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From Off-line to On-Line Models: Model Intercomparisons and Transition to Forecasting.

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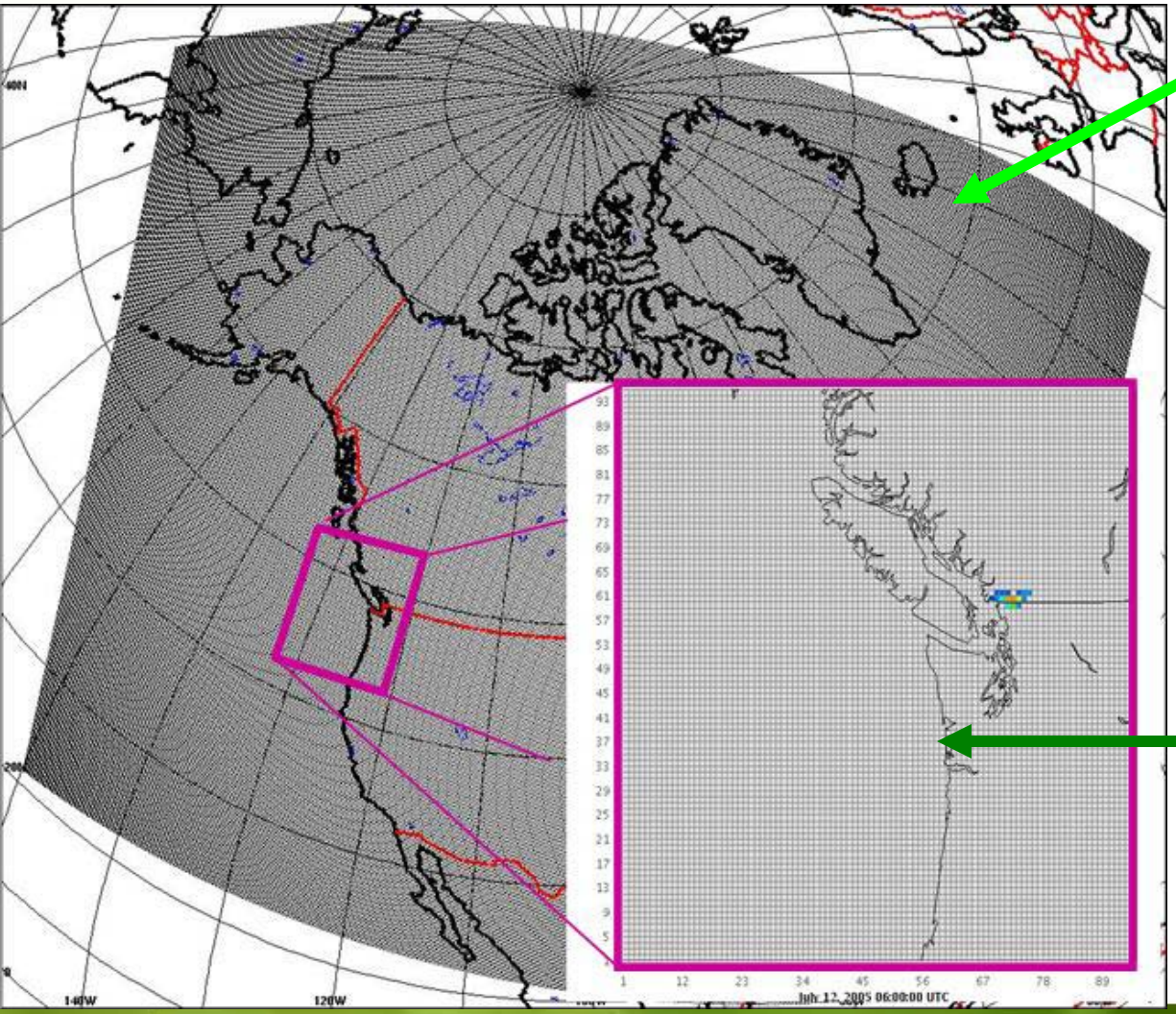
A “simple” comparison… with unexpected results

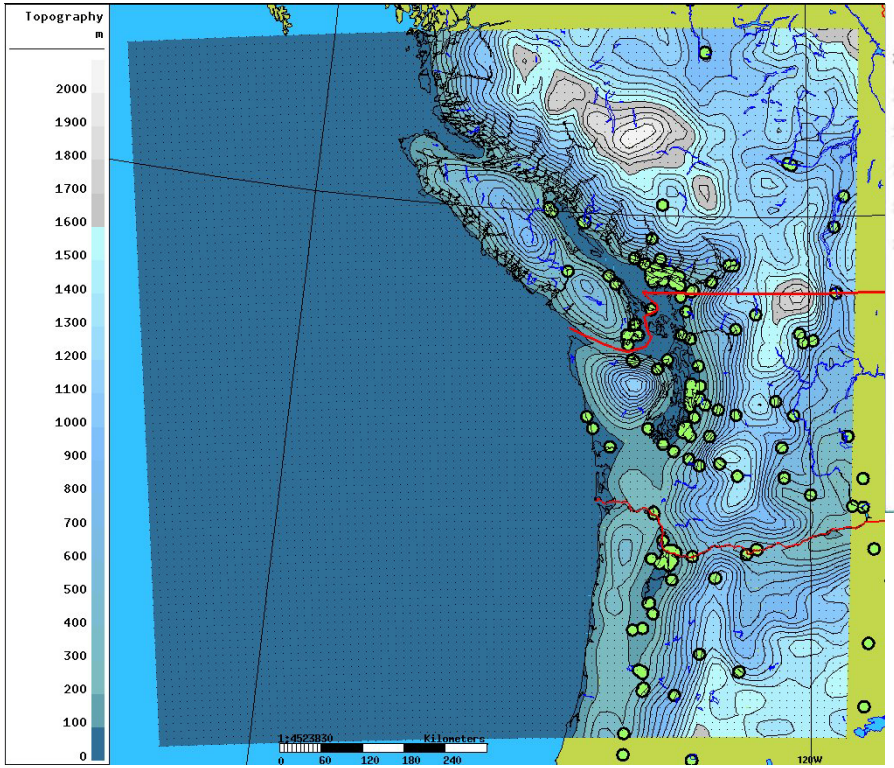
- Compare two off-line models:
  - **CMAQ** v4.6 (**C**ommunity **M**ultiscale **A**ir **Q**uality; US EPA & NOAA)
  - **AURAMS** v1.4.2 (**A U**nified **R**egional **A**ir-quality **M**odelling **S**ystem; Environment Canada). ***Progenitor of GEM-MACH’s chemistry code.***
- Domain: SW Canada, NW USA, 12km resolution.
- *Use the same inputs*: meteorology, emission inventory, emission processing system, horizontal coordinate system, model grid.
- Run models in ‘native mode’ (default model settings used, at the start)
- **How well do the models perform? What can be learned?**
- A biproduct: tech transfer to GEM-MACH15 (on-line model)



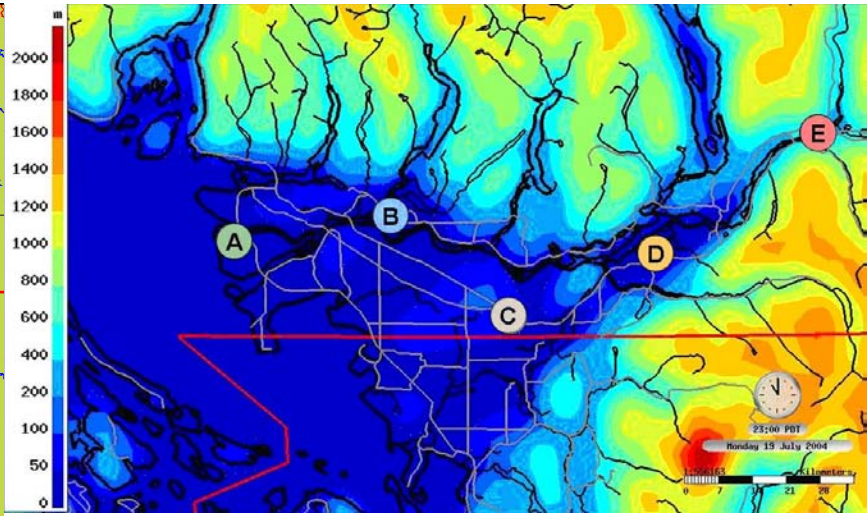
Weather inputs: GEM 3.2.2 15km weather forecasting domain.

