ARCTAS-CA
June 2008

Air Quality Simulations

California Environmental Protection Agency
Air Resources Board

Collaborators

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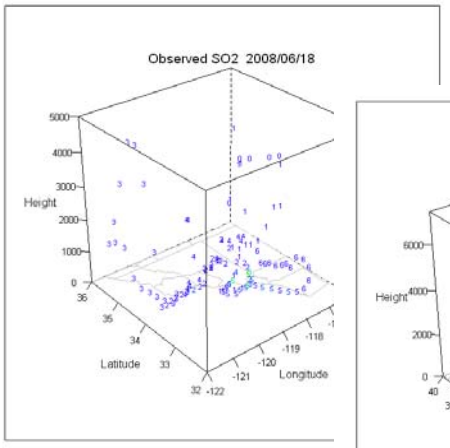
- William Brune – Penn State
- Jack Dibb – University of New Hampshire
- Greg Huey – Georgia Institute of Technology
- Jose Jimenez – University of Colorado
- Paul Wennberg – California Institute of Technology
- Armin Wisthaler – University Innsbruck
- + …….

P-3 California Flights

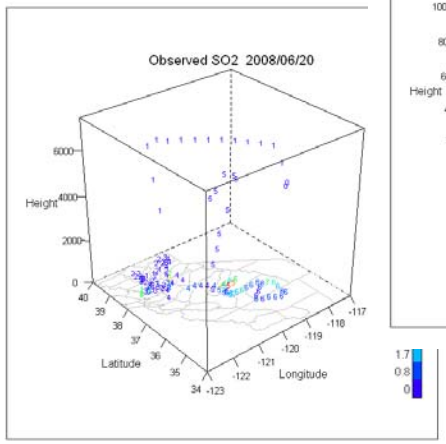
Not included in this presentation due to time limitations

Flt	Date	Track	Comments
11	22 Jun	Moffett Local	Power plant plume, CAR circles, ship plume, AERONET, Terra, sonde, smoke.
12	24 Jun	Moffett-Los Angeles-Moffett	Plume crossings for 14 ships. Profiles under Terra & Aqua. Ocean BRDF (calm & 50-kt winds). Fire plumes & pollution plumes.
13 & 14	26 Jun	Moffett-Edmonton-Cold Lake	Lake Tahoe smoke radiation study in DC-8 lidar curtain & under Terra. Lake albedo & BRDF. Central Valley smoke gradient legs.

ARCTAS-CA DC-8 Flight Patterns



06/18/08



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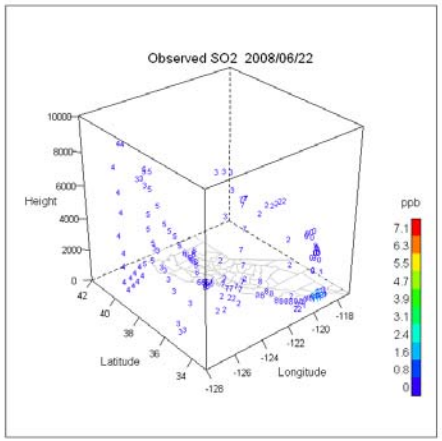

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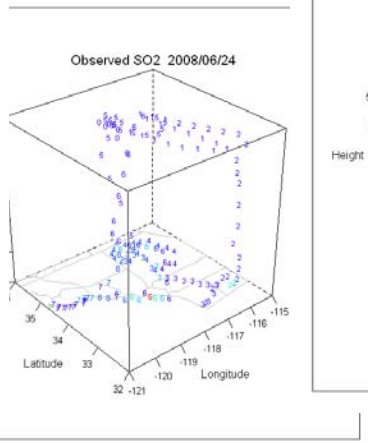

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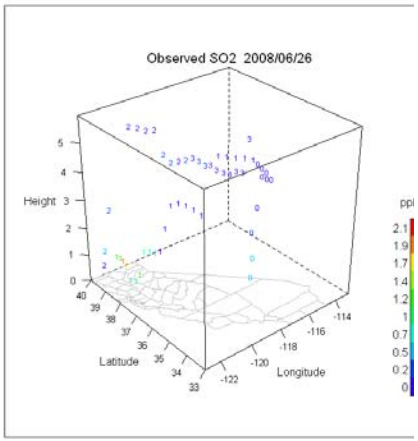

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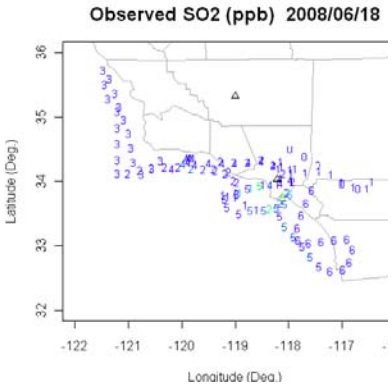
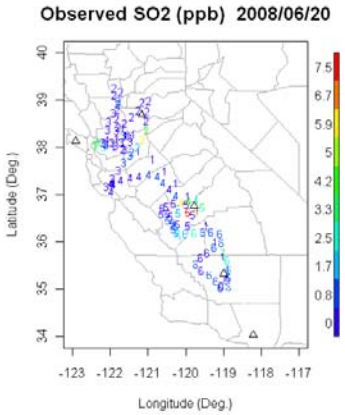
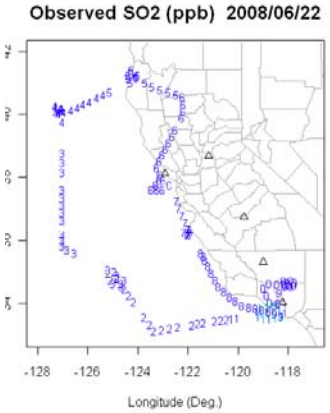
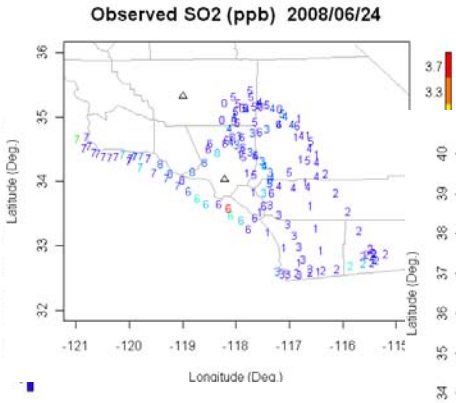
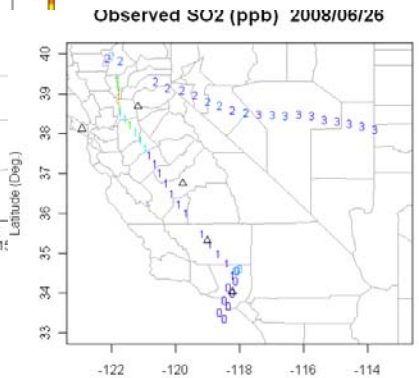






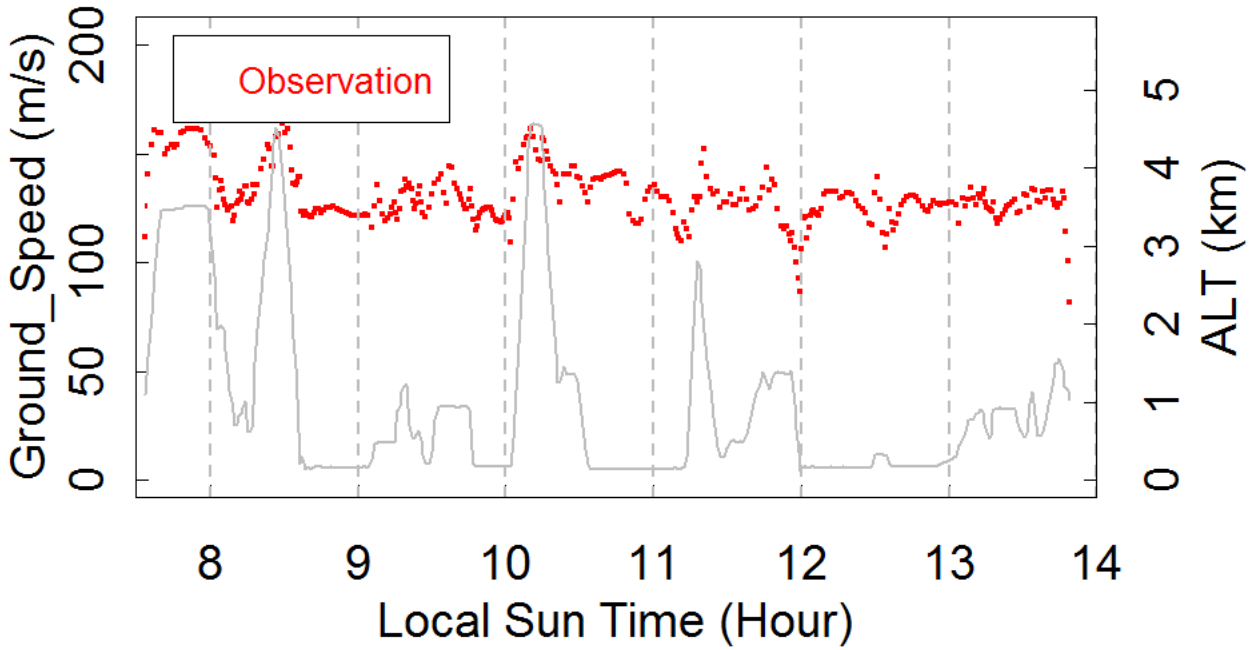




Details of Simulations

- The month of June 2008 was simulated for the entire state of California with 4×4-km horizontal grid cells and 30 vertical layers
- MM5
  - analysis nudging but no observational nudging
- CMAQ
  - v4.64
  - SAPRC99 with the AE4 aerosol module
  - MORZART June 2008 average boundary conditions
- Emissions
  - base year emissions for 2002 were projected to 2005
  - no fires in the modeling inventory yet

DC-8 Observations vs. Simulations



Aircraft moves 6-9 km per minute and horizontal grid size in the model is 4 km.

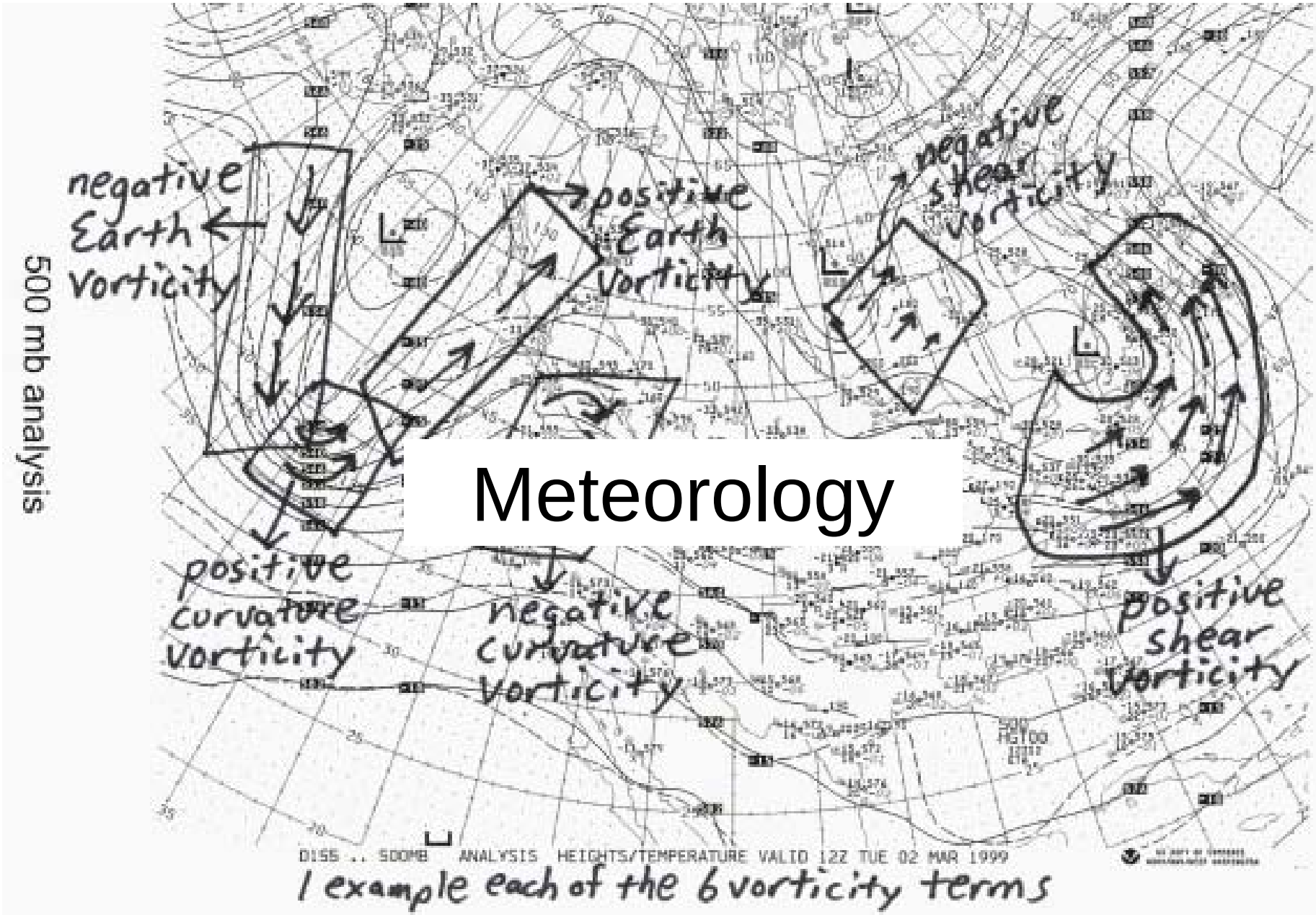
Aircraft observations are made in sub-grid-scale and averaged to a minute.

In the simulation, emissions are diluted into a grid cell and an average hourly concentration for that grid cell is simulated. Simulated concentrations are then interpolated to the average aircraft position for each minute.

