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The Sensitivity of Model Plume Rise to Emissions Inputs

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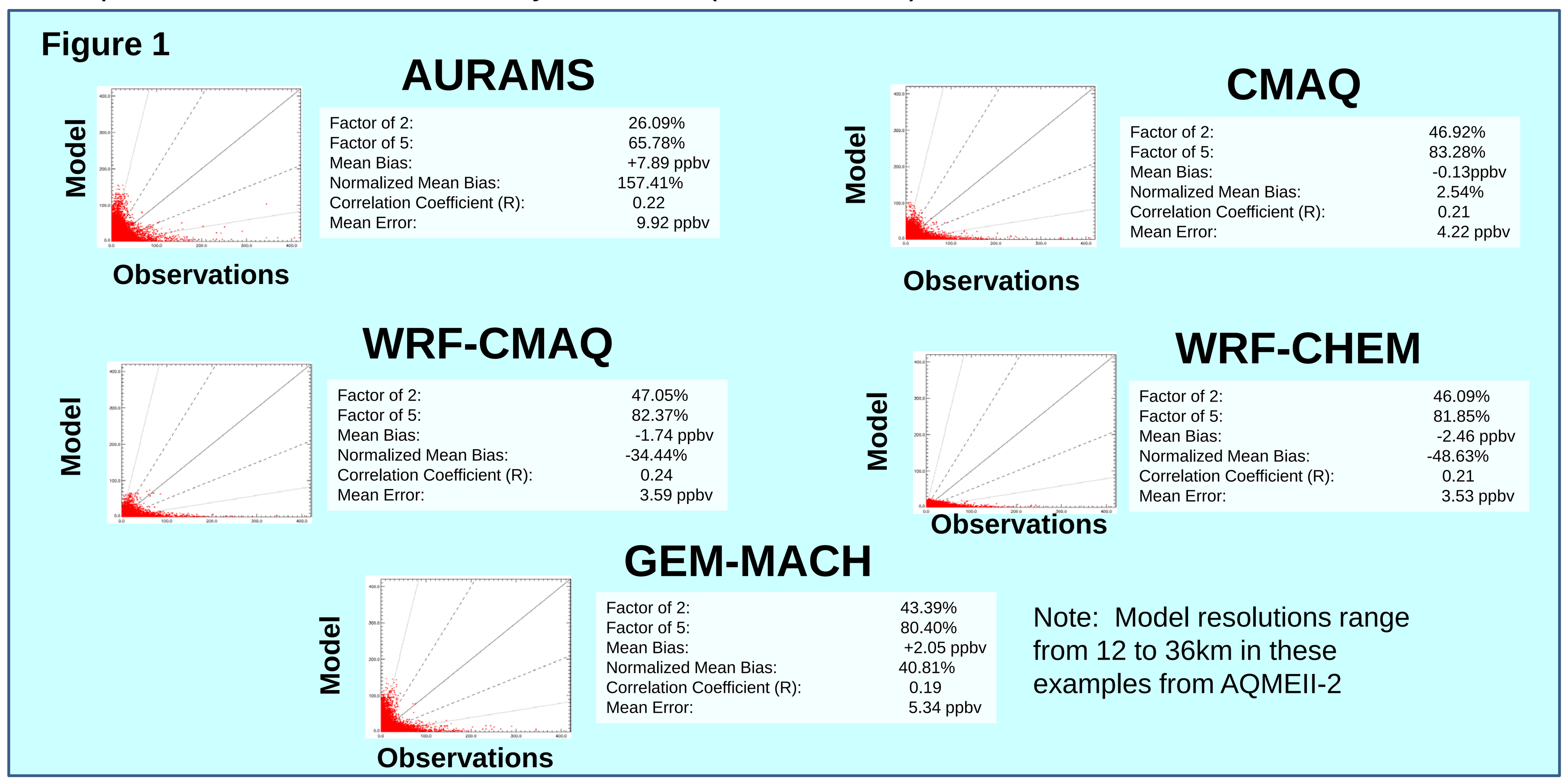
The Problem: *Most air-quality models have relatively poor performance forecasting SO_2 in North America (poor correlation, large biases etc.).*

Figure 1 shows some examples (scatterplots of daily average SO_2, model versus observations for the year 2006) from Phase 2 of the Air Quality Model Evaluation International Initiative (Makar *et al.* (a,b), 2015), in which different models' SO_2 predictions were compared to observations for the years 2006 (shown below) and 2010.