AQ model domain: 93 x 93 12km Polar stereographic

Comparison with observations: locations of stations



All stations in domain



A Vancouver Int'l Airport

B Meadowlands Elementary School (Pitt Meadows)

C Abbotsford Airport

D Chilliwack Airport

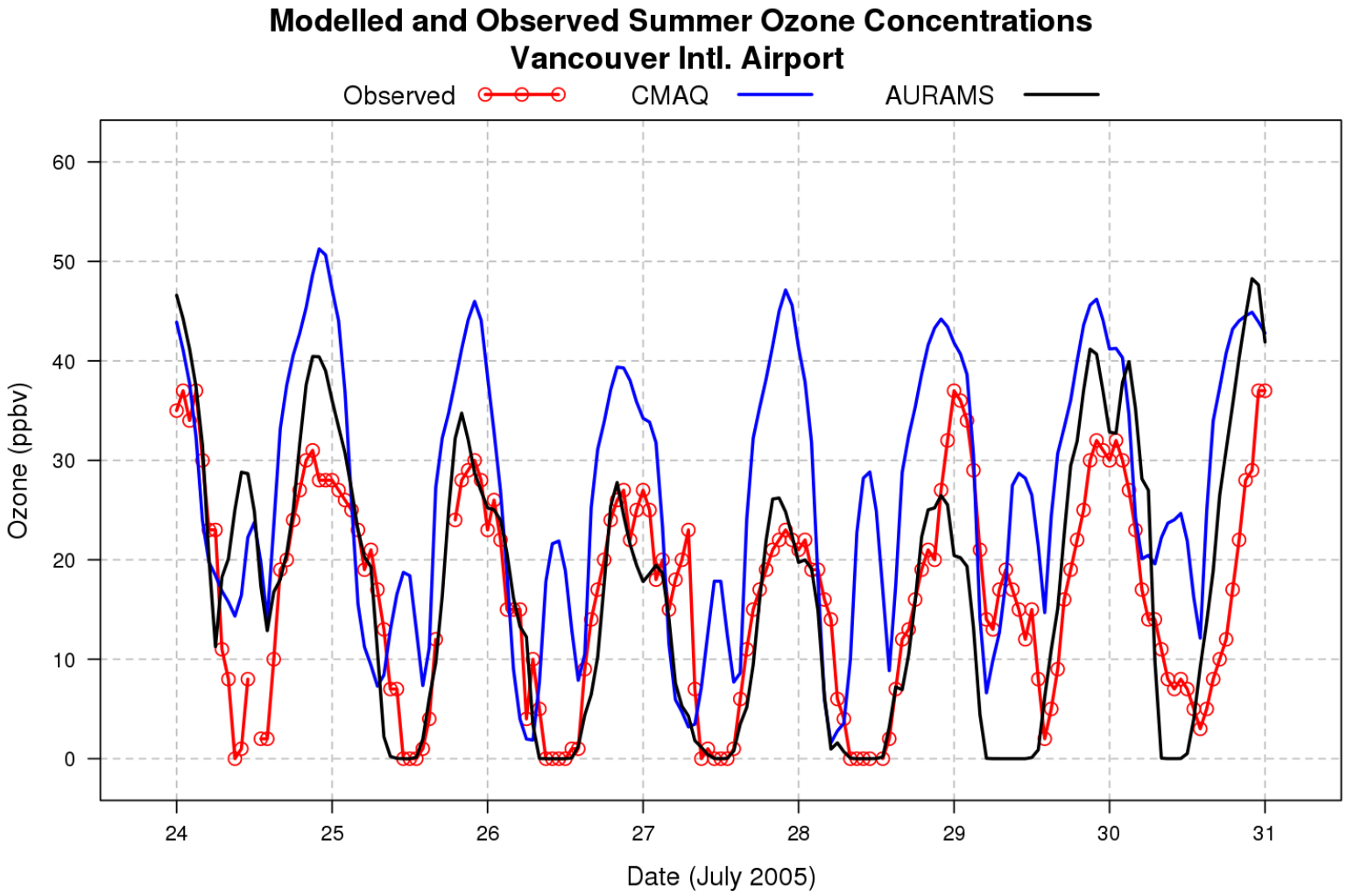
E Hope Airport

Summer 2005: stats from >200 stations, BC, Washington, Oregon.

Statistic	Ozone			PM2.5		
	Obs.	AURAMS	CMAQ	Obs.	AURAMS	CMAQ
Number of pairs		41846	41789		8657	8646
Mean	22.67	31.16	39.79	7.44	10.79	4.82
Maximum	100.00	100.21	100.48	49.00	69.94	44.49
Minimum	0.00	0.00	1.26	0.00	0.21	0.00
Y intercept (of obs vs model)		15.32	31.11		5.49	3.47
Slope (of obs vs model)		0.70	0.38		0.71	0.18
Correlation coefficient (R)		0.64	0.58		0.36	0.26
Mean Bias		8.48	17.11		3.35	-2.62
Root Mean Square Error		16.17	21.25		9.17	5.52
Normalized Mean Bias (%)		37.41	75.42		45.10	-35.20
Normalized Mean Error (%)		55.26	81.63		82.90	55.82

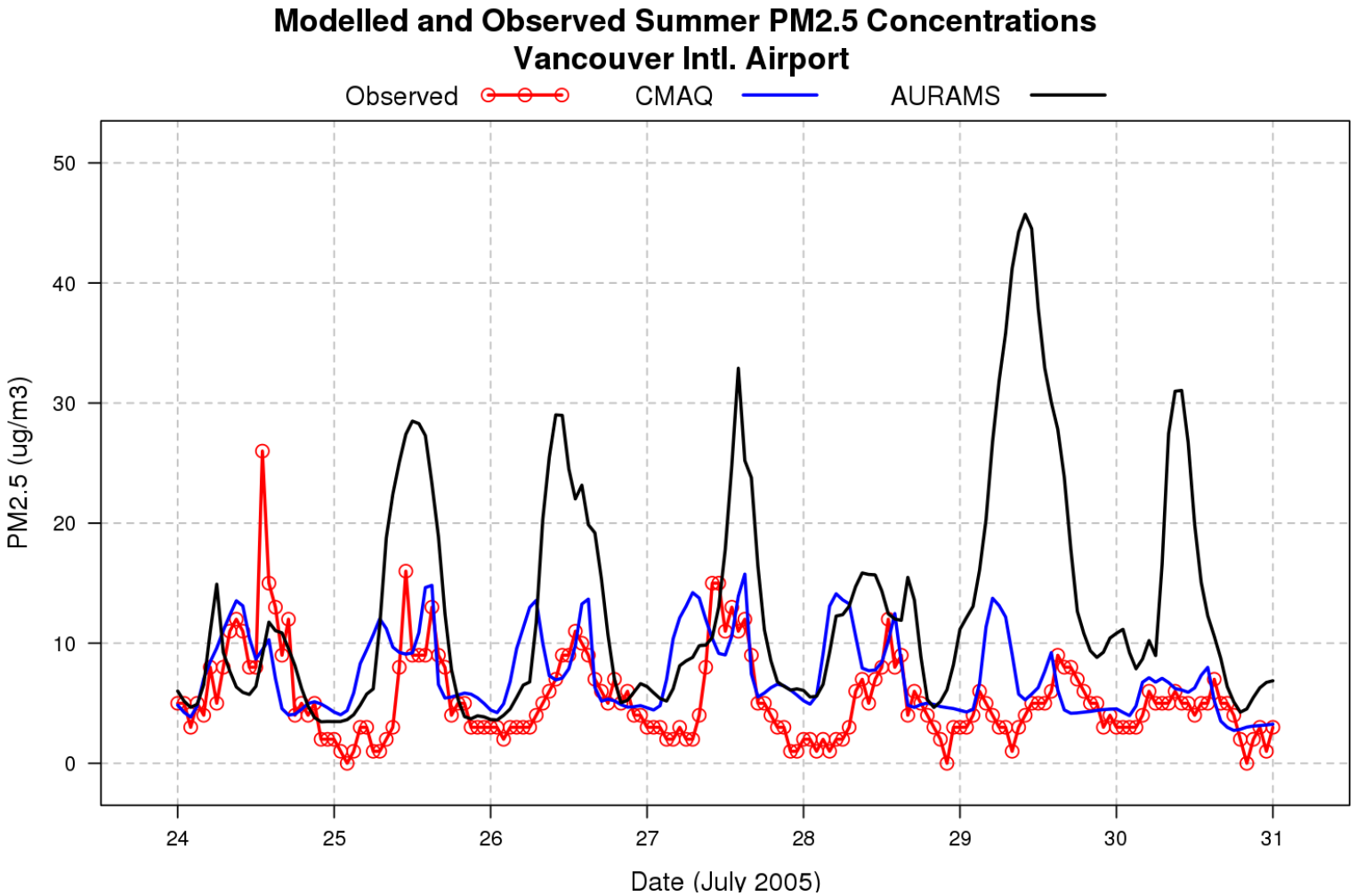
The green boxes are the better statistical values of the two. AURAMS did better for ozone, and for slope and R of $PM_{2.5}$. CMAQ did better for the rest of the $PM_{2.5}$ statistics. *Why?*