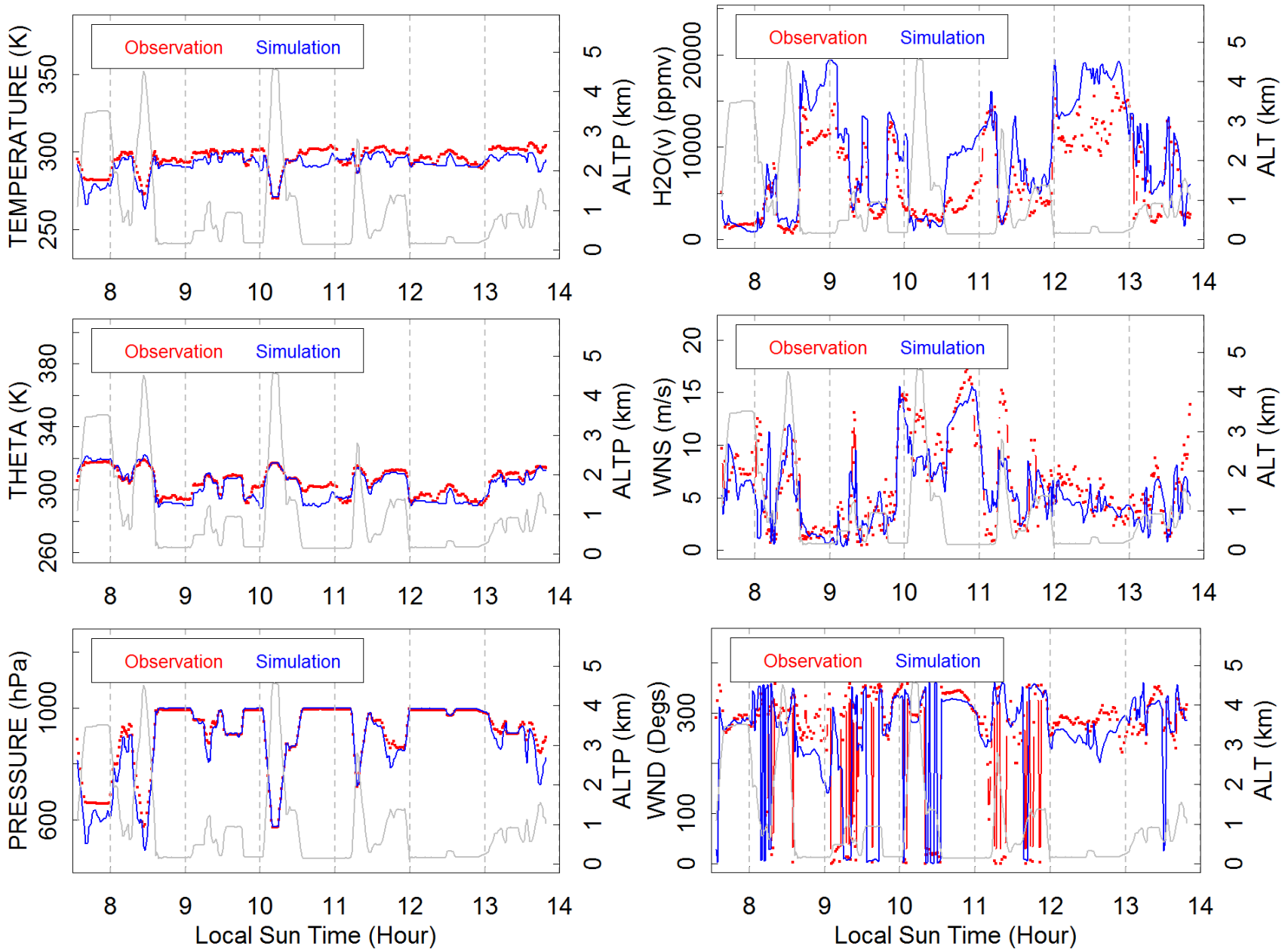
Model Performance Expectations

- Simulated and observed peak heights may not match
- Simulated and observed features should match approximately in time
- Simulated and observed trends should be similar
- Discrepancies may help improve emissions inventories
- Large discrepancies are expected where fires were (since the modeling inventory does not have fires)