Figure 1



The same models have R values for O_3 ranging from 0.54 to 0.63, and for NO_2 ranging from 0.50 to 0.63 (compare to SO_2 values from 0.19 to 0.22). Yet SO_2 mass emissions are mostly from large point sources (stacks), for which Continuous Emissions Monitoring (CEM) observations are available. *Given the high quality of the SO_2 emissions data, why are the models doing so poorly for SO_2?* Some possibilities:

- Plume rise parameterization errors
- Plume rise input errors
- Emissions information is inaccurate, or incomplete
- SO_2 oxidation rate is underestimated
- SO_2 deposition rate is overestimated

The Joint Oil Sands Monitoring Intensive Campaign: a unique dataset for testing and improving model plume rise and emissions algorithms.

Joint Oil Sands Monitoring: the governments of Canada and Alberta collaborated to implement an Integrated Oil Sands Environmental Monitoring Plan for the Canadian oil sands. Part of this plan included a measurement intensive campaign with an instrumented aircraft and ground-based supersites during August and September of 2013. 22 aircraft flights were used to sample SO_2 and other species. The GEM-MACH model was configured to run in a 3-stage nested setup (see Figure 2 (a)), with a horizontal resolution for the first two nests of 10 km, and for the final highest resolution nest of 2.5km. All of the largest sources of SO_2 in the oil sands region have hourly CEM observations – **the combined observation plus emission dataset provides a unique opportunity to evaluate and test model predictions of SO_2.**