Vancouver Airport



O_3: AURAMS is close to Observations, CMAQ creates a night-time peak that is not observed, and gets daytime peak too high.

Vancouver Airport

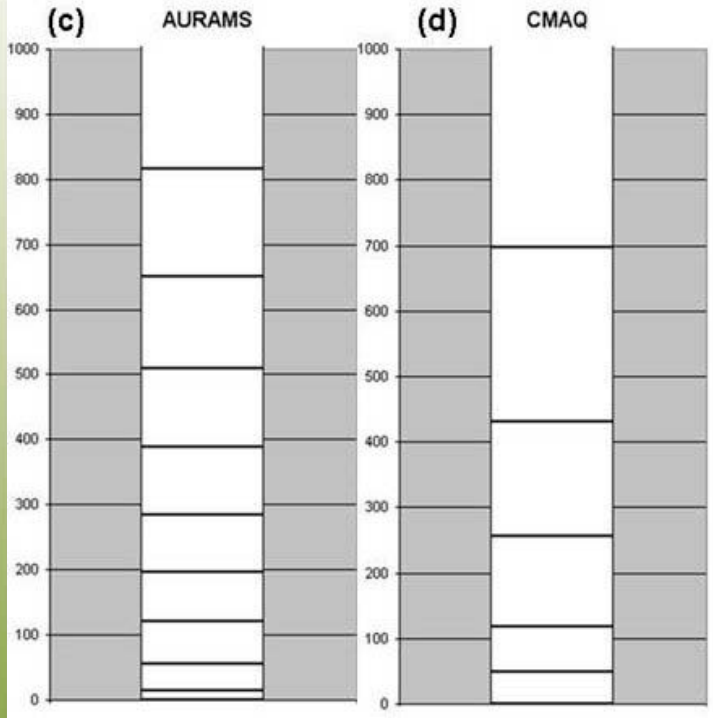


$PM_{2.5}$: CMAQ is better for peak values, AURAMS is biased very high.

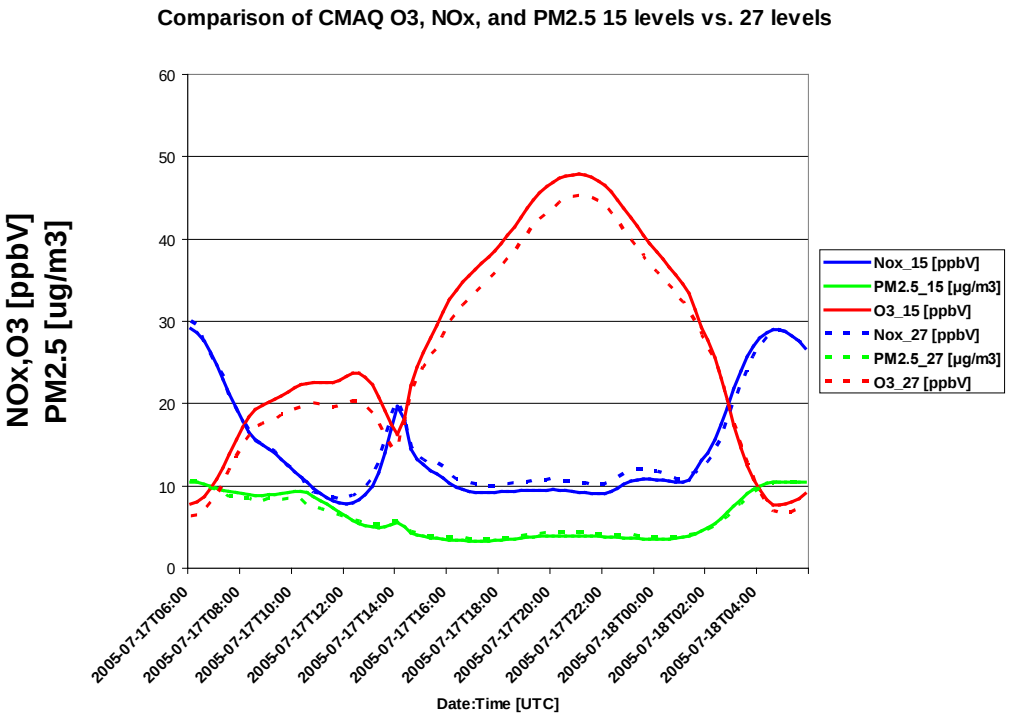
Winter results are similar… so what's happening, here?

Tried modifying CMAQ vertical structure to make it similar to AURAMS…

Native mode vertical levels



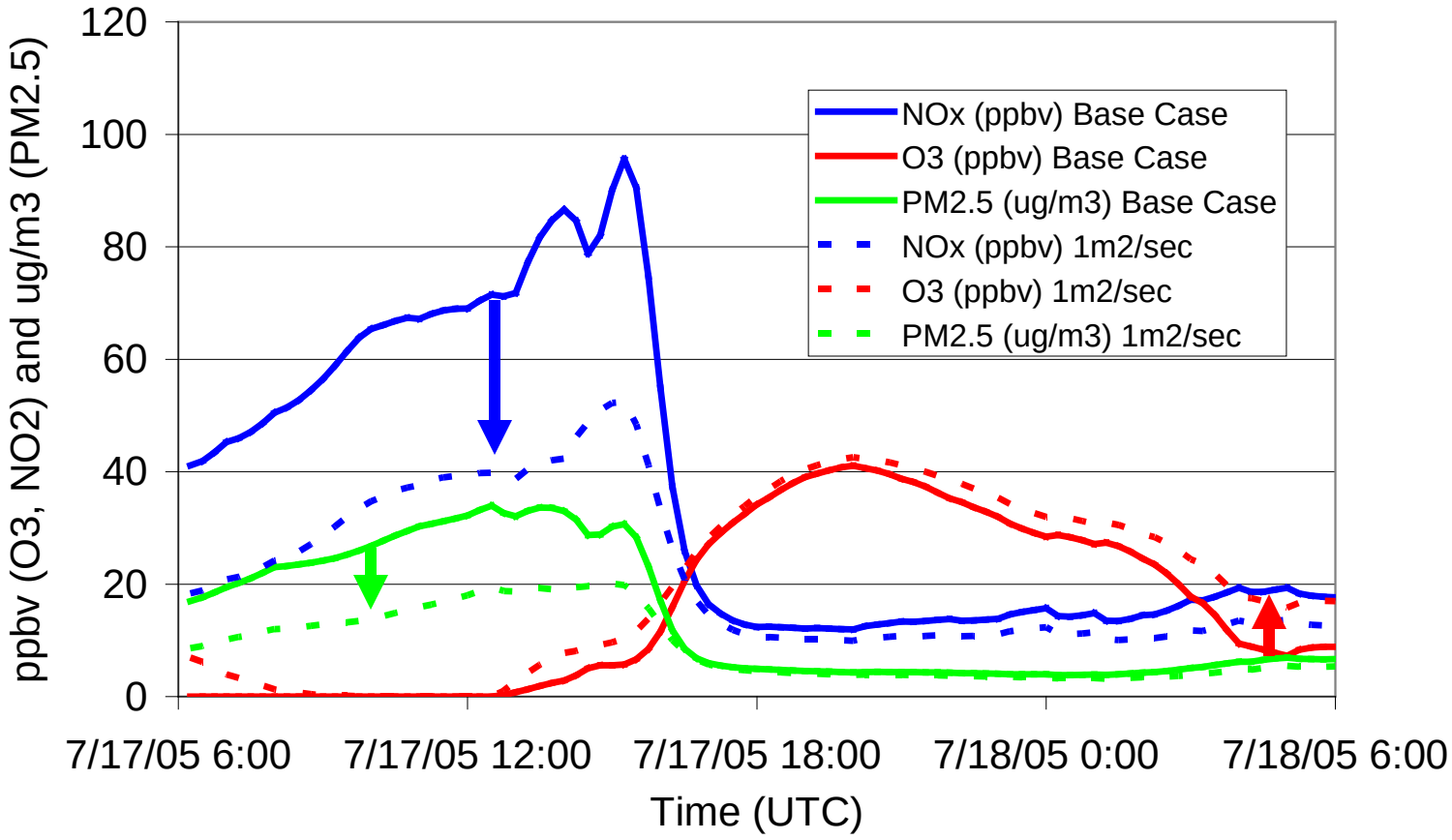
Sensitivity of number of CMAQ vertical levels