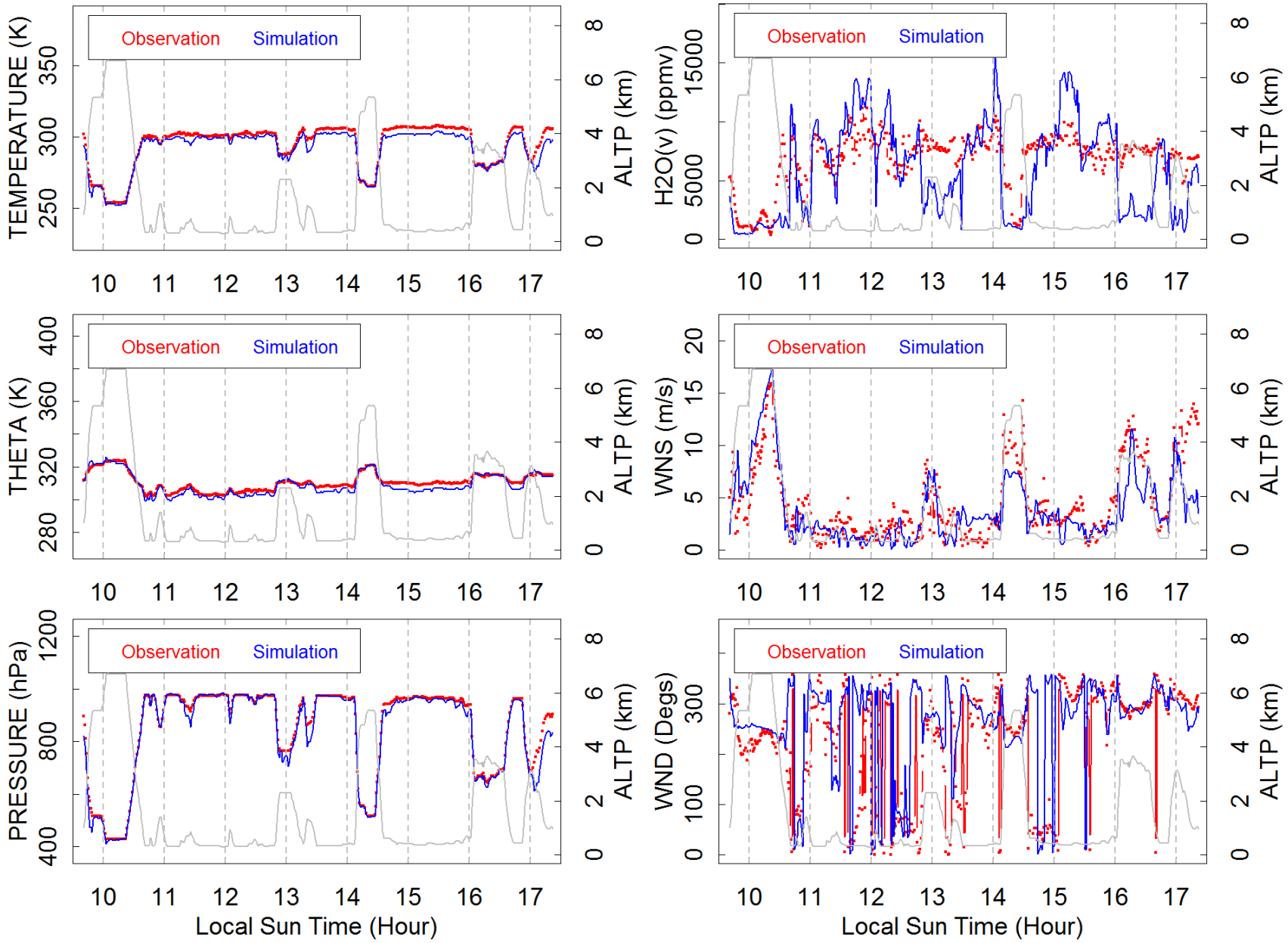
Meteorology



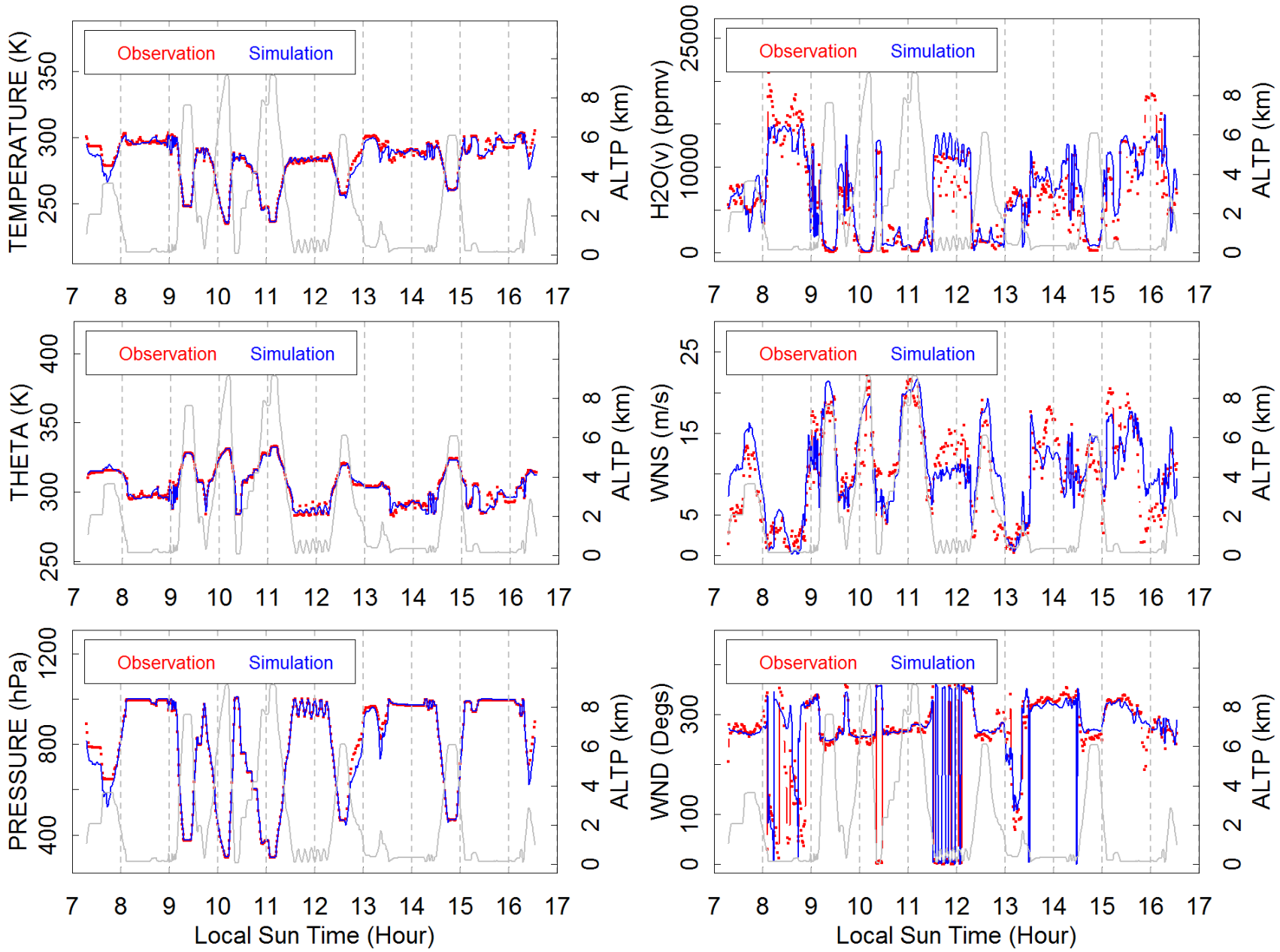
Meteorology
June 18, 2008



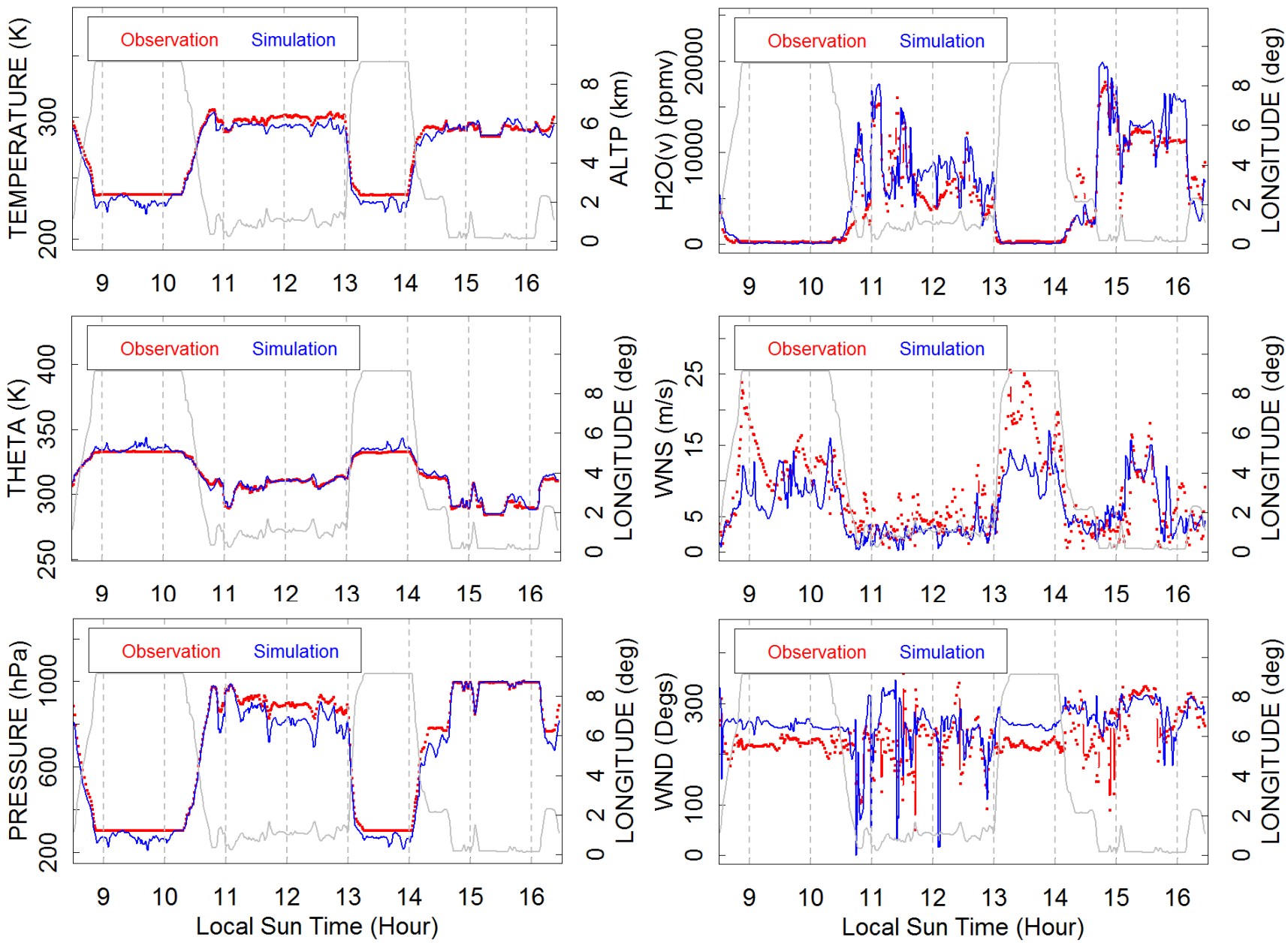
Meteorology
June 20, 2008



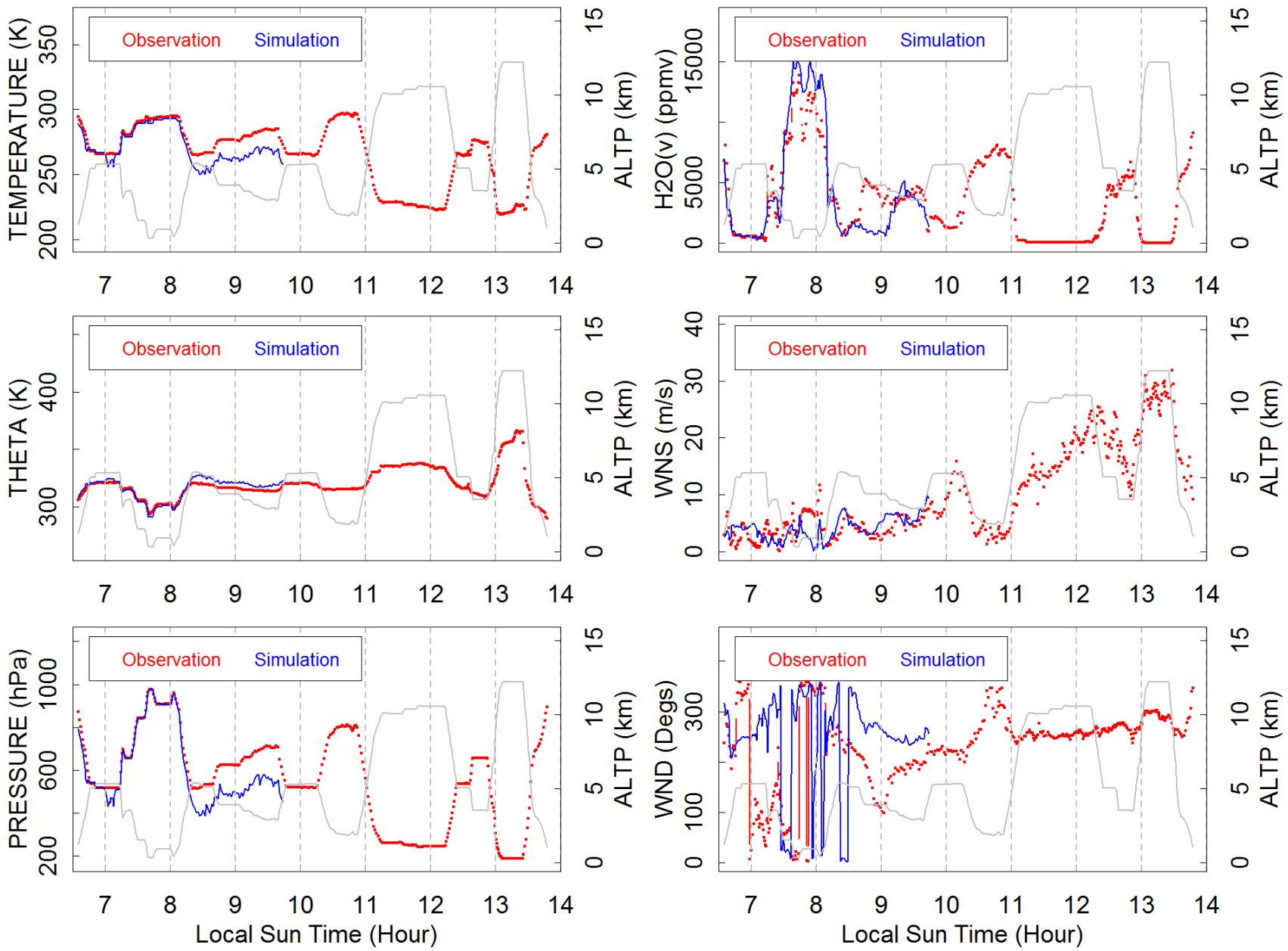
Meteorology
June 22, 2008



Meteorology
June 24, 2008



Meteorology
June 26, 2008



Ozone and Precursors

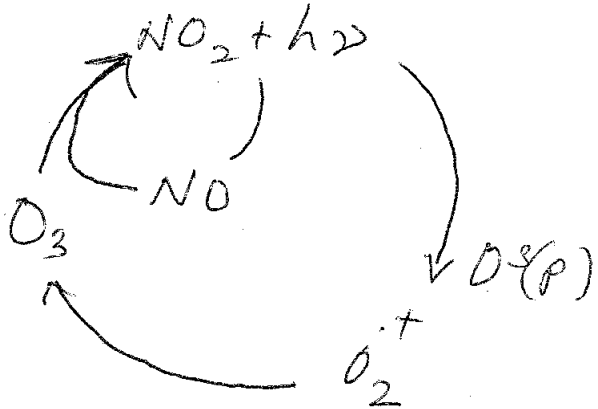
O_3 formation:

$$NO_2 \xrightarrow{h\nu} NO + O(^3P)$$

$$O(^3P) + O_2 \xrightarrow{M} O_3$$

$$O_3 + NO \rightarrow NO_2 + O_2$$

Nothing!



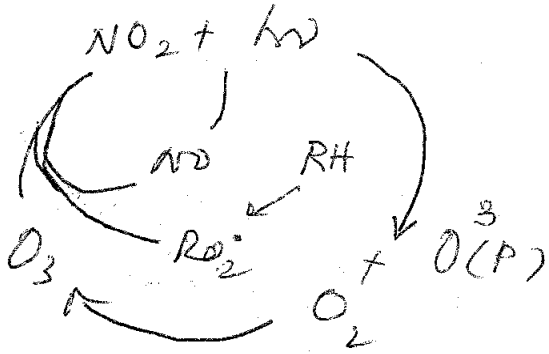
$$HCHO \xrightarrow{h\nu} HCO^{\bullet} + H^{\bullet}$$

$$H^{\bullet} + O_2$$

$$HCO^{\bullet} + O_2$$

$$HO_2^{\bullet} + NO \rightarrow NO_2 + OH^{\bullet}$$

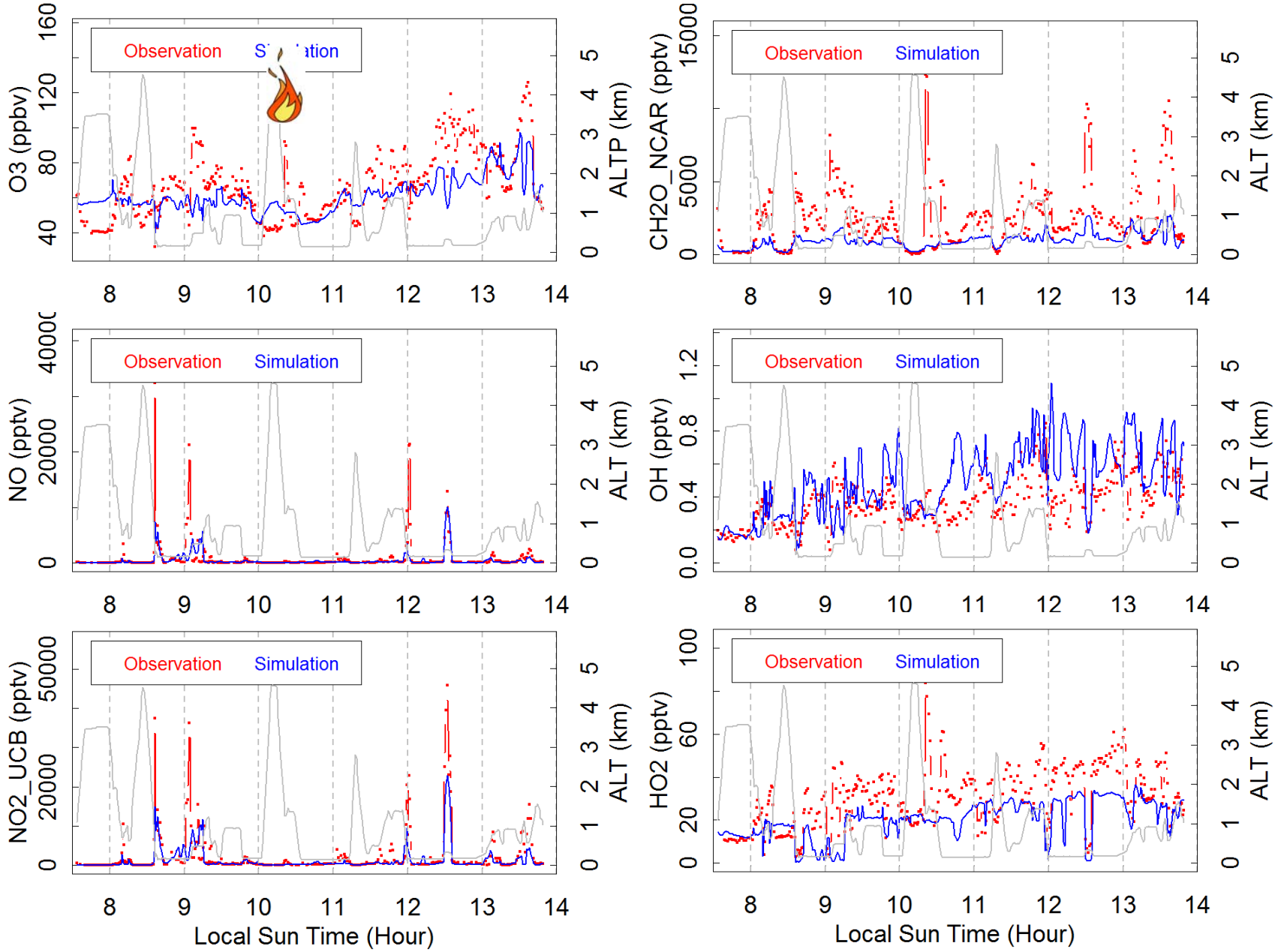
$$RO_2^{\bullet} + NO \rightarrow NO_2 + RO^{\bullet}$$



Tropospheric Concentrations

Ozone and its Precursors

June 18, 2008



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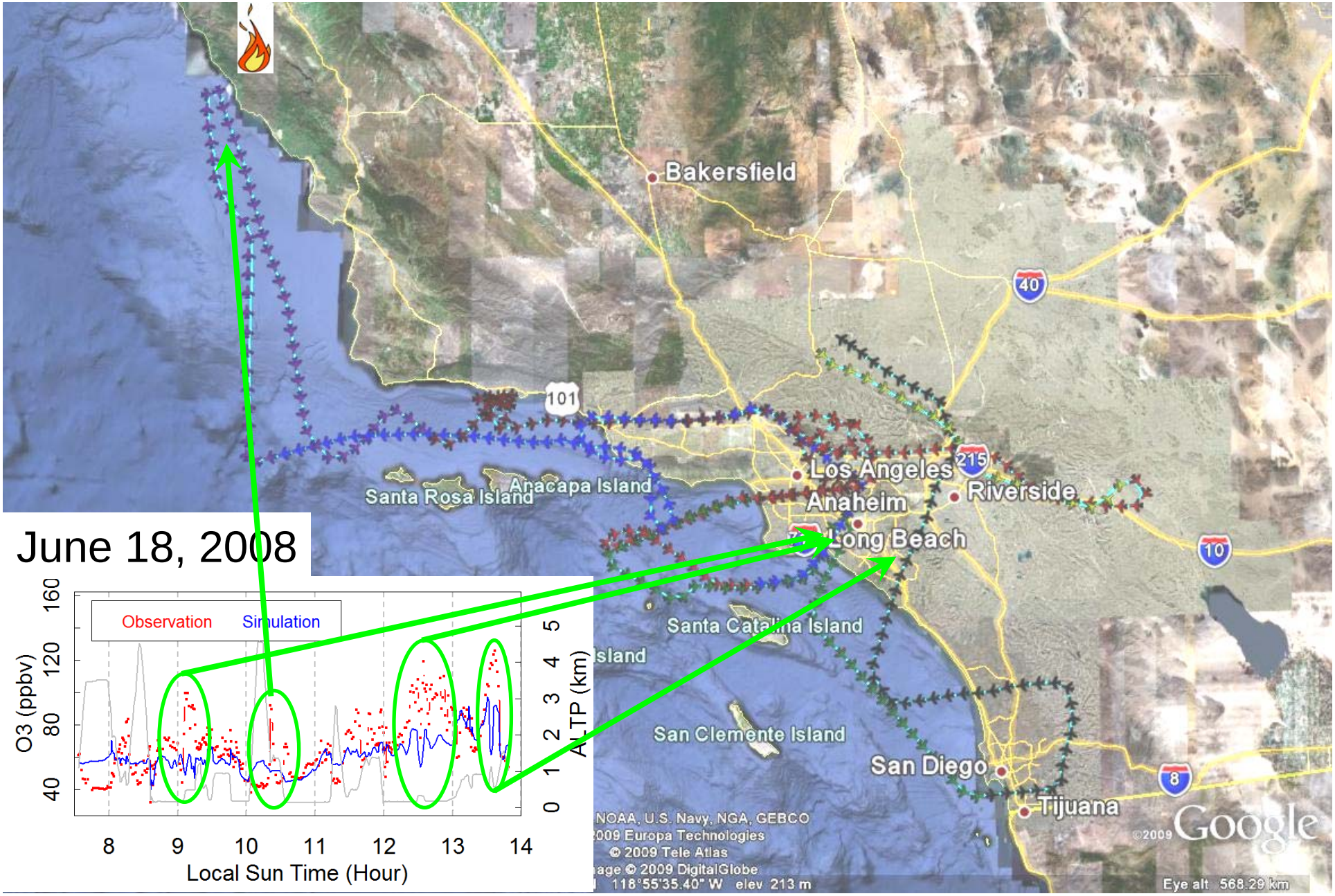
Things to Notice

- At 2-5 km, $[O_3]$ ~ 40 ppb
- No NO_x above 1 km
- Peaks in $[NO_x]$ causes $[O_3]$ to dip (with matching dips in radicals). $[O_3]$ in these areas may be VOC sensitive.
- $[O_3]$ peaks without NO_x but with abundant VOC (and HO_2) at ~ 10:30 am (emissions not in the inventory)
- Dip in modeled $[O_3]$ at 1:30 pm?