Figure 2

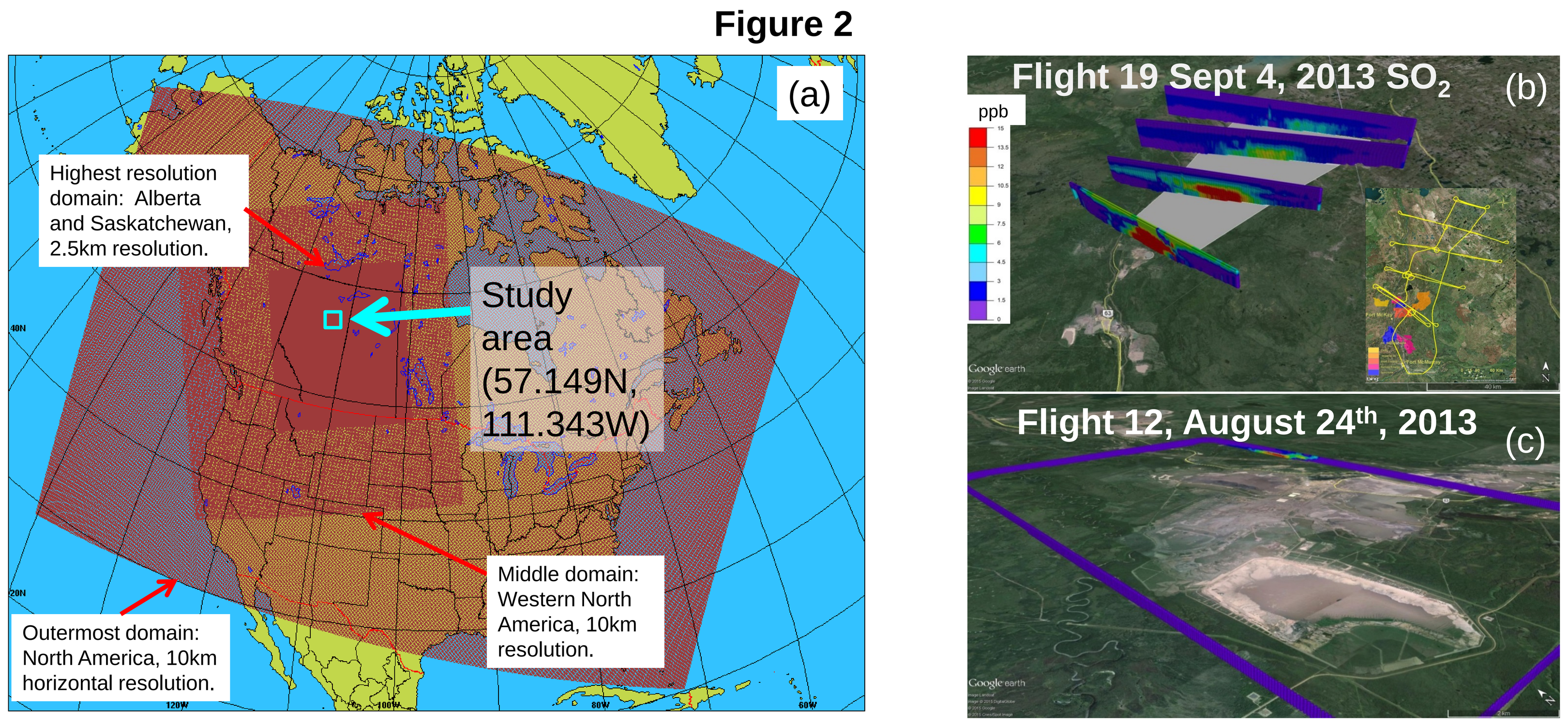


Figure 2(b) shows **observed SO_2**: reconstructed SO_2 concentration profiles from flights designed to study the chemical transformation of pollutants at successive distances downwind from oil sands sources (inset: flight path viewed from above). Figure 2(c): a second example; an emissions flight in which observations from circuits around a single facility are used to reconstruct that facility's emissions. This flight will be used as a "case study" for plume sensitivity experiments which follow.

GEM-MACH:A *comprehensive* and *coupled* air-quality model:

- ***Comprehensive***: attempts to include the main processes affecting the concentrations of atmospheric pollution
  - Gas-phase chemistry (42 species)
  - Aqueous phase chemistry and scavenging
  - Inorganic and organic particle formation
  - 2-or-12-bin sectional aerosol representation
  - 8 aerosol species (sulphate, ammonium, nitrate, primary organic carbon, secondary organic carbon, elemental carbon, crustal material, sea-salt)
  - Option for feedbacks between weather and air pollution in 12 bin mode
- ***Coupled***: a "Next Generation" model, in which meteorological and chemical processes are carried out by a single model
  - Makes use of data assimilated weather forecast data as inputs to improve forecast accuracy
  - Closely coupled meteorology and chemistry also improves accuracy
  - Options to show the effect of pollution on weather and vice versa
  - Peer models in the community: WRF-CHEM, WRF-CMAQ, COSMO-ART, COSMO-MUSCAT, MetUM-UKCA RAQ
- ***Model versions***:
  - 1.5.1: An extended version of the operational forecast model (including more detailed aerosol size distribution and the ability to calculated feedbacks between meteorology and chemistry) - used here for most simulations to date
  - 2: New model version under construction and testing

Case Study (Flight 12) : an emissions characterization flight around a single facility.

Given the proximity to the source (less than 5km), there is very little time for SO_2 deposition or chemical transformation – hence these can be eliminated as potential influences on model performance.

Observations show a well-defined plume between 250 and 500 m above ground level: Figure 3(a) shows observed SO_2 interpolated from multiple aircraft flights downwind of the facility). SO_2 emissions estimates from these observations agree with CEM emissions estimates to within 2 to 25%: most of the SO_2 mass in the plume is captured by the flights (Gordon *et al*, 2015).