… a small effect, not enough to account for the differences between the two models.

Tried running AURAMS with CMAQ's diffusion cutoff of 1 m^2s^{-1}…

Comparison of O3, NOx, and PM2.5, Base Case AURAMS versus 1m2/s diffusion constant minimum



Bingo…AURAMS starts behaving like CMAQ, with only a 24 hour run. O_3 doesn't titrate properly at night, PM drops at night.

Problem: ***these lower limits are arbitrary, and not physically realistic (though the met model may not capture urban diffusion accurately)….***

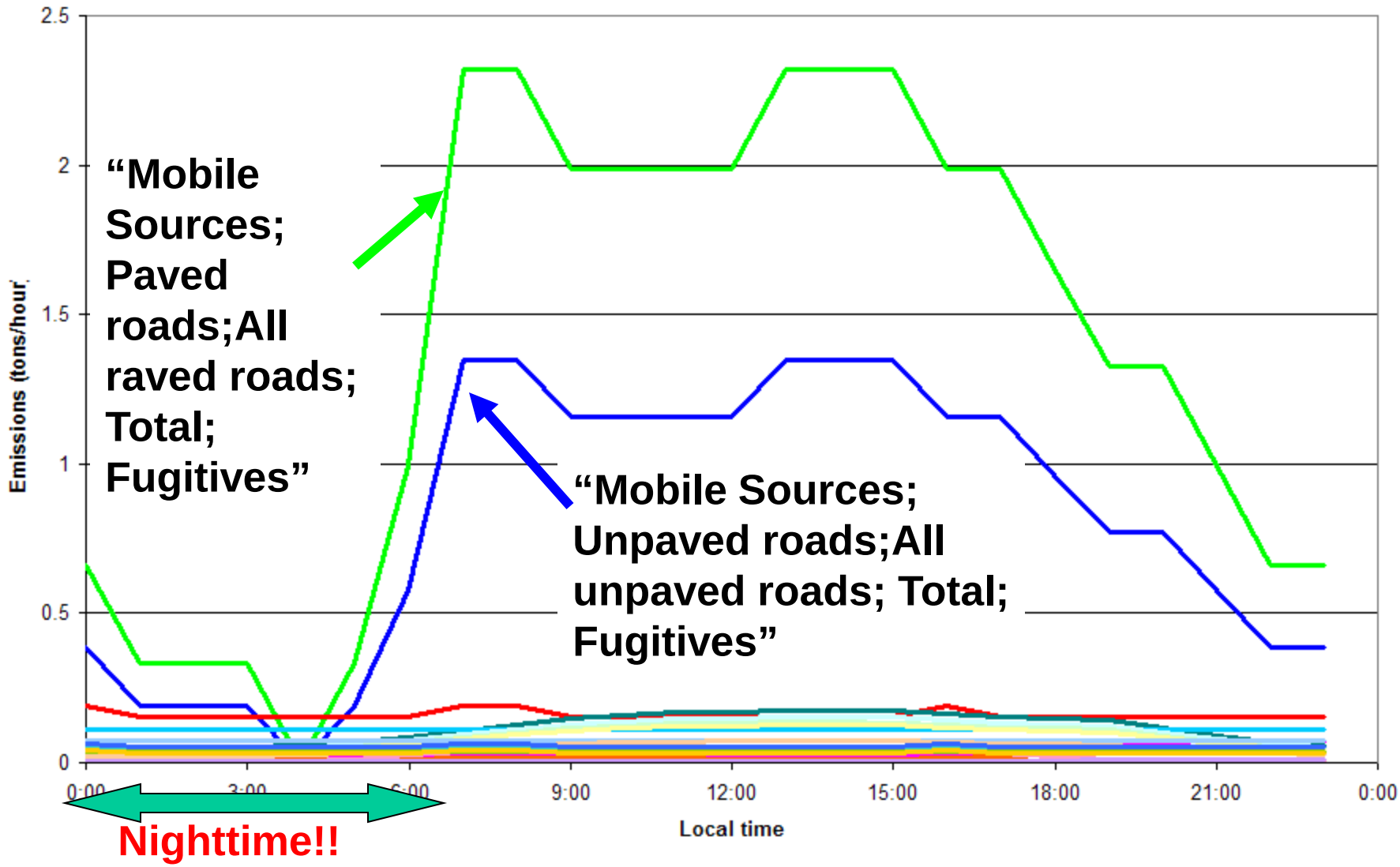
So, what <u>else</u> could be causing these problems?

Look for clues in the PM speciation:

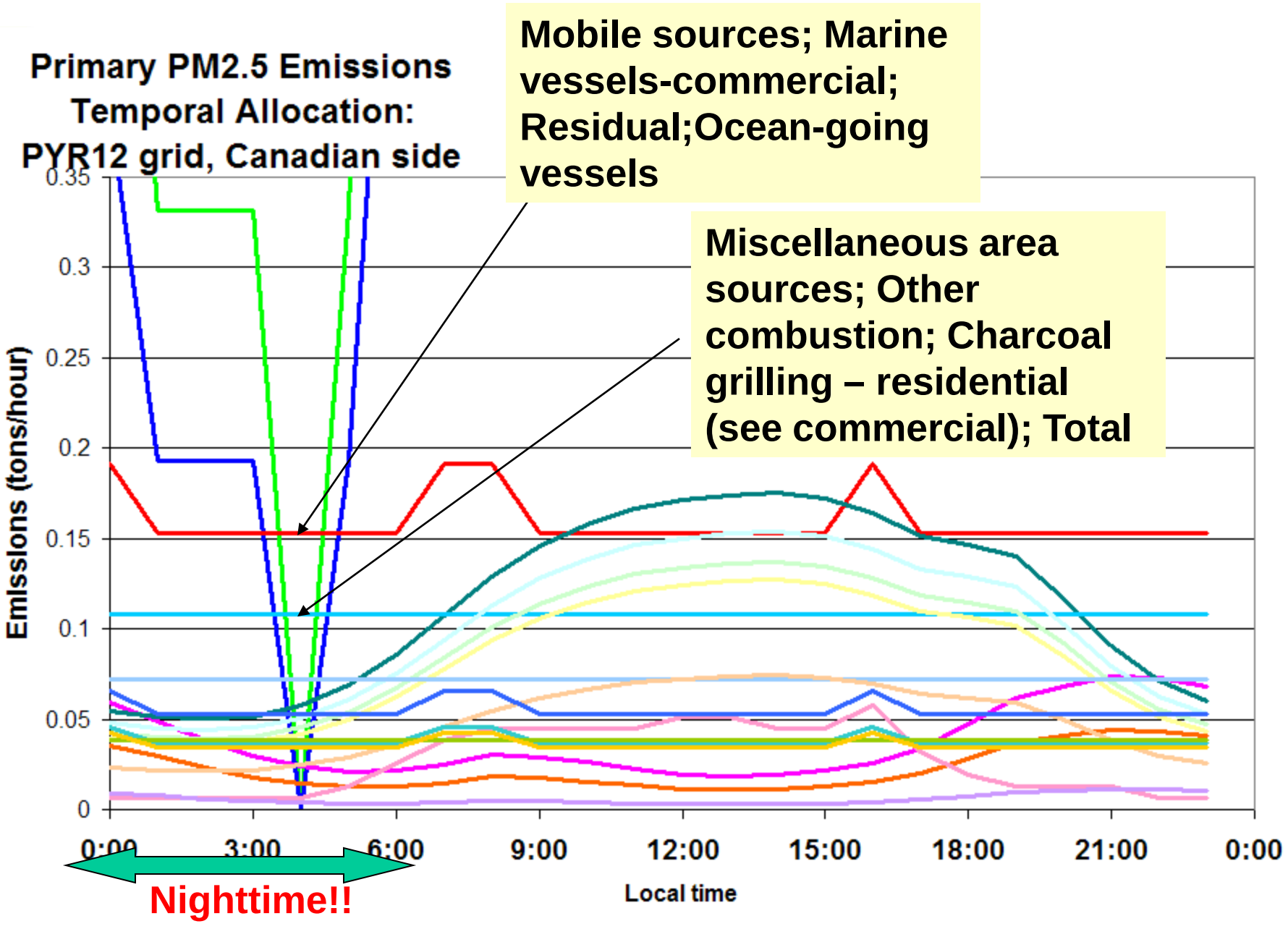
- The simulated $PM_{2.5}$ in Vancouver peaks ***at night***, and it's mostly ***primary*** (crustal material, primary organic carbon).
- → Implies emissions and/or transport aren't right.
- Ok, so let's look at the emissions…
  - Temporal Allocation?
  - Spatial Allocation?
  - Total amounts?

Emissions: *Temporal allocation*

- **Generate time series for $PM_{2.5}$ emissions on the Canadian side of the grid.**



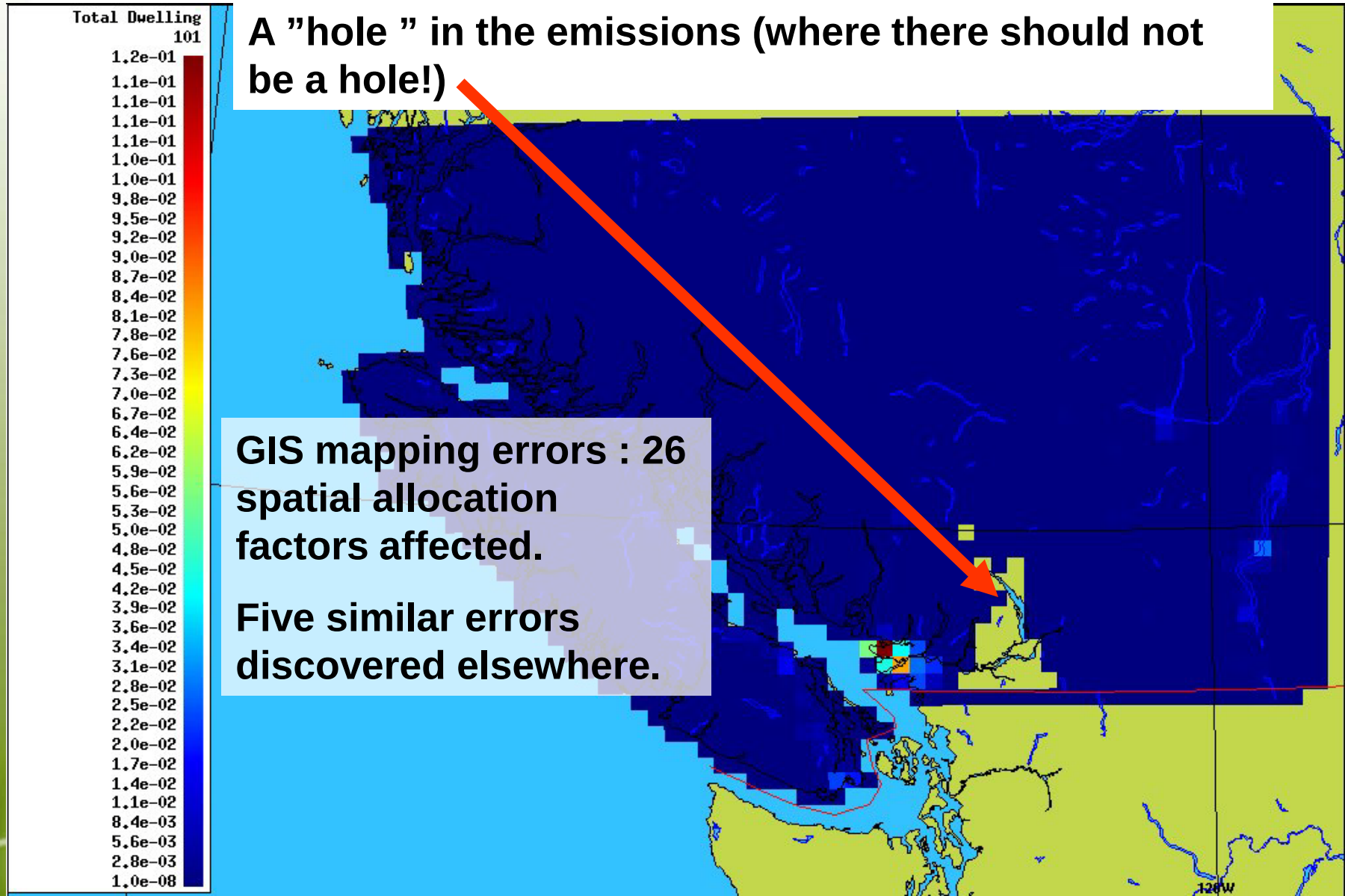
Expand the vertical scale…



Strangeness in Emission land at night…

- 2nd biggest source of primary $PM_{2.5}$ at 4 am: ***people using their barbeque grills***. Oops.
- 4th biggest source of primary $PM_{2.5}$ at 4 am: ***farm tractors***. Oops.
- I found many other issues like this
  - NO and $PM_{2.5}$ from the similar source types had dissimilar splitting factors.
  - Temporal splitting for mobile emissions were inconsistent
  - Some Ocean-going vessel types assumed constant, others have same time splitting profile as railroad diesel engines.
  - Etc., etc.
  - These are *default* SMOKE profiles, as far as I know.

Emissions issues: spatial allocations *also* had errors…



These issues led to a review of the emissions database, and several fixes

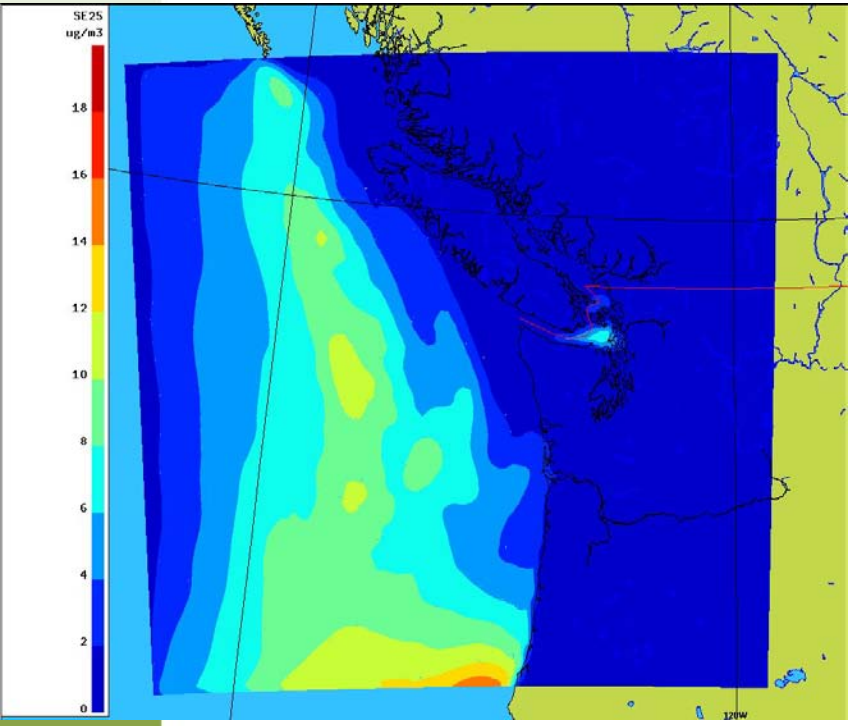
- I passed the above on to colleagues Mike Moran, Junhua Zhang, Qiong Zheng, who have been implementing fixes.
- In parallel, (Mike, Junhua, Qiong) have also added more detailed Canadian mobile emissions spatial allocation factors (see previous talk by V. Bouchet).
- New emissions were generated last week! First test is a repeat of the above comparison.