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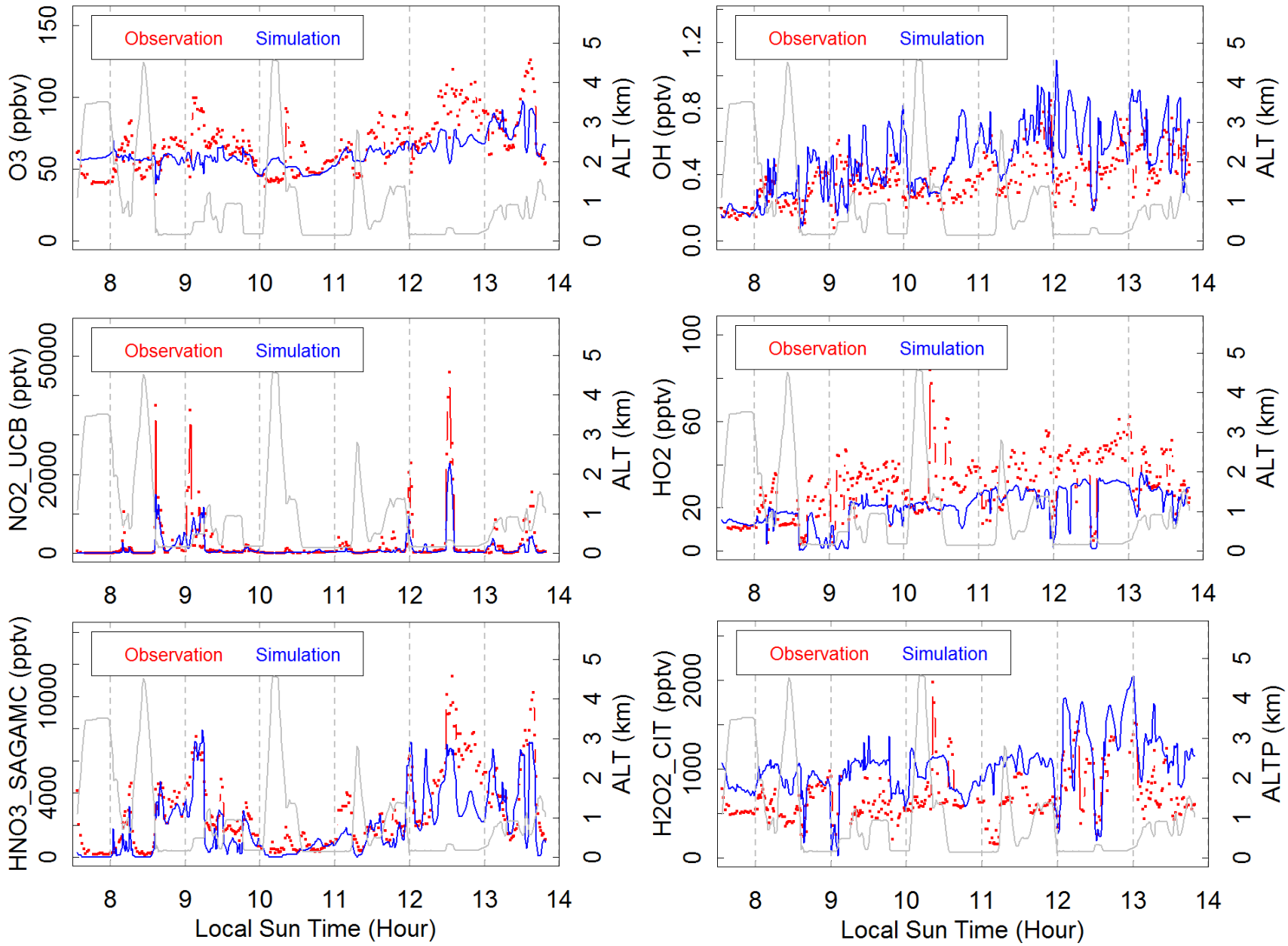
VOC and/or NOx Limitations

- Obtained an unprecedented suit of measurements that would allow one to probe inner-workings of chemistry
- Aircraft measurements are not really Lagrangian
- Is the model predicting the correct VOC and/or NOx sensitivity of O_3?
  - Are we now able to test the validity of indicator ratios (or something related to that)? If not, what are we missing (and should be measured during 2010 CalNex)?
  - Is there anything else we can look at?

Precursor Limitations

June 18, 2008



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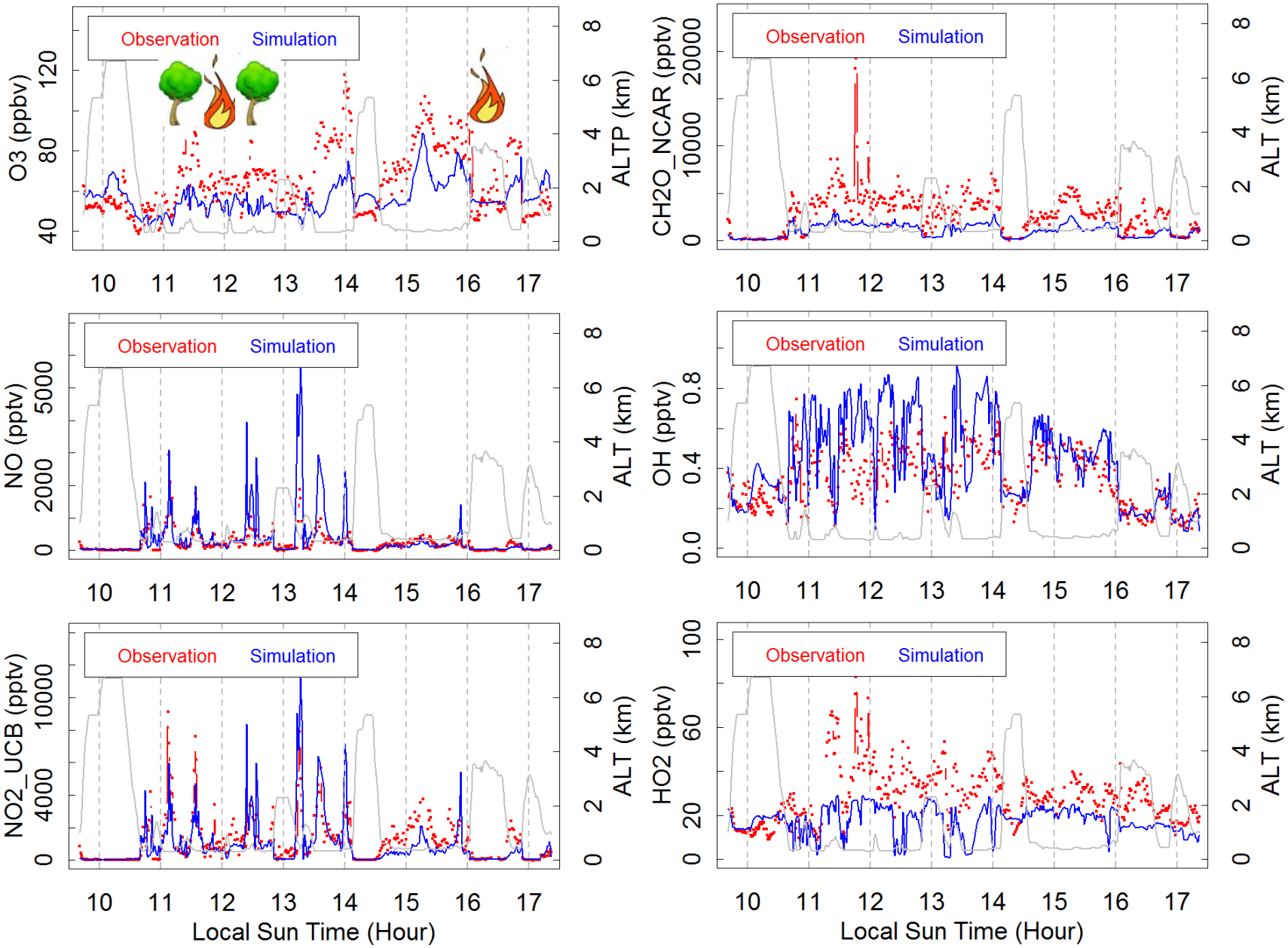
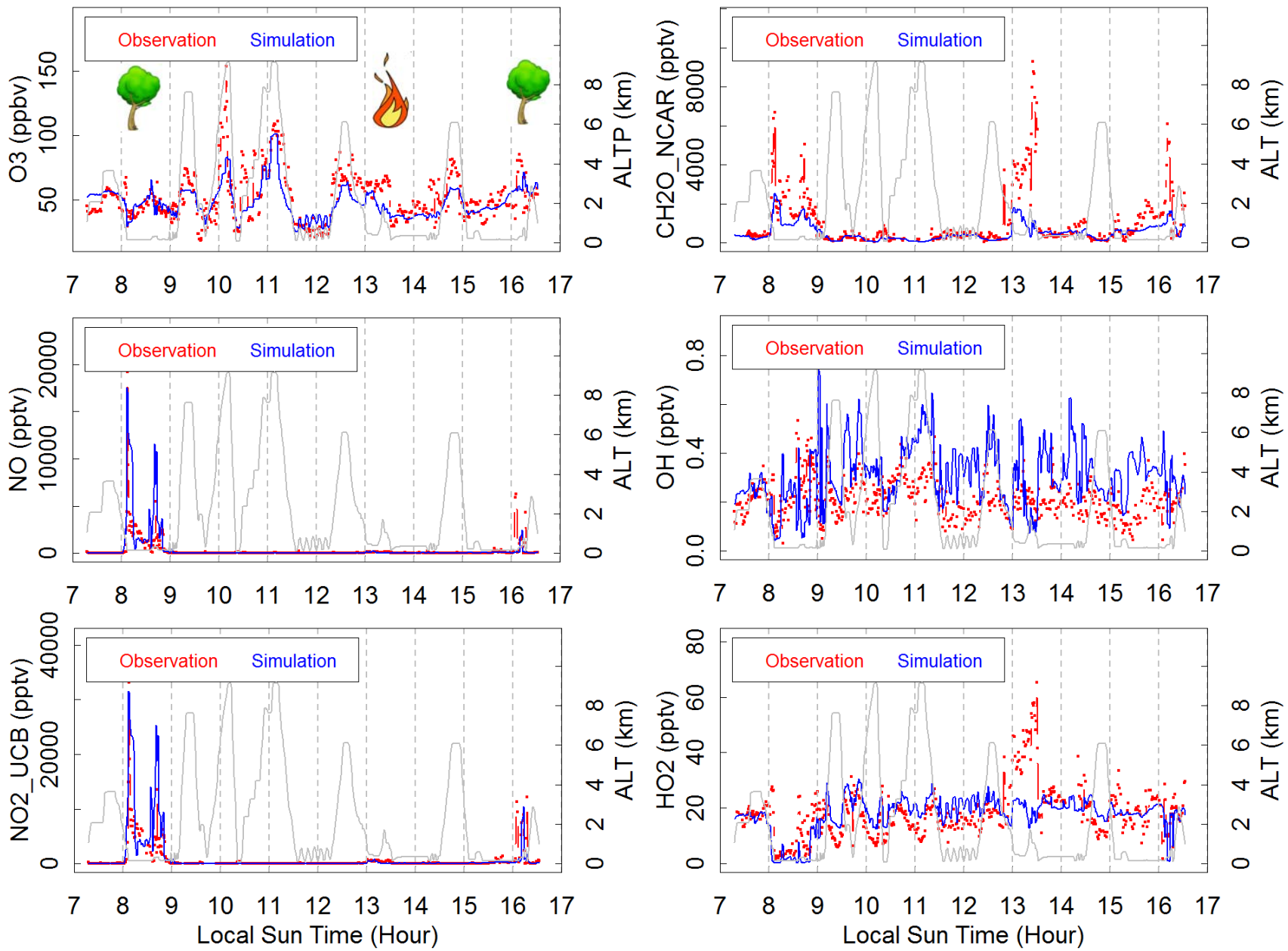
Ozone and its Precursors

June 20, 2008



Ozone and its Precursors

June 22, 2008



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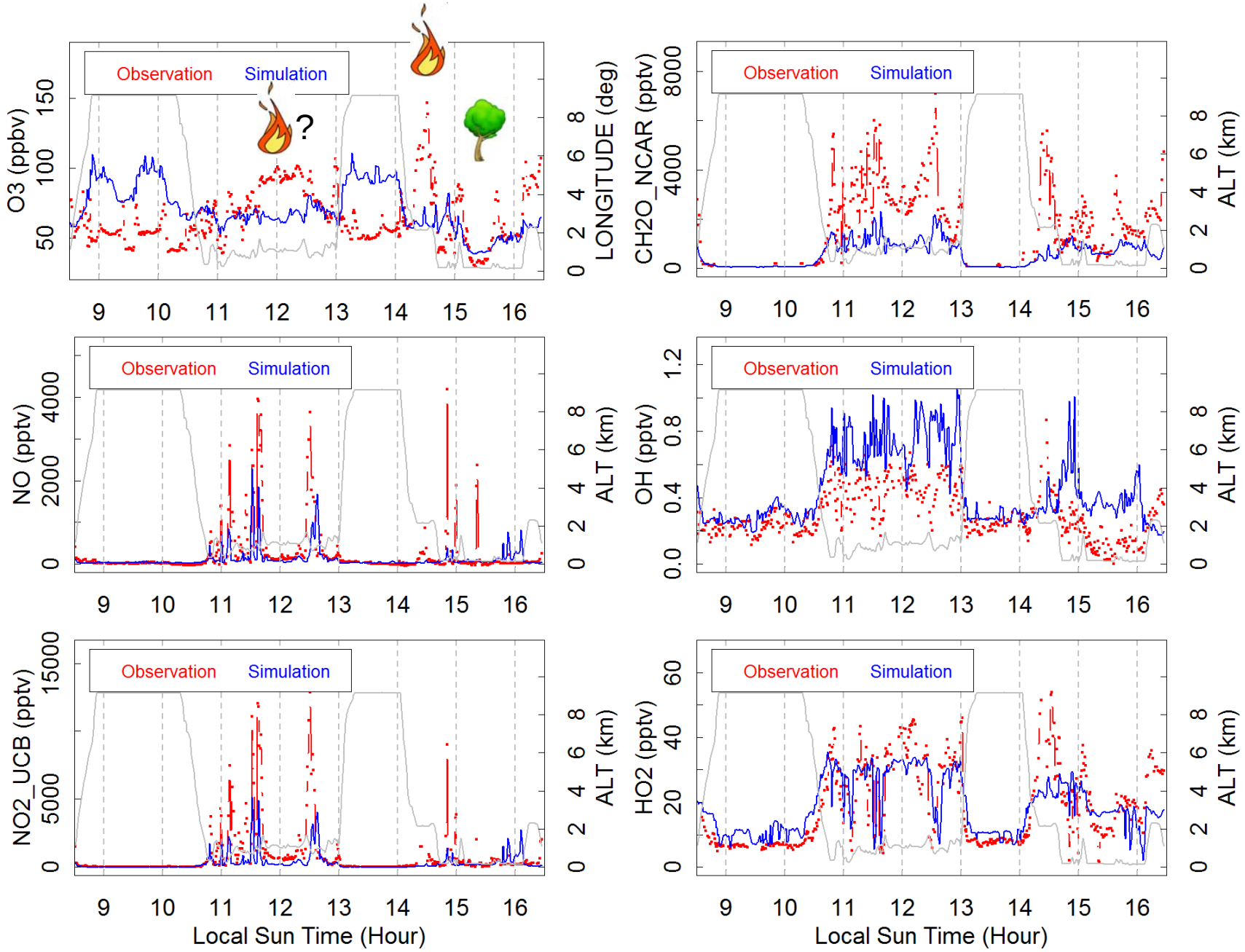
Ozone and its Precursors