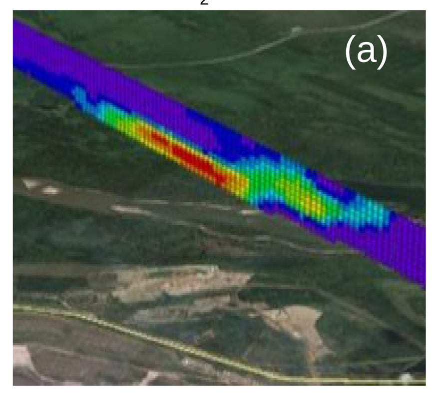
The model-predicted SO_2 concentrations are compared to observed values in the Figure 3(b). The x-axis is *time*, the y-axis is height: the colour contours are the model's predictions of SO_2 concentrations in the vertical column *along the aircraft flight path*. The observed concentrations along the aircraft's flight are also plotted with the same colour scale as the model values at the actual aircraft elevations and times. The predicted model plume height (800m) is higher in elevation than the observed plume height (500m). The correlation coefficient is poor – this is due to the predicted spatial location of the plume being slightly different from the observations; <u>a small error in the wind direction</u> has the model plume located slightly before or after its measured location on the timeline below, and this problem can be seen in all of the simulations.

(continued in next column, above right)

(Case Study, continued, from below left)

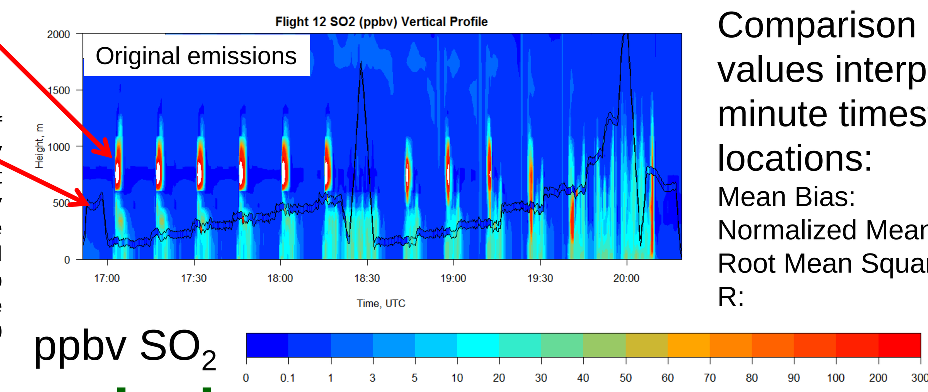
Figure 3

Observed SO_2 concentrations



Model plume maximum, at each circuit around the facility, is at 800m.

Aircraft observations of SO_2. The aircraft is slowly gaining in elevation as it flies around the facility during the first half of the flight.. The observed plume, however, shows up as hot-spots in the observations between 250 and 500m



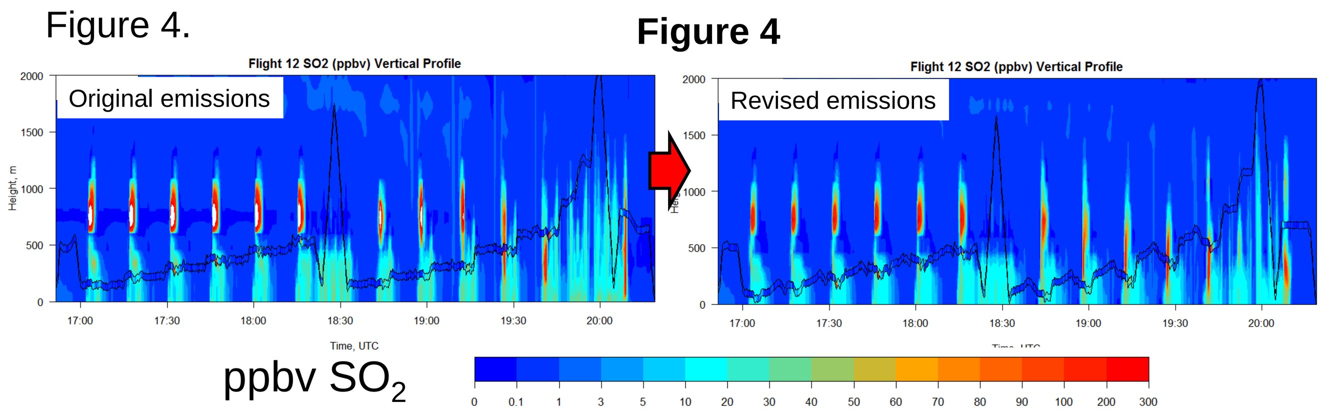
Comparison between model values interpolated from 2 minute timestep to aircraft locations:

Mean Bias: +3.1 ppbv
Normalized Mean Bias: +72.4%
Root Mean Square Error: 21.0 ppbv
R: 0.148

Scenario 1: Improve the emissions

The above simulations made use of Canadian 2010 National Pollutant Release Inventory annual values for Oil Sands facilities, where the hourly emissions are assumed to be constant with time. Note that Canadian major point source emissions are reported on an annual total basis under current regulations. However, emissions are reported to Alberta Environment and Parks as hourly CEM records. The 2013 CEM records for SO_2 and NO_x were obtained from Alberta Environment and Parks and used in the model. The results of this test are shown in Figure 4.

Figure 4



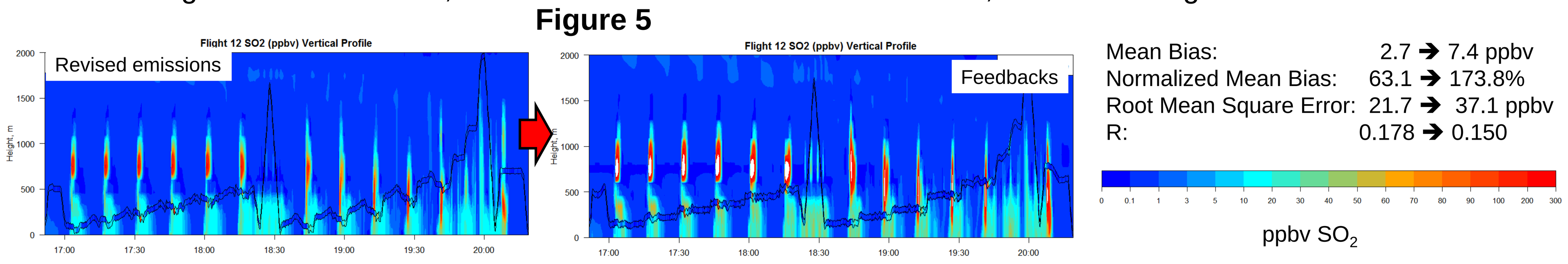
Mean Bias: 3.1 → 2.7 ppbv
Normalized Mean Bias: 72.4 → 63.1%
Root Mean Square Error: 21.0 → 21.7 ppbv
R: 0.148 → 0.178

The CEM data improved the performance for SO_2 slightly, reducing the bias. However, the plume height remained unchanged.

Scenario 2: Effects of feedbacks between weather and AQ

Another version of the model has the capability to include the effect of aerosol scattering and absorption of incoming solar radiation on weather, and of aerosols on cloud formation and cloud-related radiative balance.. The effect of using these "feedbacks", and the new emissions from Scenario 1, is shown in Figure 5.

Figure 5



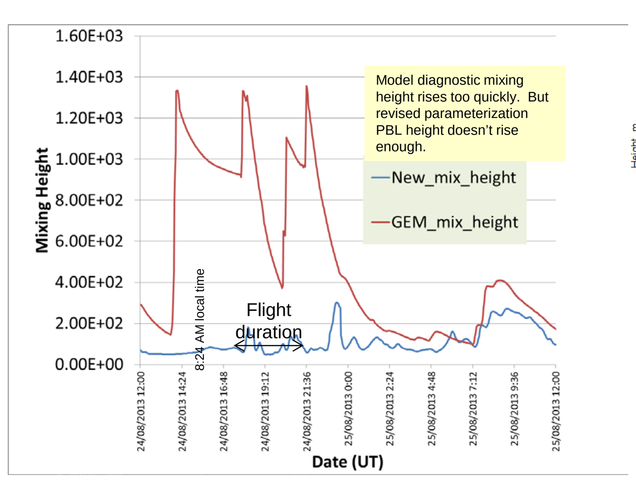
Mean Bias: 2.7 → 7.4 ppbv
Normalized Mean Bias: 63.1 → 173.8%
Root Mean Square Error: 21.7 → 37.1 ppbv
R: 0.178 → 0.150

