deposition Comparisons of Simulations and Observations

Monitoring Station	Acidic Sulphur Wet Deposition			Acidic Nitrogen Wet Deposition		
	Observed Wet Deposition (eq/ha/yr)	Predicted Wet Deposition (eq/ha/yr)	Percent Difference	Observed Wet Deposition (eq/ha/yr)	Predicted Wet Deposition (eq/ha/yr)	Percent Difference
Fort McMurray (Athabasca Valley)	276	229	-17%	124	178	44%
Fort McKay	132	213	61%	81	215	165%
Cold Lake	162	120	-26%	178	167	-6%

6. ACID DEPOSITION SIMULATION COMPARISON BETWEEN CMAQ AND CALPUFF

Figure 8 and Figure 9 exhibit CALPUFF modelling result for annual total nitrogen deposition and annual total sulphur deposition, respectively. The CALPUFF simulations illustrate similarity in spatial distribution patterns of nitrogen deposition and sulphur deposition to CMAQ modelling results (as shown in the bottom of Figure 3). Some local inconsistency between the simulation results from the two models may partly be the consequence of different approaches of processing area sources and other non-point sources for the two models.

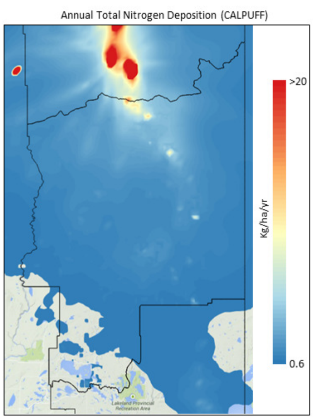

Figure8. Modelling Results for Annual Total Nitrogen Deposition Simulated by CALPUFF

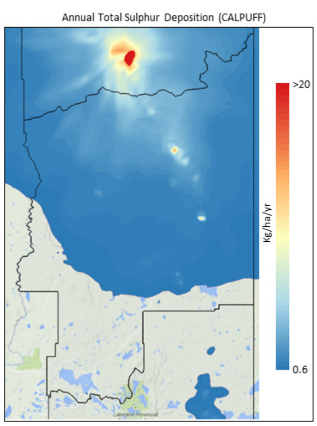

Figure9. Modelling Results for Annual Total Sulphur Deposition Simulated by CALPUFF

7. CONCLUSIONS

The WRF modelling and its evaluation indicate the model performs reasonably well and that the WRF modelling result is sufficient to support CMAQ and CALPUFF modelling.

The 2010 CMAQ modelling shows some consistency between simulations and observations of air quality, particularly for the temporal patterns and peak values. Therefore the model performs well to be used as a range-finding tool, and the modelling results for the 2010 baseline year can be used as a benchmark in comparison to future development scenarios in next study.

The acidic deposition simulations performed by CMAQ and CALPUFF models demonstrate some consistency in spatial patterns of nitrogen deposition and sulphur deposition simulated by these two models.

8. REFERENCES

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2. Environ and Novus, 2014. Development of Air Emissions Inventories and Inputs to Support Air Quality Modelling of Selected Pollutants using Community Multiscale Air Quality (CMAQ) and Long Range Dispersion CALPUFF Model for the South Athabasca Oil Sands Area (SAOS). Novato, CA; Guelph, Ontario. July.