June 24, 2008



Ozone and its Precursors

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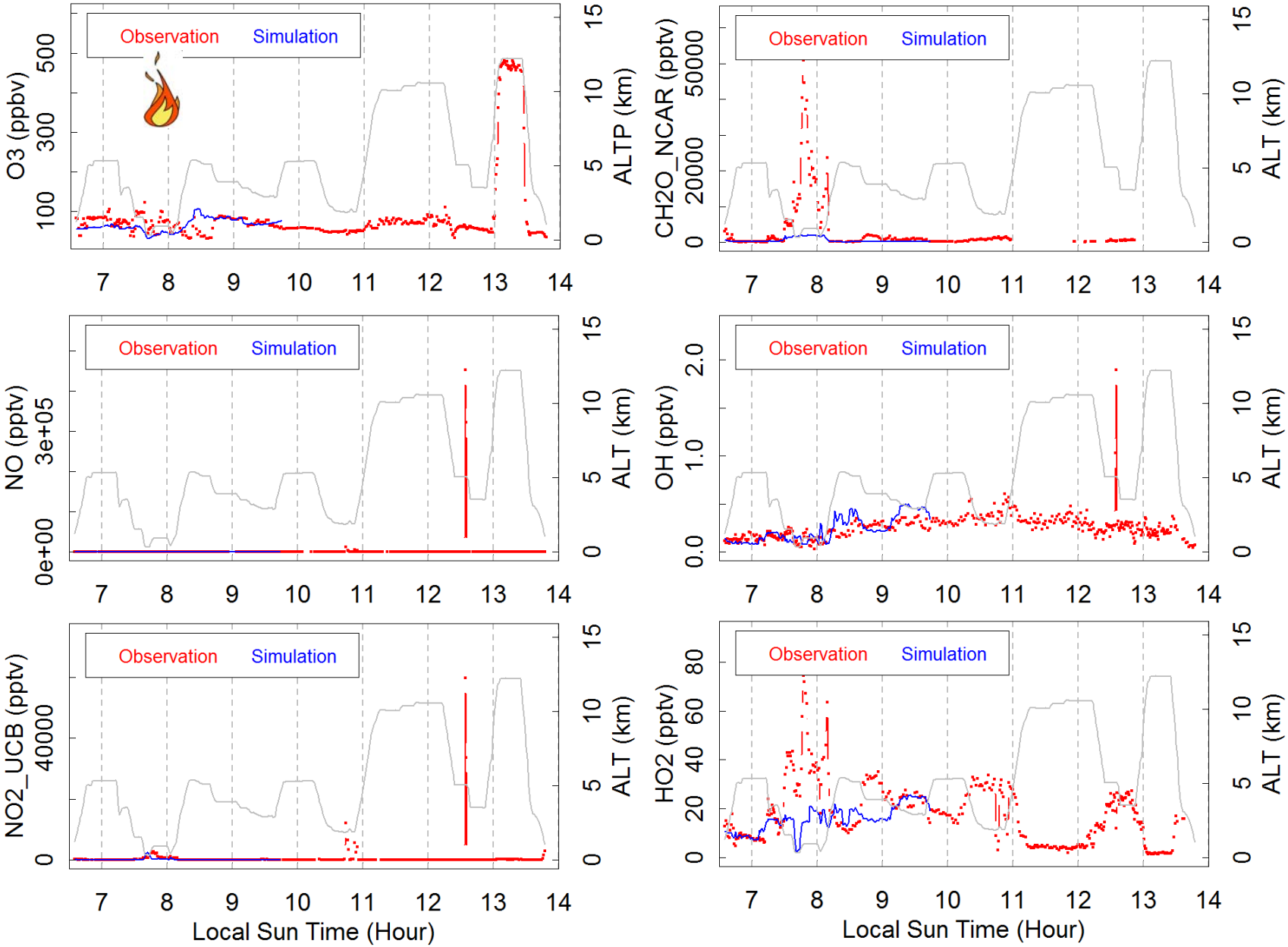
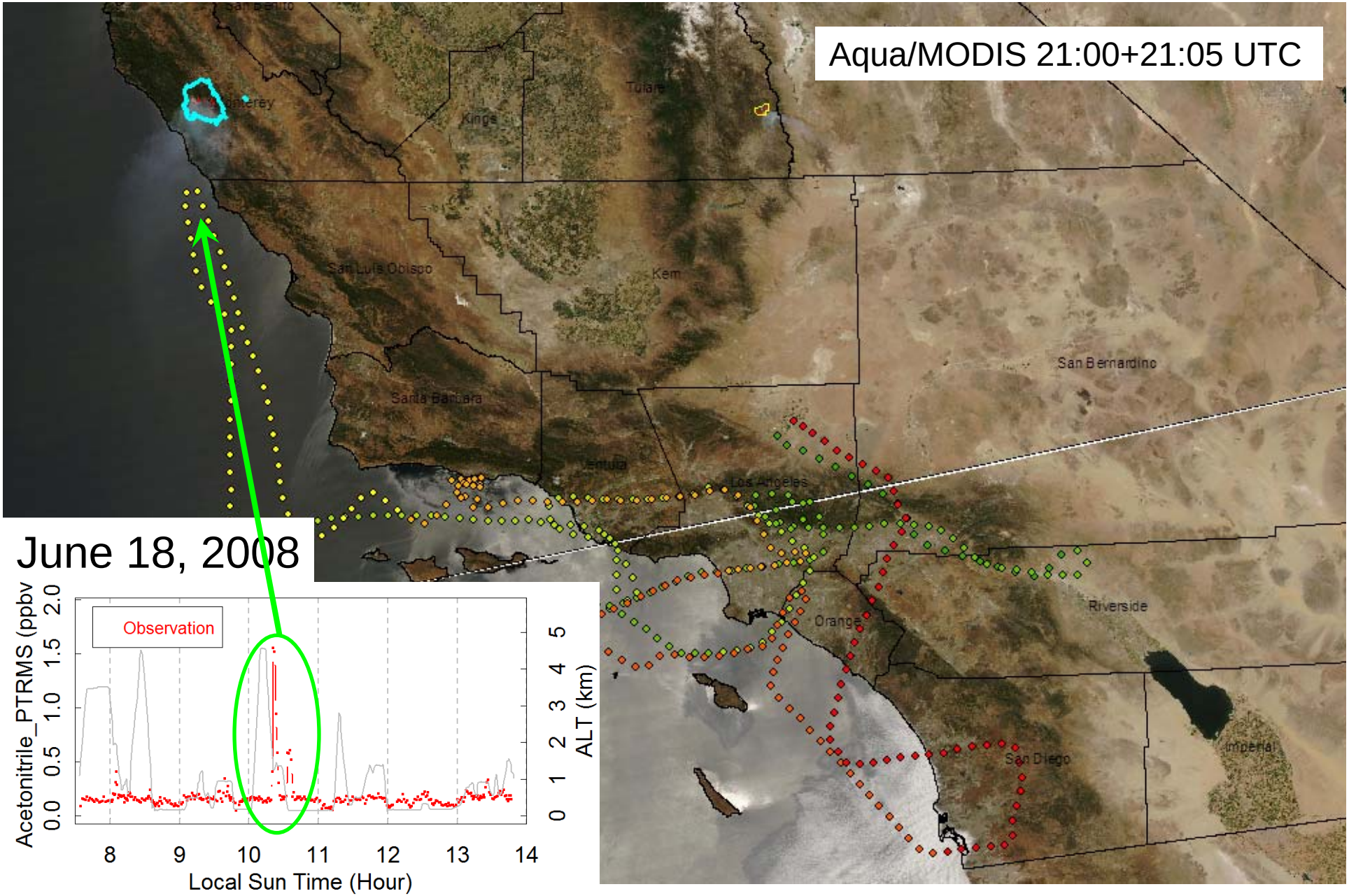


Wild Fires



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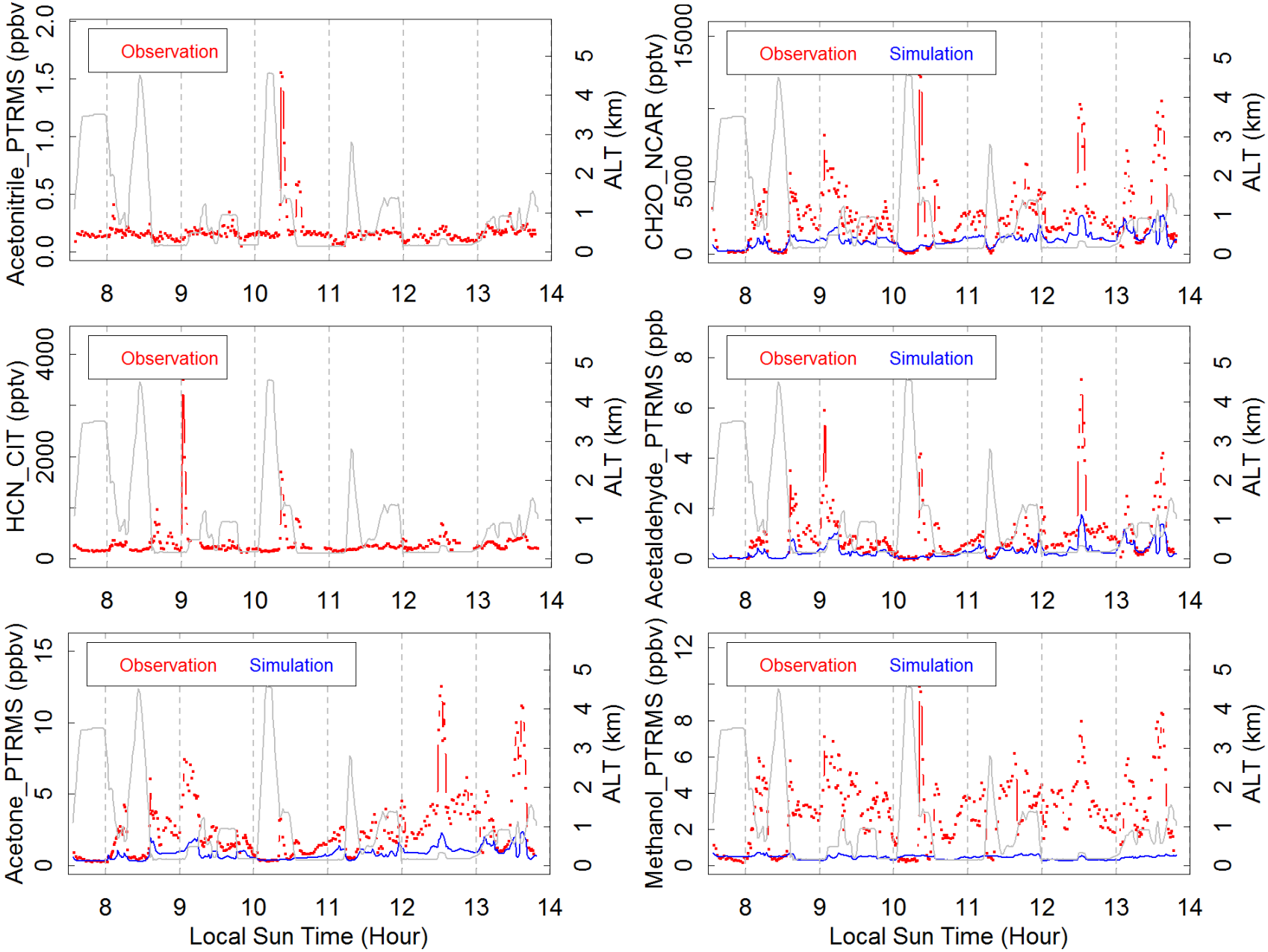
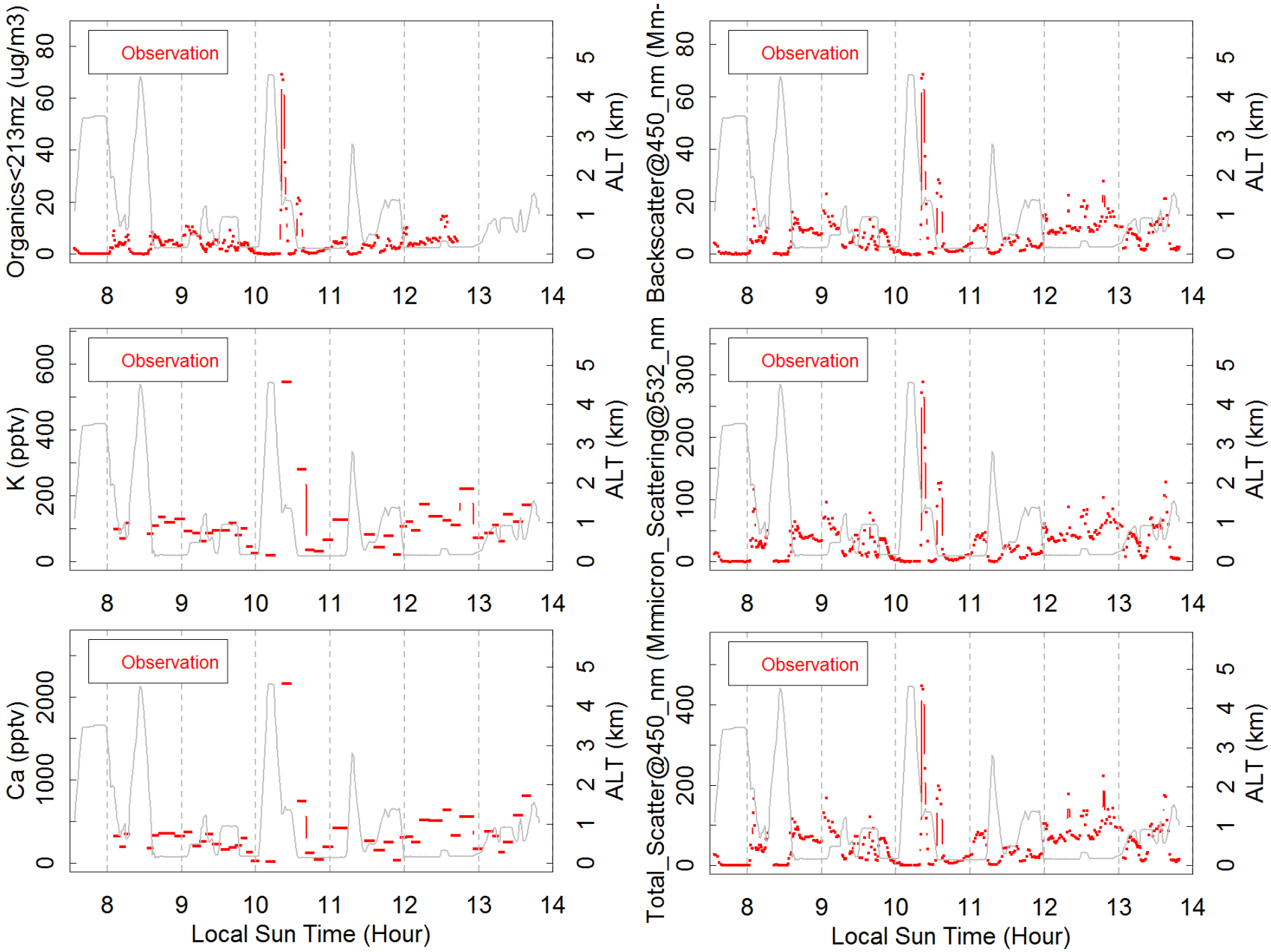
Wildfire Signature
June 18, 2008