AURAMS operator splitting scenarios:

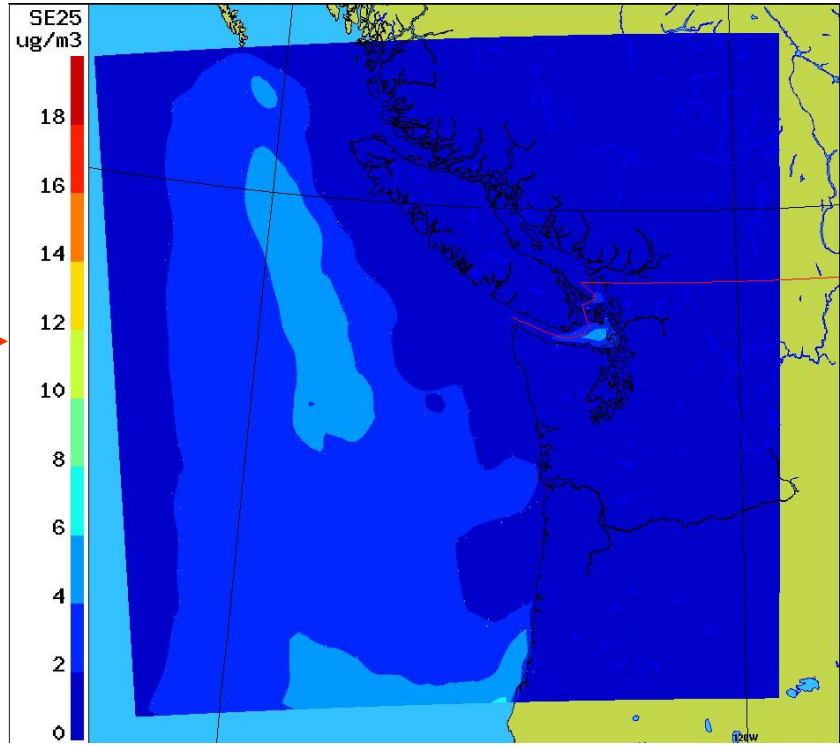
The order of AURAMS operations was modified, 7 tests:

- 7 tests, in which the order of AURAMS operators, and the type of operator splitting (forward versus centred) was varied.
- Substantial effect on model results!

A long-standing problem with AURAMS (and GEM-MACH): sea-salt positive bias; factor of 3 too high compared to observations…



Base Case



Scenario

… was fixed by using better operator splitting.

Operator splitting tests: O_3

Statistics	Obs.	CM AQ	AURAMS_ 1	AURAMS_ 2	AURAMS_3	AURAMS_4	AURAMS_5	AURAMS_ 6	AURAMS_7
Number of Pairs		41789	41846	41846	41846	41846	41846	41846	41846
Mean	22.67	39.79	31.24	32.32	27.29	27.67	31.32	29.89	31.59
Maximum	100	100.48	100.78	98.39	100.41	112.85	97.66	102.73	102.52
Minimum	0	1.26	0.000037	0.000097	0.000056	0.000039	0.000081	0.000061	0.00029
Y-intercept (a) of observations versus model line		31.11	15.37	17.04	10.86	8.62	15.02	13.59	15.13
Slope (b) of observations versus model line		0.38	0.7	0.67	0.72	0.84	0.72	0.72	0.73
Correlation Coefficient(R)		0.58	0.64	0.65	0.68	0.69	0.66	0.64	0.66
Mean Bias		17.11	8.56	9.65	4.62	5	8.64	7.22	8.92
Root mean Square Error		21.25	16.24	16.38	13.62	14.59	15.98	15.71	16.18
Normalized Mean Bias (%)		75.42	37.77	42.54	20.36	22.05	38.12	31.84	39.32
Normalized Mean Error (%)		81.63	55.55	56.57	45.86	48.57	54.63	53.13	55.25

Operator splitting tests: $PM_{2.5}$

Statistics	Obs	CMAQ	AURAMS_1	AURAMS_2	AURAMS_3	AURAMS_4	AURAMS_5	AURAMS_6	AURAMS_7
Number of Pairs		8646	8657	8657	8657	8657	8657	8657	8657
Mean	7.44	4.82	10.81	11.34	14.34	19.48	11.63	11.32	12
Maximum	49	44.49	70.06	71.17	100.66	126.89	71.98	71.37	74.23
Minimum	0	0.0006	0.22	0.21	0.22	0.26	0.22	0.18	0.21
Y-intercept (a) of observations versus model line		3.47	5.51	5.9	7.52	9.79	6.07	5.73	6.07
Slope (b) of observations versus model line		0.18	0.71	0.73	0.92	1.3	0.75	0.75	0.8
Correlation Coefficient(R)		0.26	0.36	0.35	0.31	0.35	0.35	0.36	0.37
Mean Bias									4.56
Root mean Square Error									10.22
Normalized Mean Bias (%)		-35.2	45.36	52.43	92.82	161.93	56.35	52.16	61.31
Normalized Mean Error (%)		55.82	82.99	89.08	123.95	178.93	91	88.06	93.21

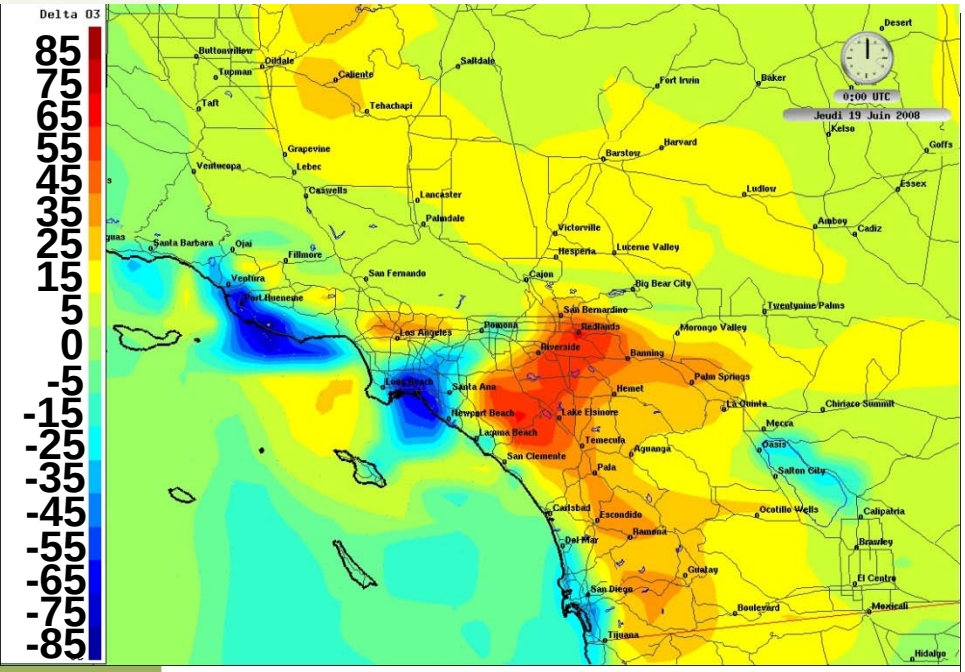
Of course, it's hard to get the $PM_{2.5}$ right, when the primary $PM_{2.5}$ dominates, and the $PM_{2.5}$ *emissions* are wacky.

