Fine Scale Model Evaluation using 2010 CALNEX Field Study Data: Meteorology, Inorganic and Organic PM2.5

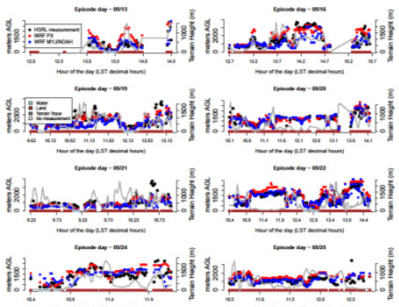
Baker, KR and Kelly, JT – U.S. Environmental Protection Agency, Research Triangle Park, NC

Kirk Baker | baker.kirk@epa.gov

Background

Ozone and particulate matter less than 2.5 microns in diameter (PM2.5) have been associated with negative health effects in humans. Many counties in California have been designated non-attainment for the 8-hour ozone and particulate matter (PM) National Ambient Air Quality Standards (NAAQS). These areas must develop emissions control plans to reduce pollution to acceptable levels. Emission control scenarios are often developed using complex emissions and photochemical transport models that use output from prognostic meteorological models such as the Weather Research and Forecast model (WRF).

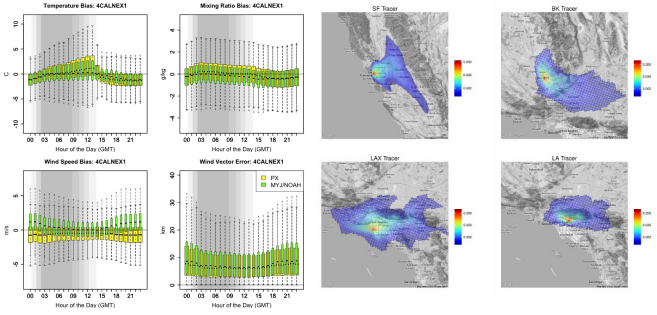
Meteorology



Sigma	Level	Estimated Height (m)
0.000	34	17554
0.050	33	14780
0.100	32	12822
0.150	31	11282
0.200	30	10002
0.250	29	8901
0.300	28	7932
0.350	27	7064
0.400	26	6275
0.450	25	5553
0.500	24	4885
0.550	23	4264
0.600	22	3681
0.650	21	3136
0.700	20	2619
0.740	19	2226
0.770	18	1941
0.800	17	1665
0.820	16	1485
0.840	15	1308
0.860	14	1134
0.880	13	964
0.900	12	797
0.910	11	714
0.920	10	632
0.930	9	551
0.940	8	470
0.950	7	390
0.960	6	311
0.970	5	232
0.980	4	154
0.985	3	115
0.990	2	77
0.995	1	38
1.000	0	0

Mixing layer height estimated by HSRL, WRF-PX, and WRF-MYJ/NOAH for 8 different flights in southern and central California during the CalNex field study.

	May-June 2010	
	WRF PX	WRF MYJ/NOAH
Version	3.2*	3.3.1
Longwave radiation	RRTMG	RRTM
Shortwave radiation	RRTMG	Goddard
Surface Layer	Pleim-Xiu	Monin-Obukhov (Janjic)
Land Surface	Pleim-Xiu	NOAH
Boundary Layer	ACM2	Mellor-Yamada-Janjic
Cloud Microphysics	Morrison 2-moment	Thompson
Cumulus	Kain-Fritsch	Grell 3D ensemble



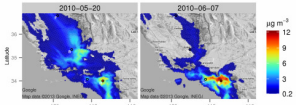
Distribution of observed and modeled wind vector error, wind speed bias, temperature bias, and water vapor mixing ratio by hour over all surface monitor locations in California.

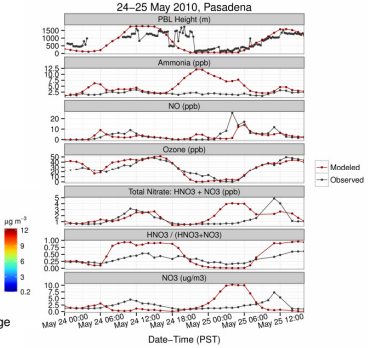
Aggregated inert tracer endpoints for June 2010 released from 4 locations: San Francisco (top left), Bakersfield (top right), Los Angeles airport (bottom left), and Pasadena (bottom right).

Baker, K.R., Misenis, C., Obland, M.D., Ferrare, R.A., Scarino, A.J., Kelly, J.T., 2013. Evaluation of surface and upper air fine scale WRF meteorological modeling of the May and June 2010 CalNex period in California. Atmospheric Environment 80, 299-309.