Wildfire Markers
June 18, 2008



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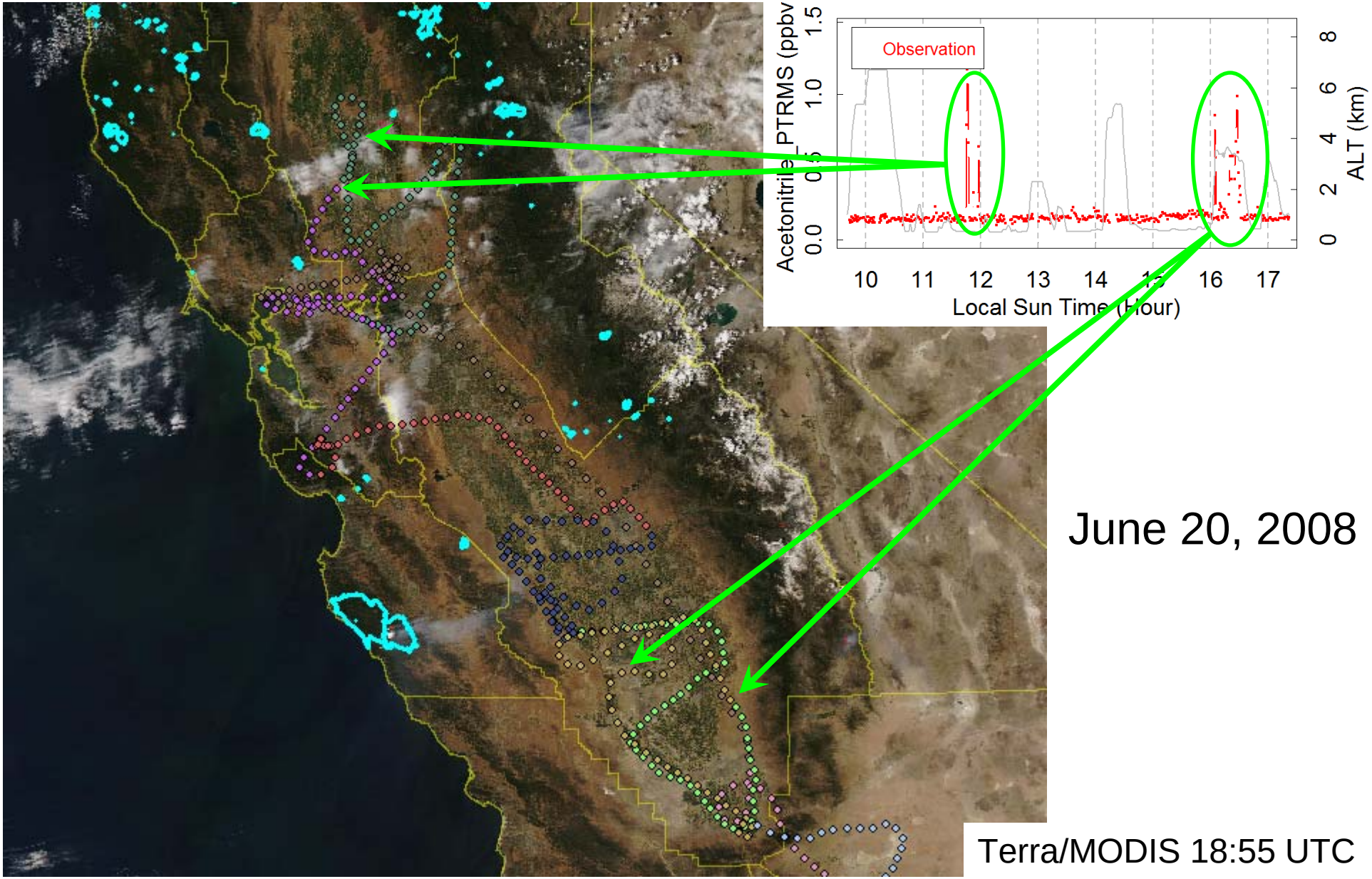
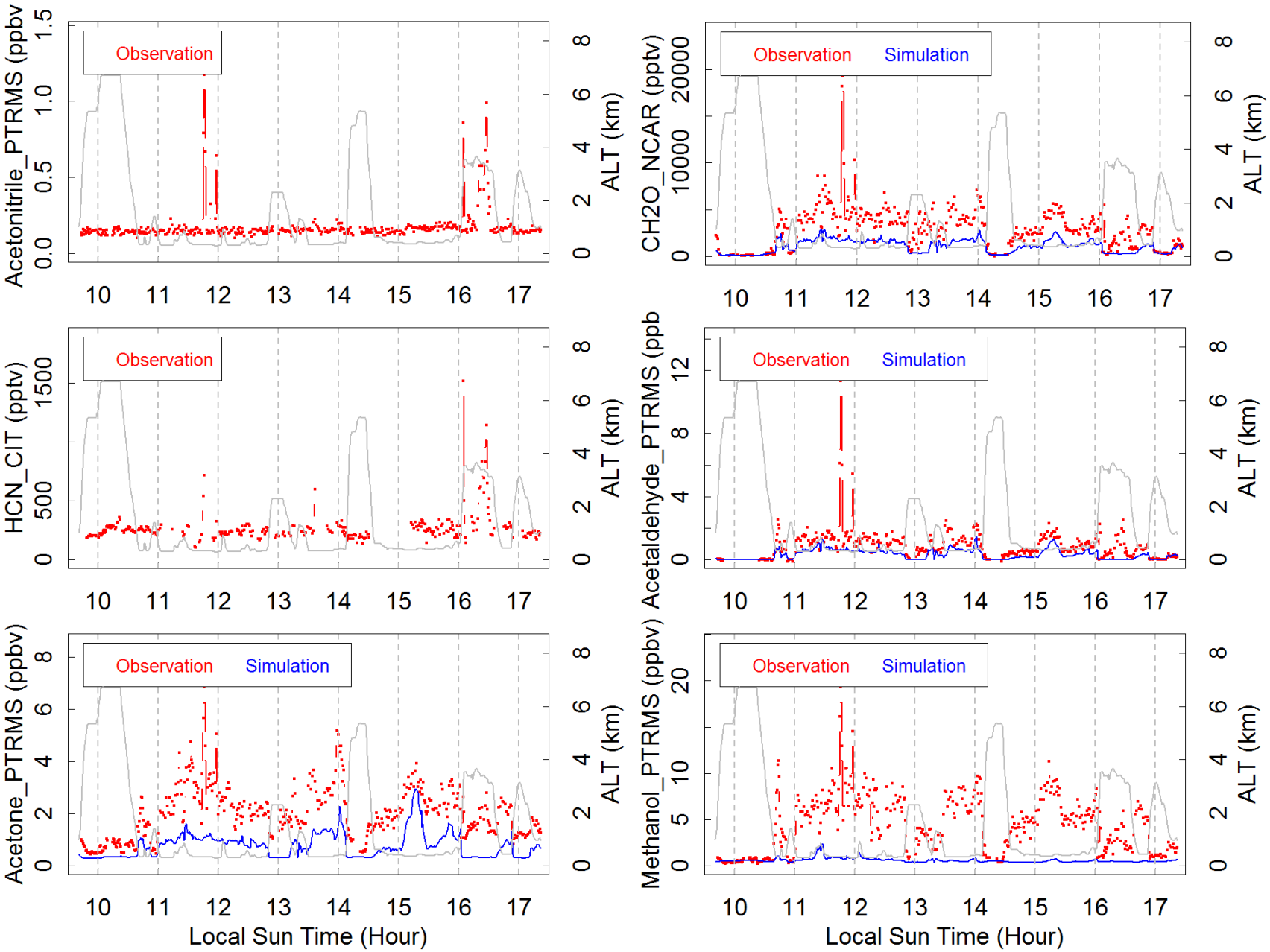
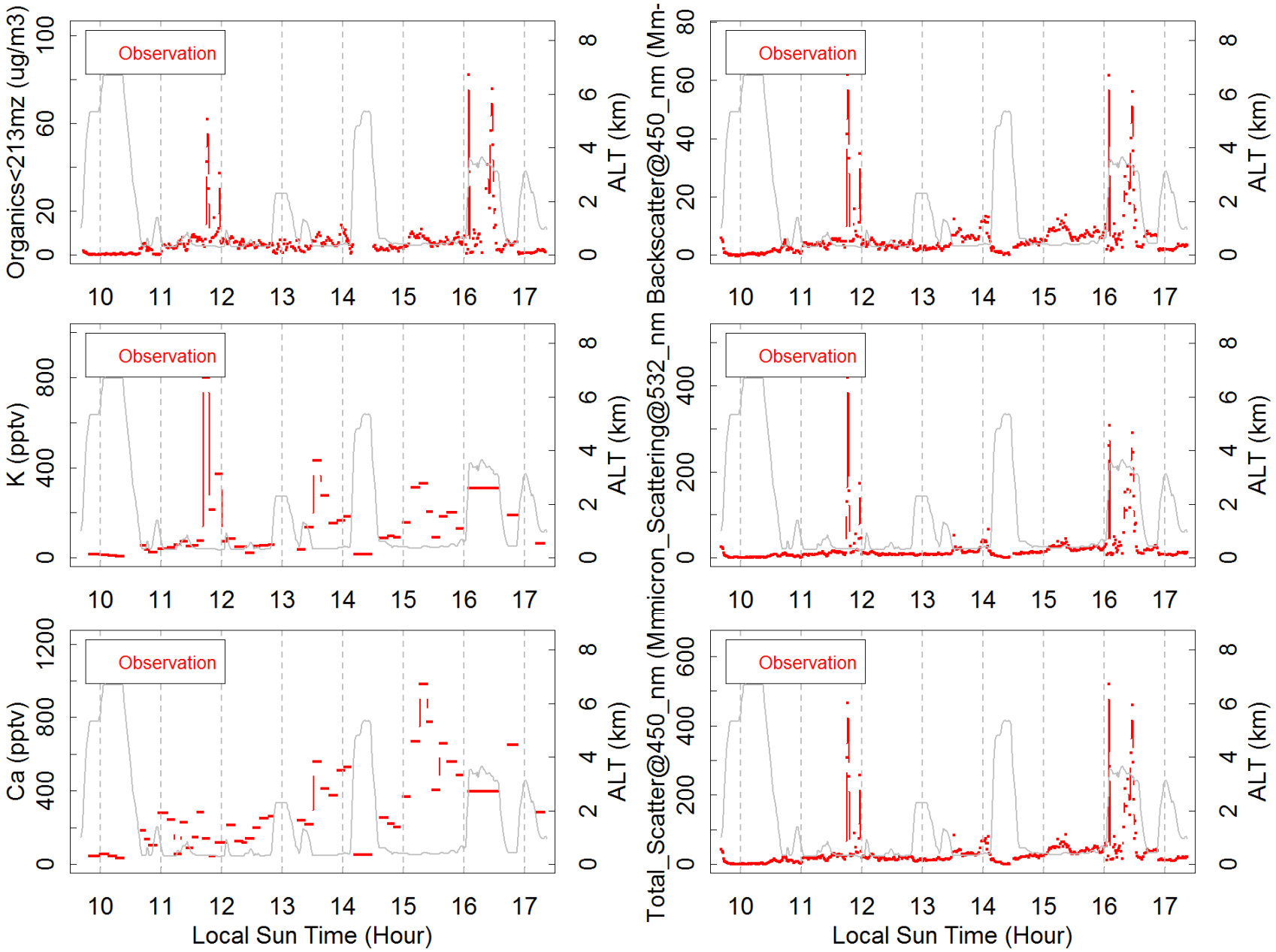

Observation
Acetonitrile_PTRMS (ppbv)
0.0
0.5
1.0
1.5
ALT (km)
0
2
4
6
8
10
11
12
13
14
16
17
Local Sun Time (Hour)
June 20, 2008
Terra/MODIS 18:55 UTC