Porting to the On-Line model GEM-MACH15

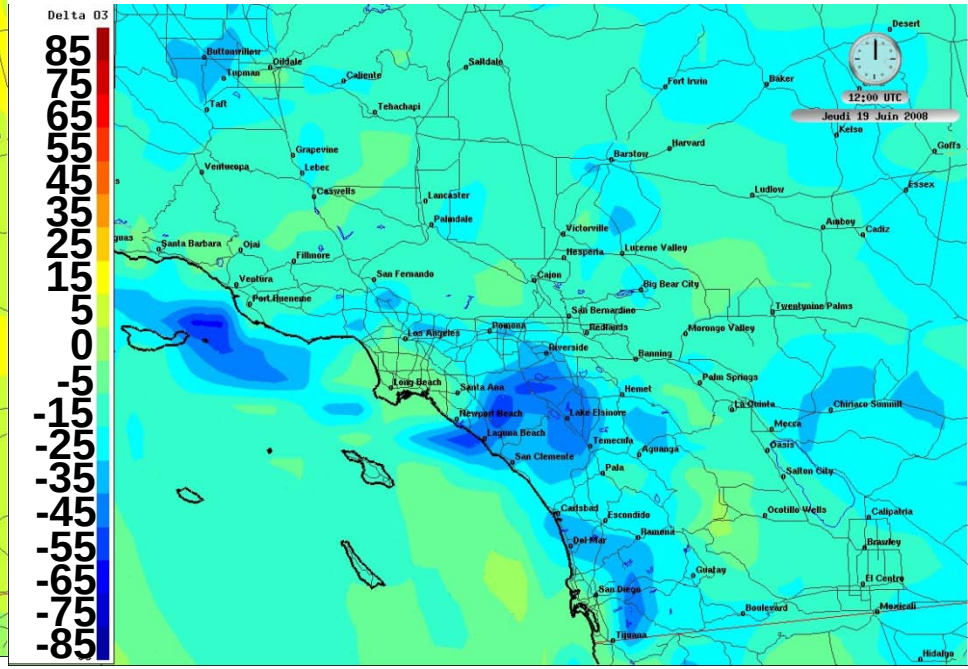
- Current work: repeating the same operator tests with the on-line AQ forecast model GEM-MACH
- Definitely a large impact on results!
- Example, post-spinup for a standard summer cycling run:

Difference in GEM-MACH15 O_3 forecast for Los Angeles, 0Z and 12Z, June 19, 2008 (Scenario – Base Case, ppbv)

0 Z (5 pm)



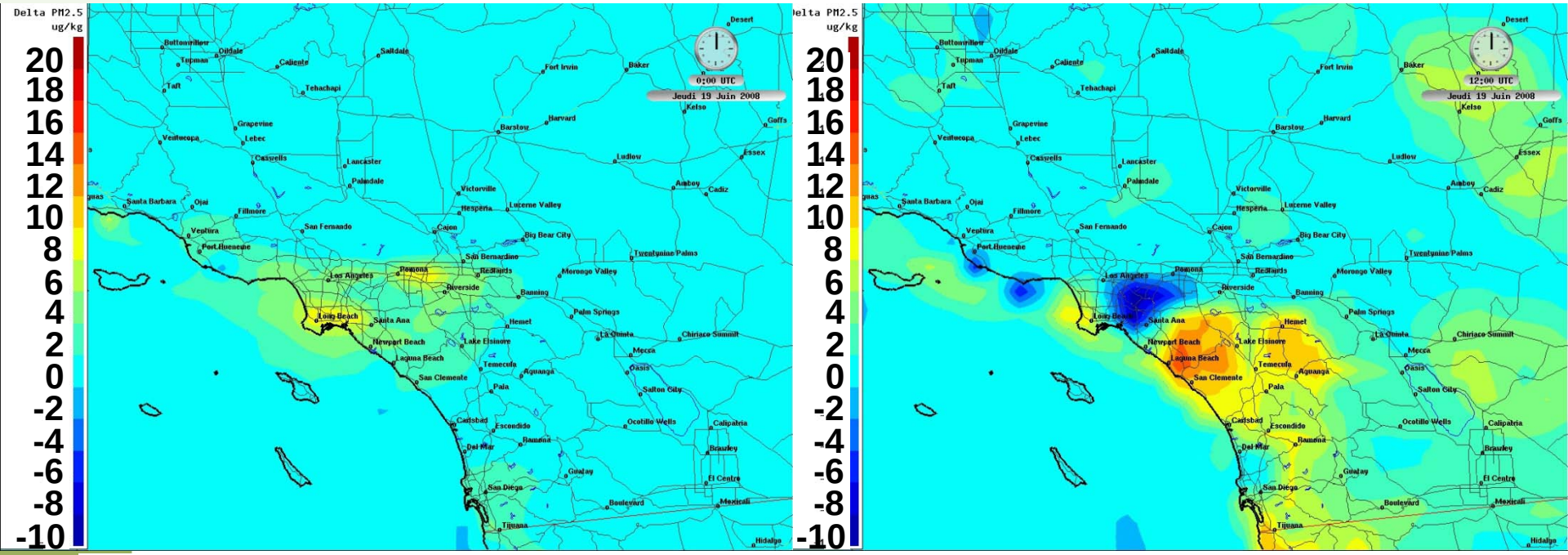
12 Z (5 am)



- Locally, this particular snapshot shows ozone differences of up to +/- 80 ppbv.
- Does not necessarily mean the new forecast is better – need to do the statistical analysis, yet.

Difference in GEM-MACH15 $PM_{2.5}$ forecast for Los Angeles, 0Z and 12Z, June 19, 2008 (µg/kg).