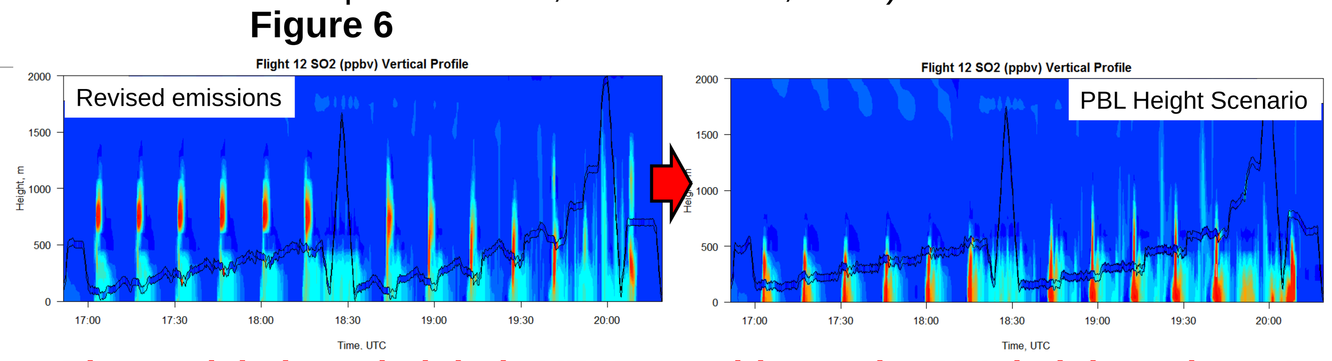
Feedbacks made SO_2 for this particular flight *worse* (Though $PM_{2.5}$ and NO_x improved – see my talk, Thursday morning).

Scenario 3: Sensitivity to diagnostic PBL height

The above tests did not alter the predicted *height* of the plume. The model's plume rise equation depends on the value of the Planetary Boundary Layer (PBL) height, which is a diagnostic output from the weather forecast part of the model. The model's PBL values look unrealistically high in the night and morning hours. Figure 6 shows how the model responds to a different diagnostic calculation for PBL height is used (PBL given as where the Bulk Richardson number relative to the lowest model level drops below 0.5, Aliabadi *et al*, 2015).

Figure 6





The model plume height is VERY sensitive to the PBL height estimate!

Mean Bias: 2.7 → 6.2 ppbv
Normalized Mean Bias: 63.1 → 145.7%
Root Mean Square Error: 21.7 → 30.8 ppbv
R: 0.178 → 0.123

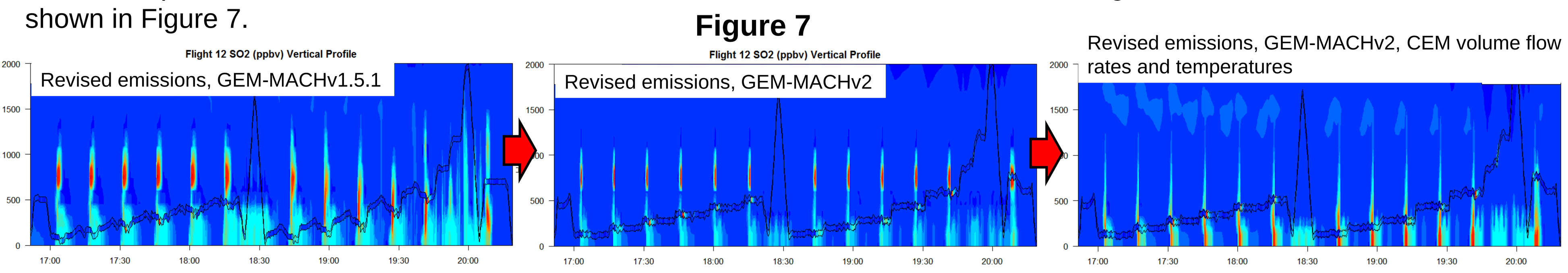
However, this estimate results in worse stats. and the observed plume is *not* fumigating.