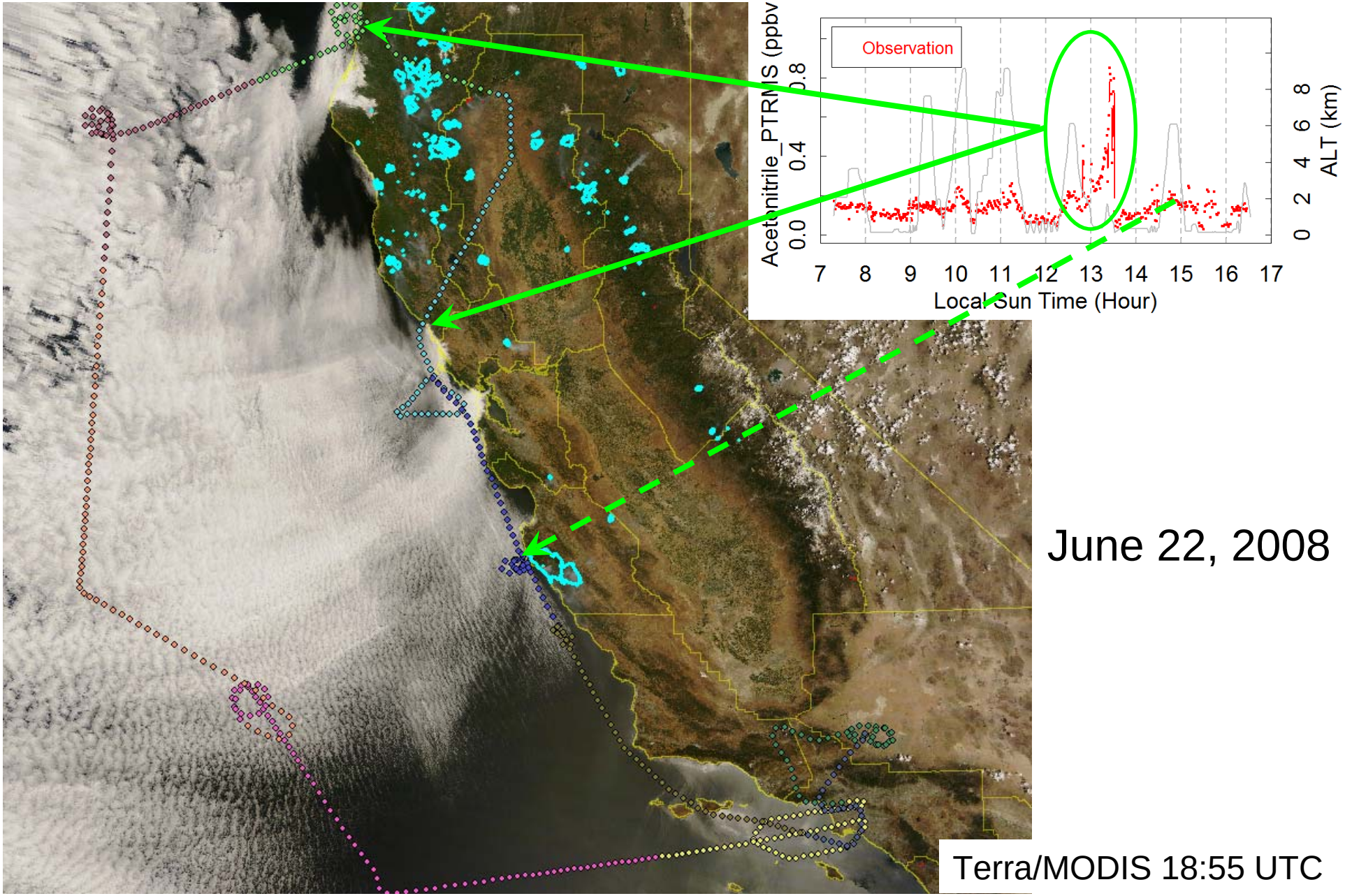
Wildfire Signature
June 20, 2008



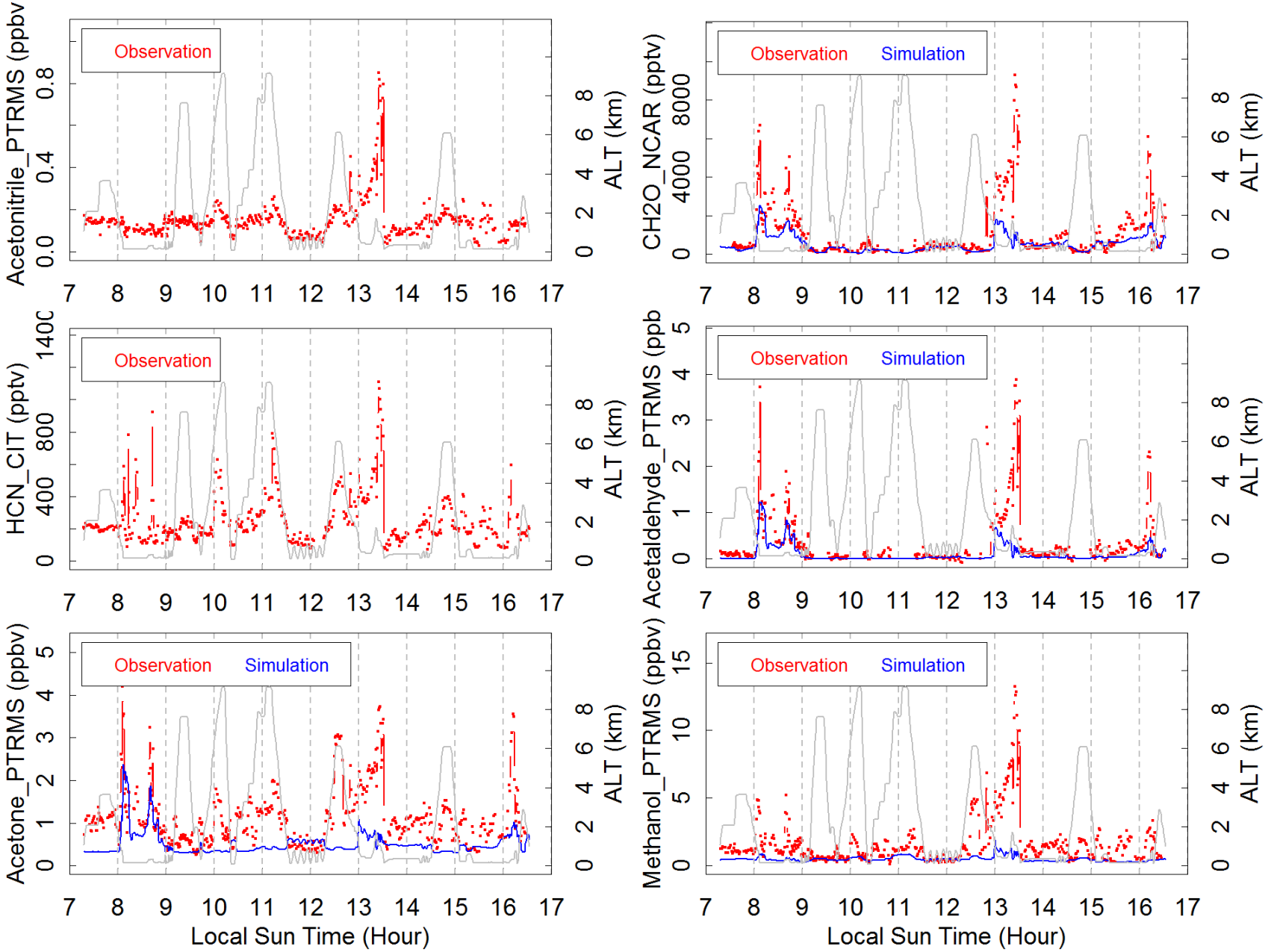
Wildfire Markers

June 26, 2008

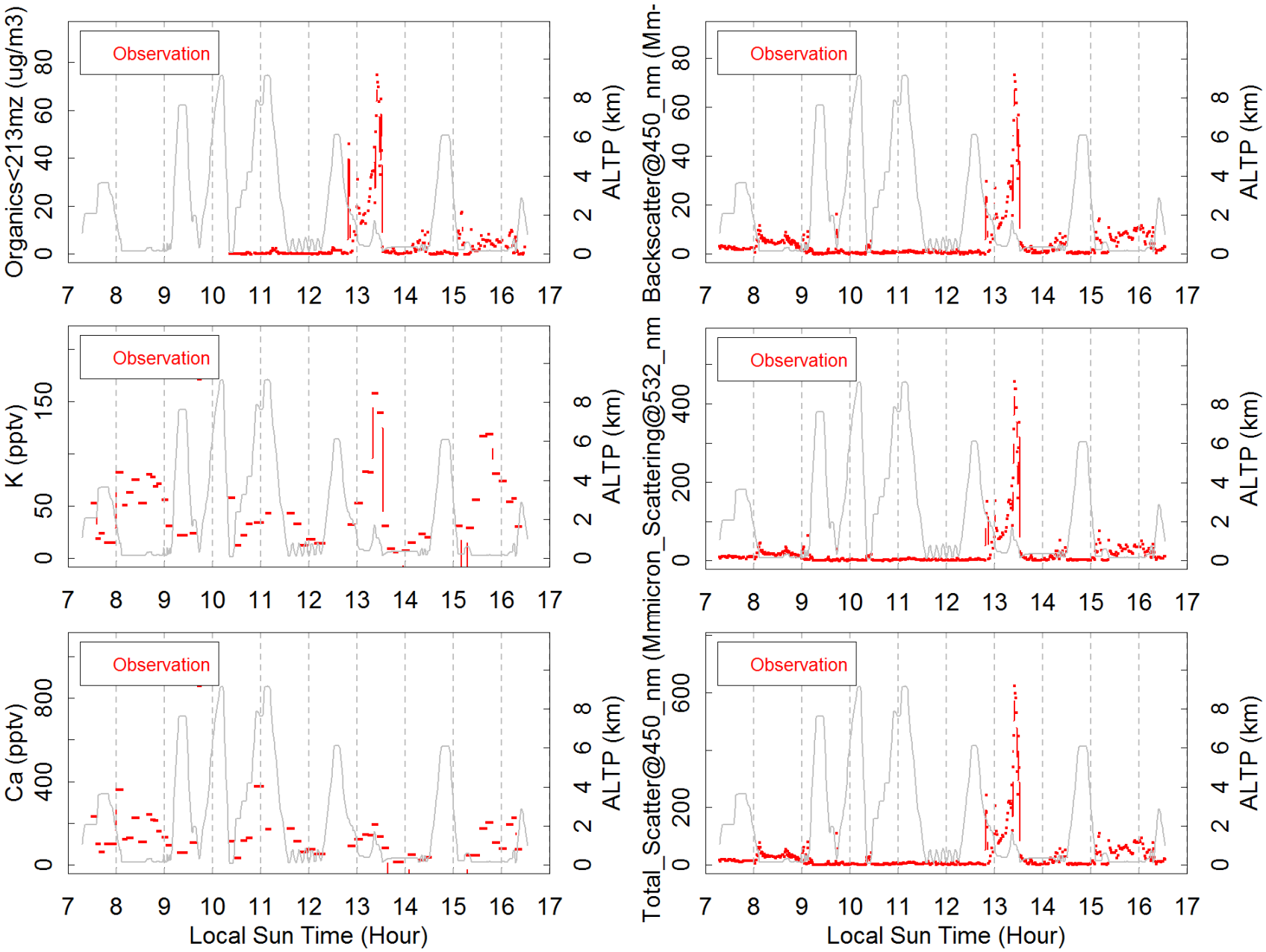



Observation
Acetonitrile_PTRMS (ppbv)
0.0
0.4
0.8
ALT (km)
0
2
4
6
8
7
8
9
10
11
12
13
14
15
16
17
Local Sun Time (Hour)
June 22, 2008
Terra/MODIS 18:55 UTC

Wildfire Signature
June 22, 2008



Wildfire Markers
June 22, 2008



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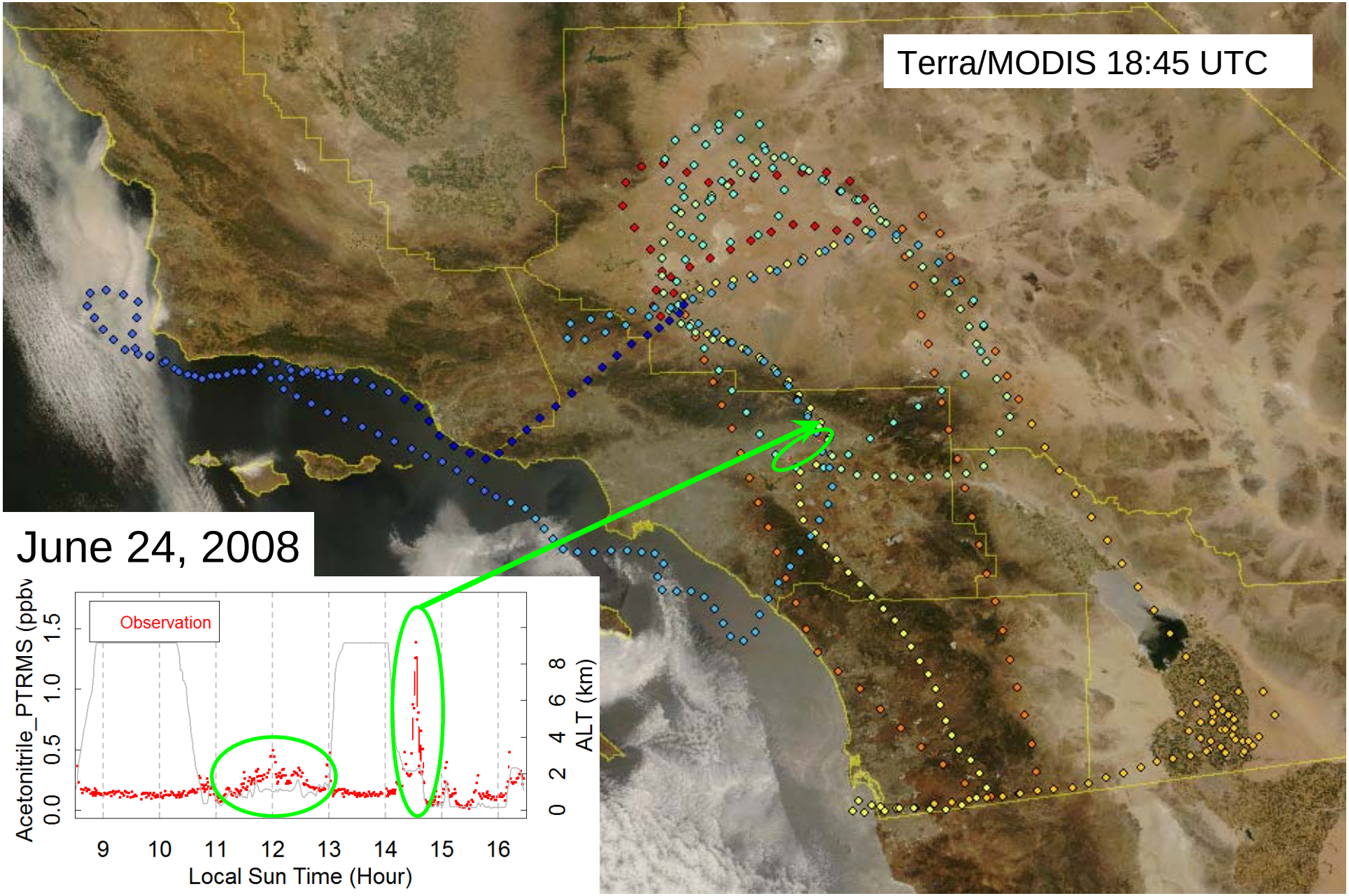