Precursors & Inorganic PM2.5

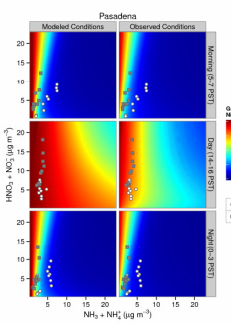
- Modeled PBL collapses too early in the evening on 24 May 2010 and leads to NH3 and NO overprediction
- Estimated NO overprediction leads to excessive titration of modeled O3 and production of HNO3 via N2O5
- Estimated total nitrate partitions too much to the particle phase during night causing nighttime NO_3^- peak



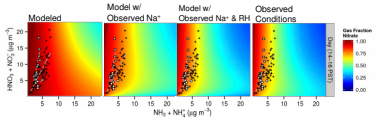


Modeled and measured (circles) daily average PM2.5 nitrate ion.

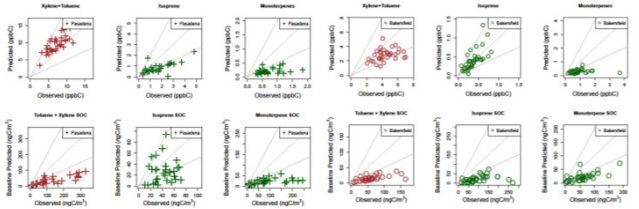
Kelly, J.T., Baker, K.R., Nowak, J.B., Murphy, J.G., Markovic, M.Z., VandenBoer, T.C., Ellis, R.A., Neuman, J.A., Weber, R.J., Roberts, J.M., 2014. Fine-scale simulation of ammonium and nitrate over the South Coast Air Basin and San Joaquin Valley of California during CalNex-2010. Journal of Geophysical Research: Atmospheres 119, 3600-3614.



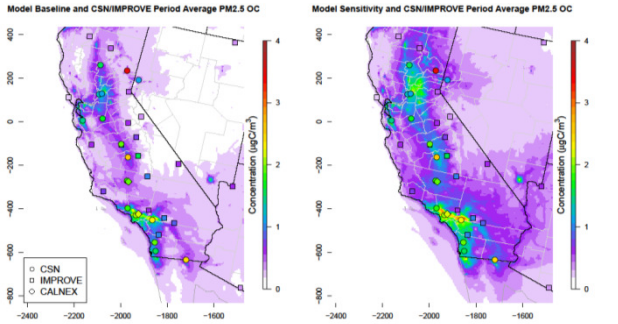
- ← ISORROPIA II calculations of GFN constrained by average modeled values (left) and observed values (right)
- ← During morning and night, GFN gradients based on modeled and observed conditions are similar but total ammonia is over-predicted (top and bottom)
- ← During the day, ISORROPIA II predicts higher GFN for average modeled conditions than for average observed conditions (middle)
- ↓ Daytime gas fraction of nitrate is sensitive to Na^+ and RH
- ↓ Under-predictions of Na^+ and, to a lesser degree, RH could explain daytime over-predictions of GFN



Precursors & Organic PM2.5



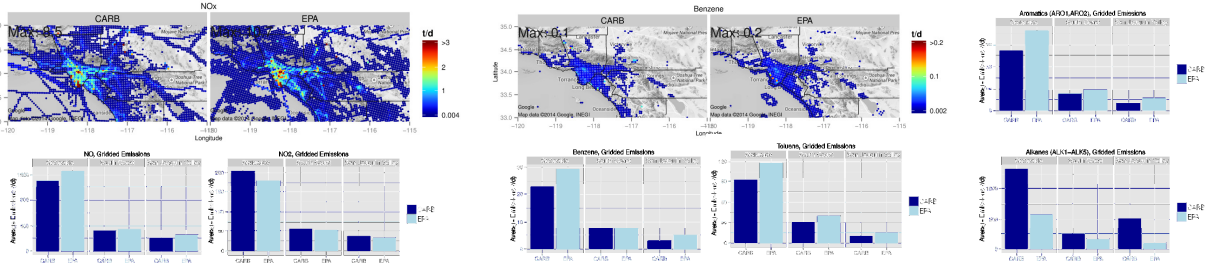
Comparison of CMAQ-predicted and measured VOC (daily average of hourly samples) and corresponding SOC species (daily 23-hr average samples). Comparison points outside the gray lines indicate model predictions are greater than a factor of 2 different from the measurements.



May-June 2010 average observed and modeled PM2.5 organic carbon. Measurements are from both CalNex locations and routine networks including CSN (circles) and IMPROVE (squares). Left panel shows baseline model predictions and right panel shows model estimates with increased SOA yields.

KR Baker, AG Carlton, TE Kleindienst, JH Offenberg, MR Beaver, AH Goldstein, DR Gentner, JB Gilman, JA de Gouw, PL Hayes, JL Jimenez, HOT Pye, JT Kelly, M Woody, M Jaoui, M Lewandowski, YH Lin, CL Rubitschun, JD Surratt, 2014. Gas and aerosol carbon in California: comparison of measurements and model predictions in Pasadena and Bakersfield. Submitted: Atmospheric Chemistry & Physics Discussion.

Ongoing related work: EPA and CARB emissions comparison



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