The plume rise algorithm is clearly very responsive to the PBL height parameterization used. This is worth investigating further, given the relatively poor performance of GEM's diagnostic PBL height estimate in the evening and early morning (Fig. 11, Brunner *et al*, 2015).

Scenario 4: Sensitivity to volume flow rate and temperature.

Scenario 2 used CEM-derived emissions of SO_2 mass per hour, but the volume flow rate and temperature of each stack are assumed to be constant throughout the year. While time-varying volume flow rates and temperatures are available in CEM records, they are not reported to the NPRI, and have not been used to date in air-quality model simulations. The table at left below shows that the yearly reported values for these two parameters and the hourly observations can be very different. The <u>*measured volume flow rates are ½ the reported values*</u>, and the temperatures (degrees K) are 10% lower than reported. *This will reduce plume rise.* Here, version 2 of GEM-MACH was also used. The effect of using the measured volume flow rates is shown in Figure 7.

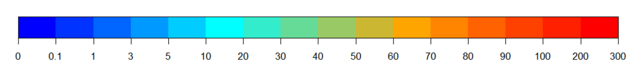
Figure 7



***Observed* (CEM) volume flow rates and temperatures** →

Date	Hour	Flow (m3/s)	Temp (K)
20130824	16:00	579.04	471.45
20130824	17:00	579.04	471.18
20130824	18:00	574.69	471.82
20130824	19:00	574.69	472.86
20130824	20:00	584.69	473.02
20130824	21:00	584.69	474.50
20130824	22:00	593.66	474.07
		1171.5	513.2

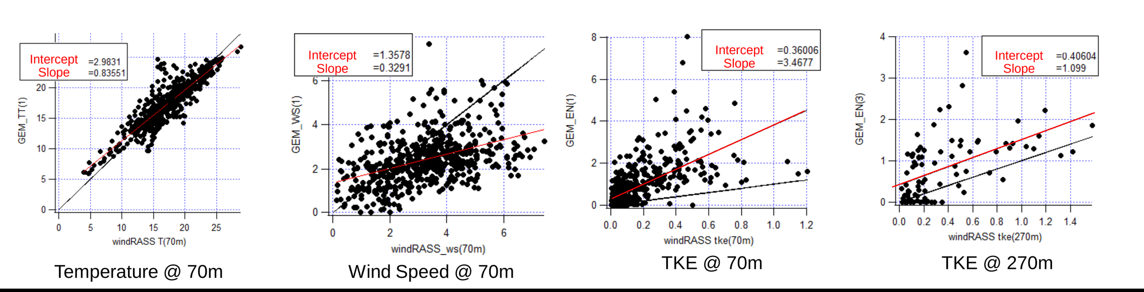
NPRI Annual *Reported* Volume flow rates and temperatures → 1171.5, 513.2



Mean Bias: +2.7 → -1.4 → +1.6 ppbv
Normalized Mean Bias: 63.1 → -33.7 → +37.7%
Root Mean Square Error: 21.7 → 23.5 → 24.5 ppbv
R; 0.178 → 0.001 → 0.009

GEM-MACH v2 reduced the bias but also reduced R. Using the measured volume flow rates and temperatures has a similar effect to the PBL height reduction, bringing down the plume and resulting in fumigation.

What additional factors might influence the model's plume dispersion? Ground-based observations at the surface indicate that while GEM-MACH temperature performance is good, the model is biased low for surface wind speed but high for turbulent kinetic energy (see scatterplots at right). The positive biases in TKE may influence the model results, increasing the extent of downwind mixing.



Next Steps and Future Directions

While the above tests did not improve the model results across all statistics, they show that the model plumes are very *sensitive* to the diagnostic PBL height, the observed volume flow rates and observed stack temperatures. The latter two parameters are included in CEM hourly observations, but these hourly values are usually not reported or used for modelling. Poor correlation coefficients seem to be due to small errors in direction or strength. These and the causes for the TKE overestimate will be investigated in future work.

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