0 Z (5 pm) **12 Z (5 am)**

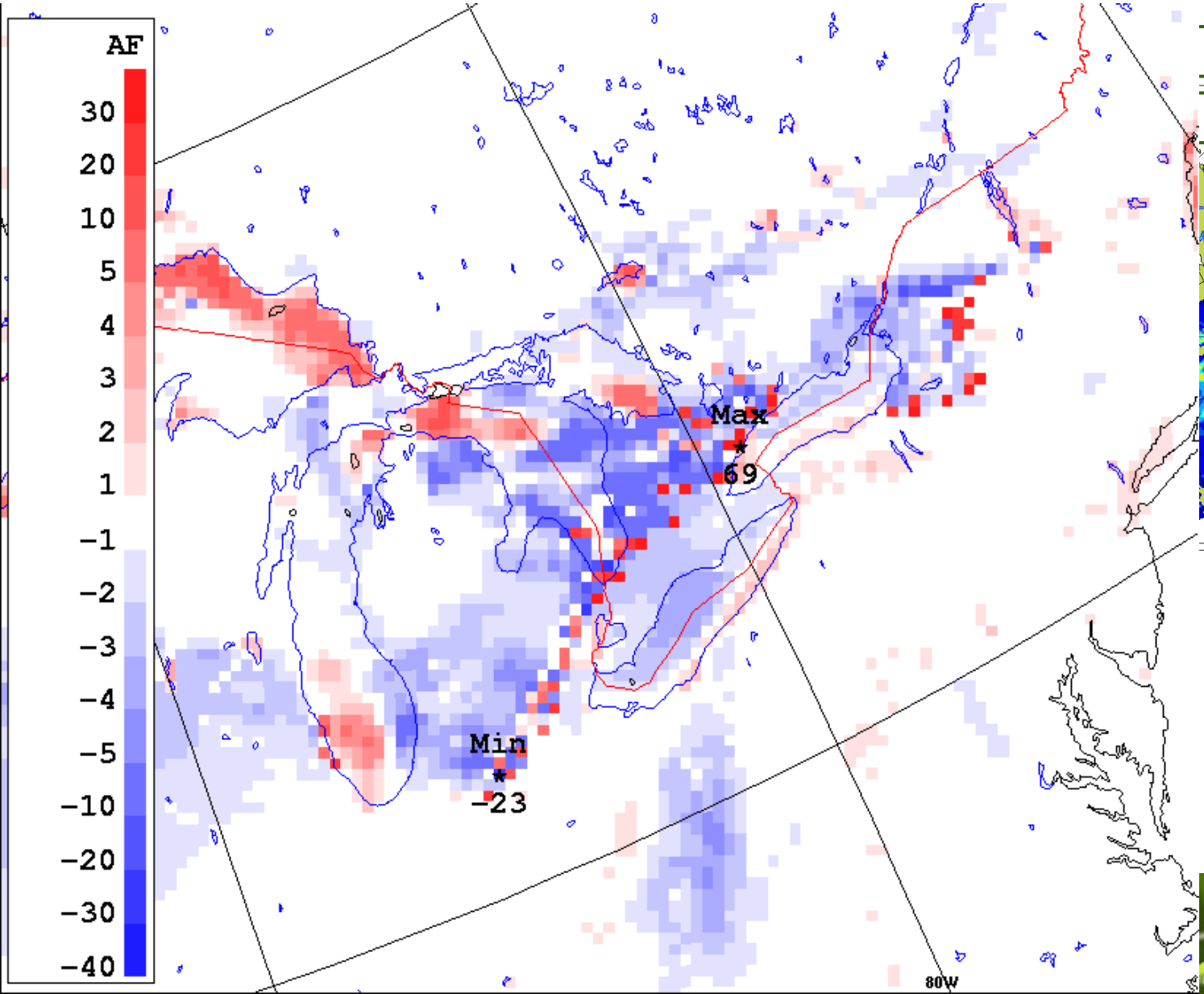


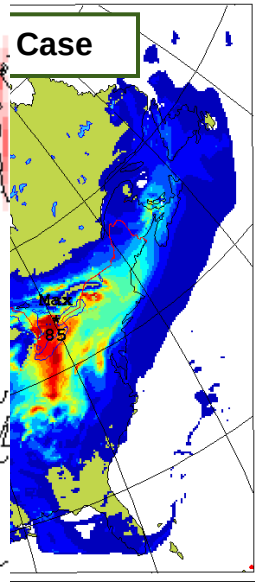
- Increases and decreases, depending on time and location.
- Does not necessarily mean the new forecast is better – need to do the statistical analysis, yet.

Current work: Particle settling and deposition algorithm update.

- Look for bugs and you will find them…
- Original AURAMS particle settling velocity algorithm:
  - Only appropriate for particles with diameters < 19 μm
  - Was being applied to all particles, included those that were activated (CCN).
- Result: activated particles had supersonic velocities (!)
- Fixed by using correct settling velocity formula for small droplets.
- Also modified the settling velocity code: new code uses Lagrangian transport…

Ported into GEM-MACH: fixed “hole problem” at the surface…

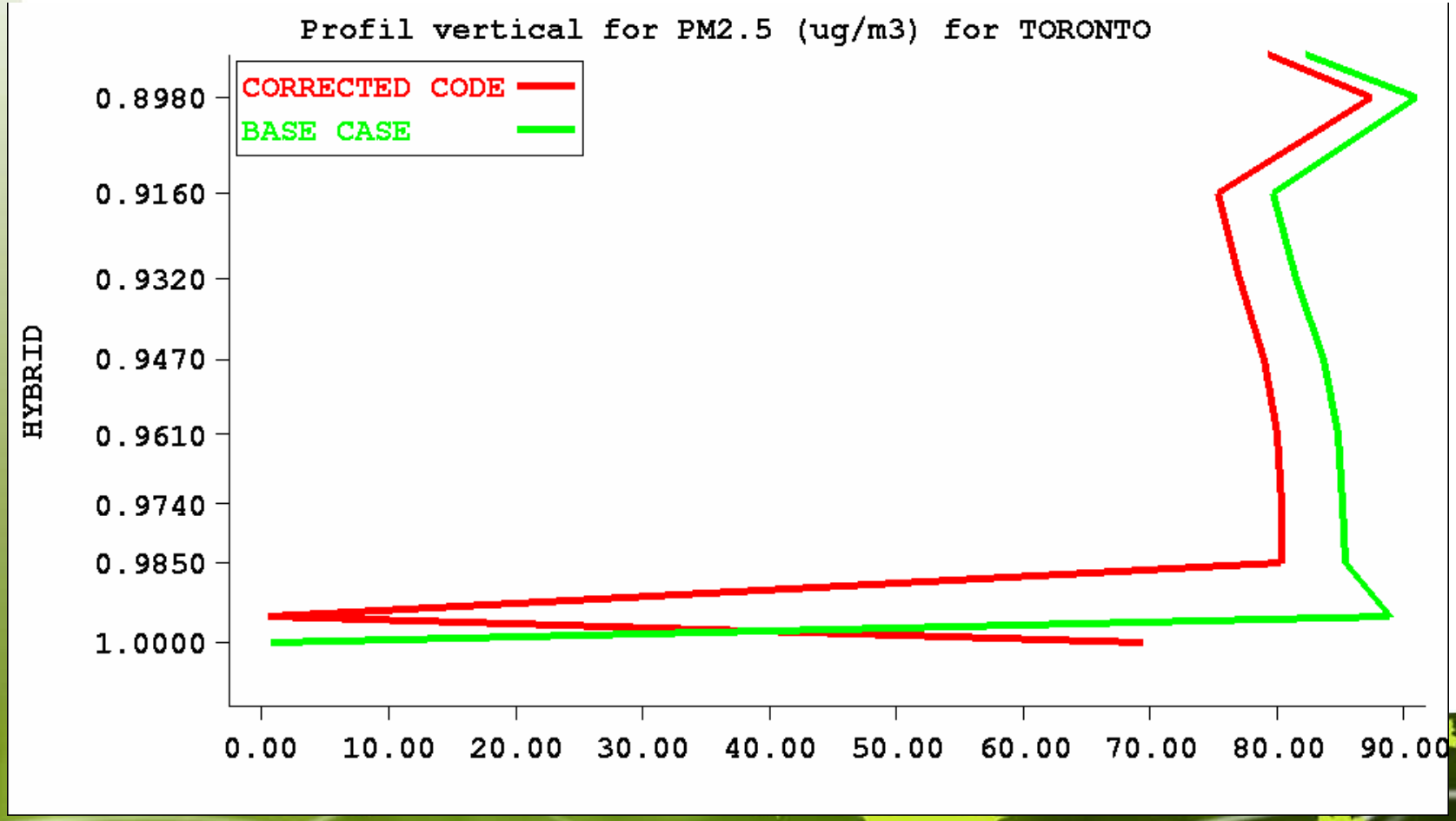




Red spots are those where problem occurred (PM2.5 holes)

Holes still showing up in the column. Ok or not? TBD…

Forecast for 16UTC July 18th 2011, by 2011-07-18 00utc run



Conclusions (1)

- A comparison of CMAQ and AURAMS at 12km resolution has been completed.
- Statistics shows AURAMS performance better for O_3, CMAQ better for $PM_{2.5}$ (except for correlation coefficient and slope)
- A look at the local situation shows that the PM biases occur at night, and are due to primary PM.
- At least part of CMAQ's "improved" $PM_{2.5}$ bias is due to the use of $1 m^2 s^{-1}$ as a diffusion minimum (right result, wrong reason)
- This lower limit reduces night-time O_3 performance (misses titration).

Conclusions (2)

- Emissions inventory analysis suggest up to half of nighttime primary PM emissions should not be there due to temporal allocation errors, and spatial allocation also has problems.
- Operator splitting improvements gets rid of the sea-salt bias in AURAMS, improves O_3 predictions.
- Operator splitting improvements make $PM_{2.5}$ “same to worse”, ***but*** primary PM emissions are wacky.
- Porting to GEM-MACH15: underway, and large effects are seen. Stats: stay tuned! (AMS, New Orleans, end of January)

Take-home message:

- Beware the local minimum in model error!
- It may be hiding other problems in the model, or in its inputs.