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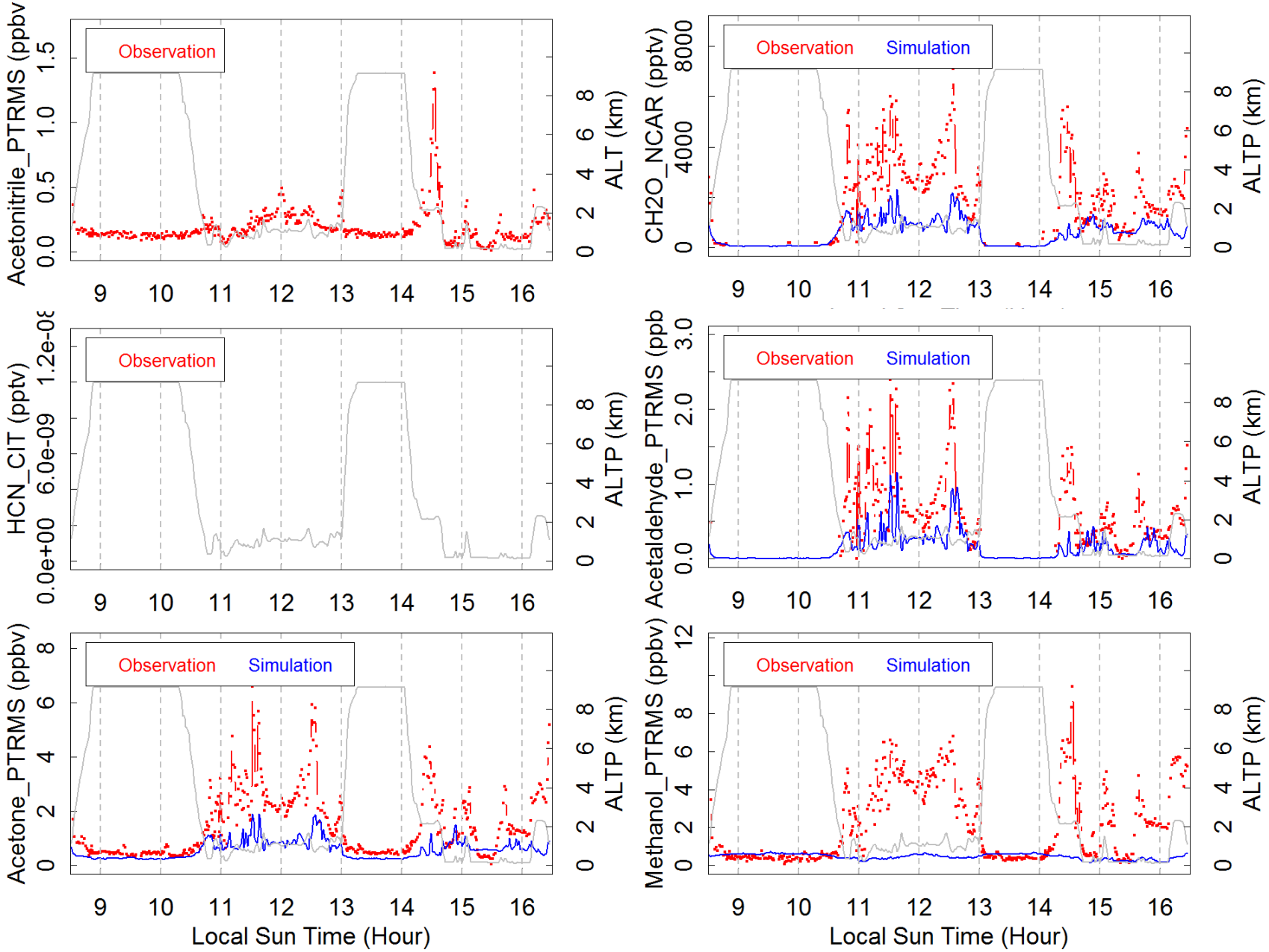
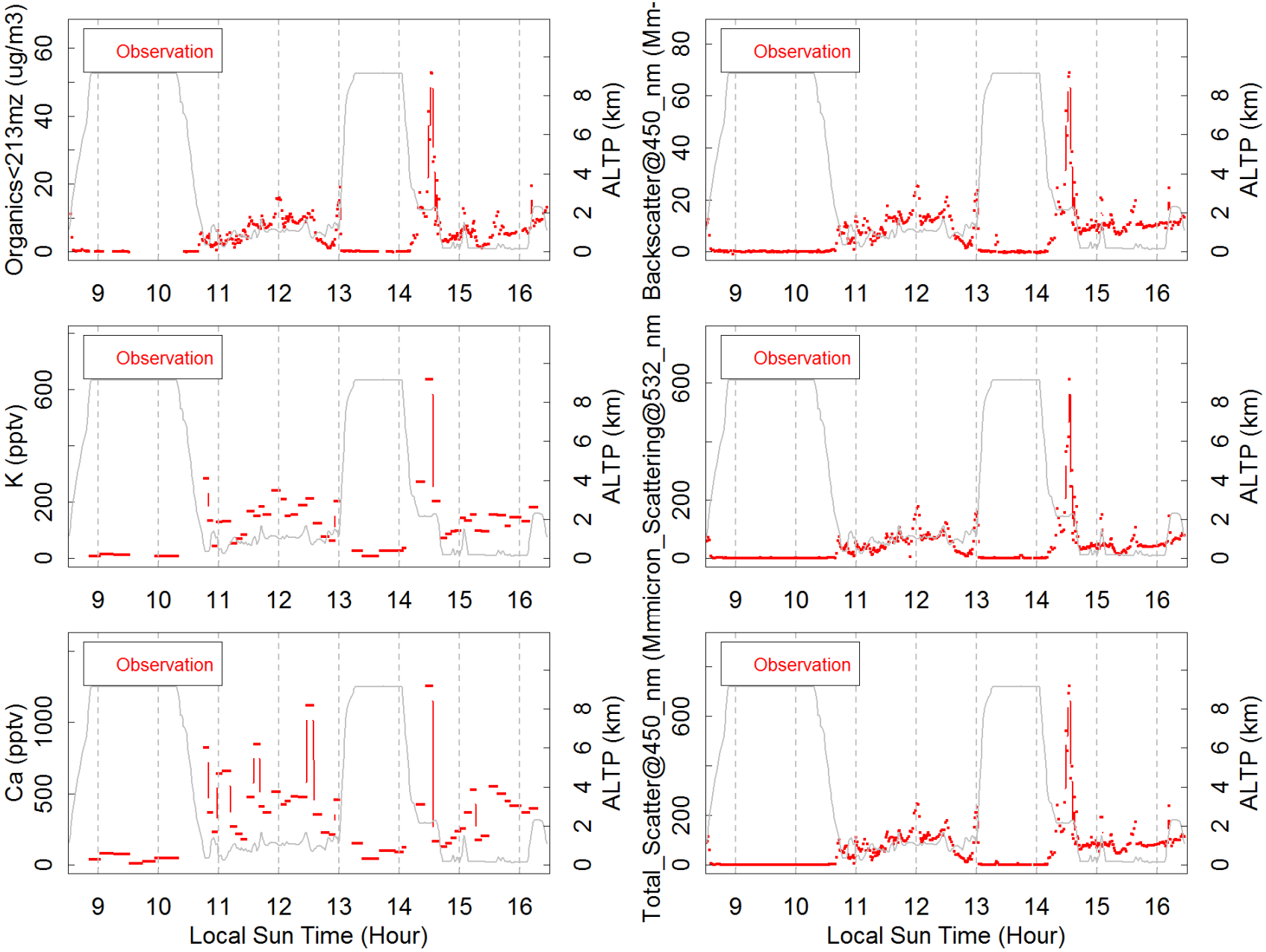
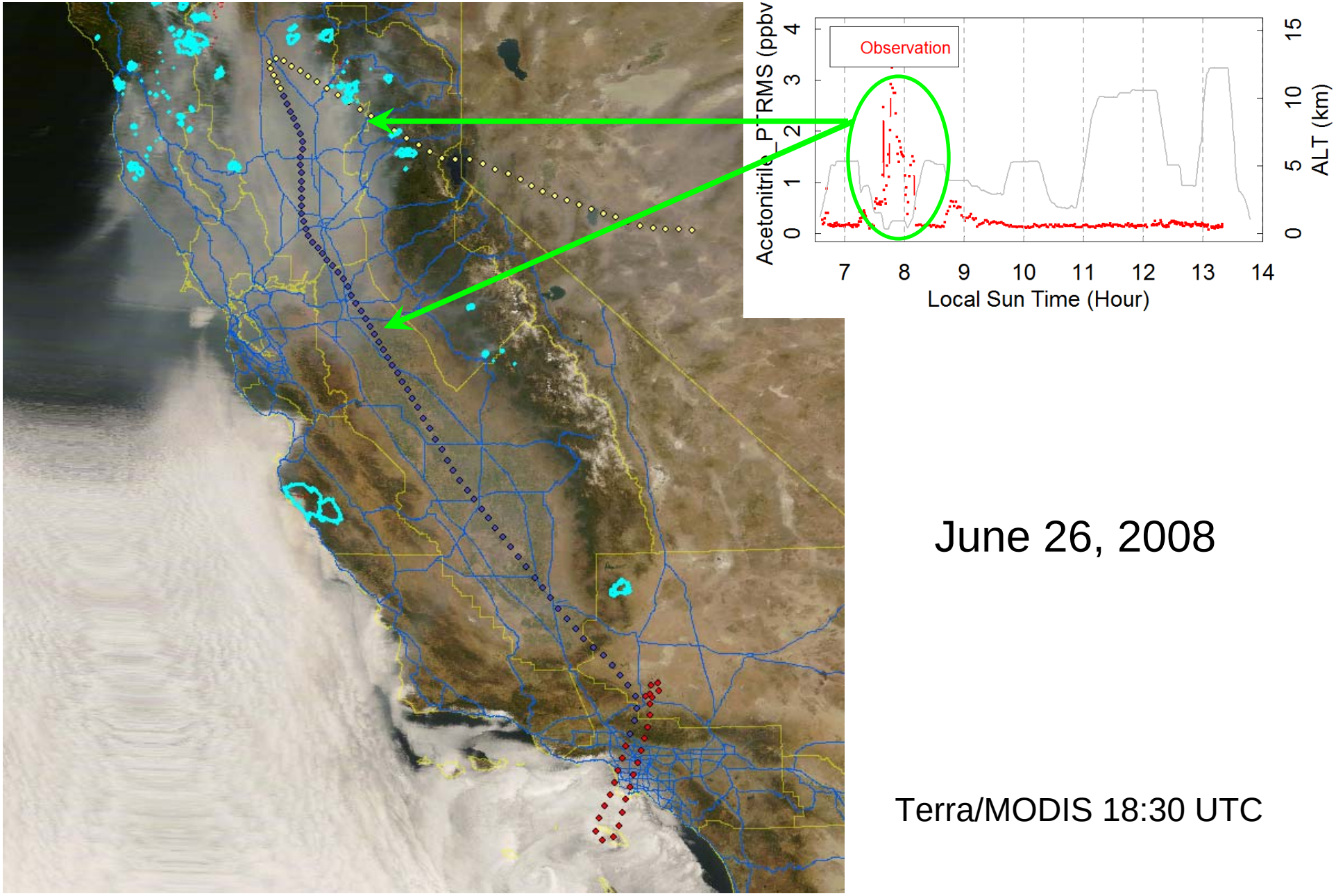
Wildfire Signature
June 24, 2008



Wildfire Markers
June 24, 2008



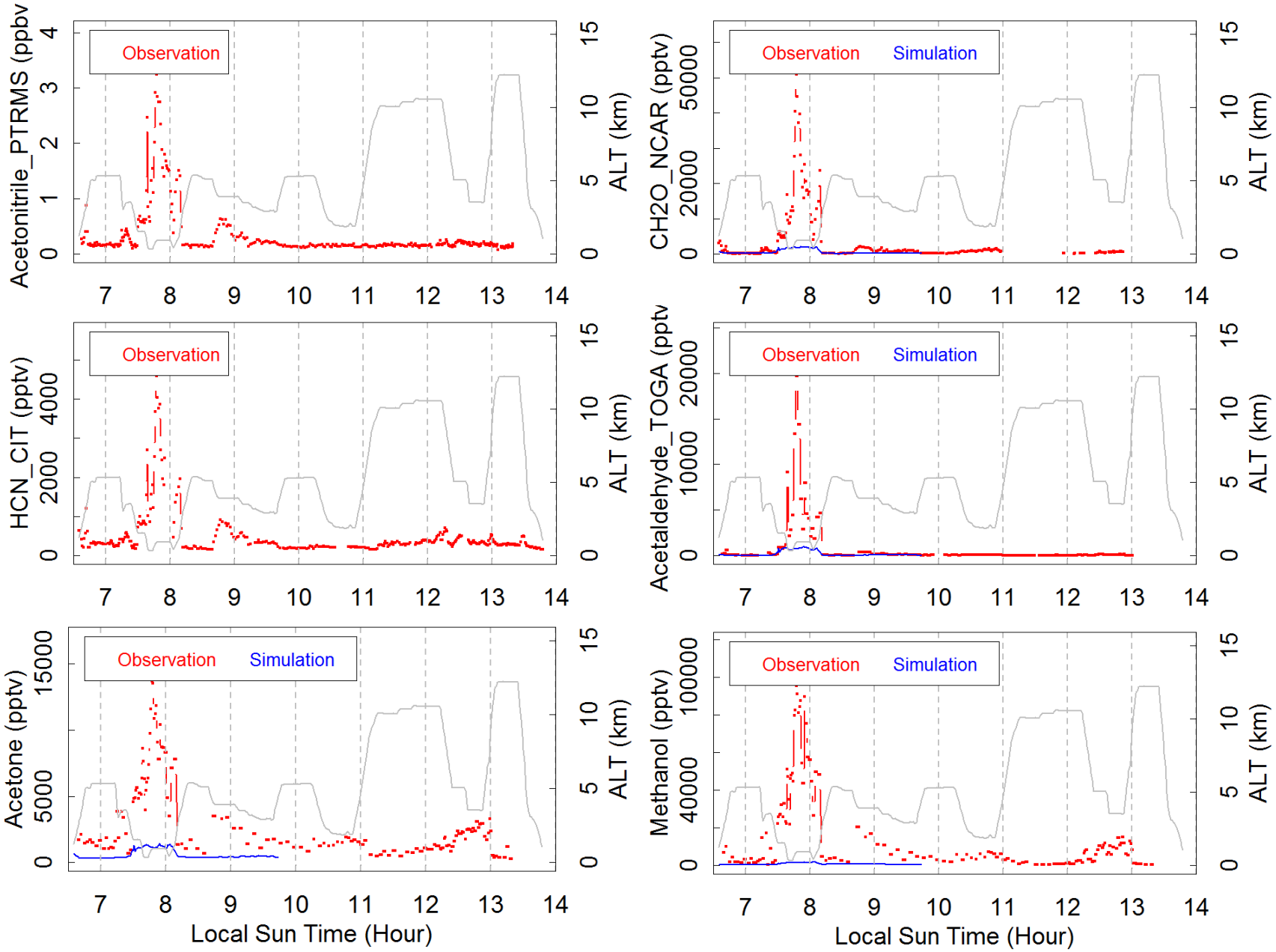


June 26, 2008

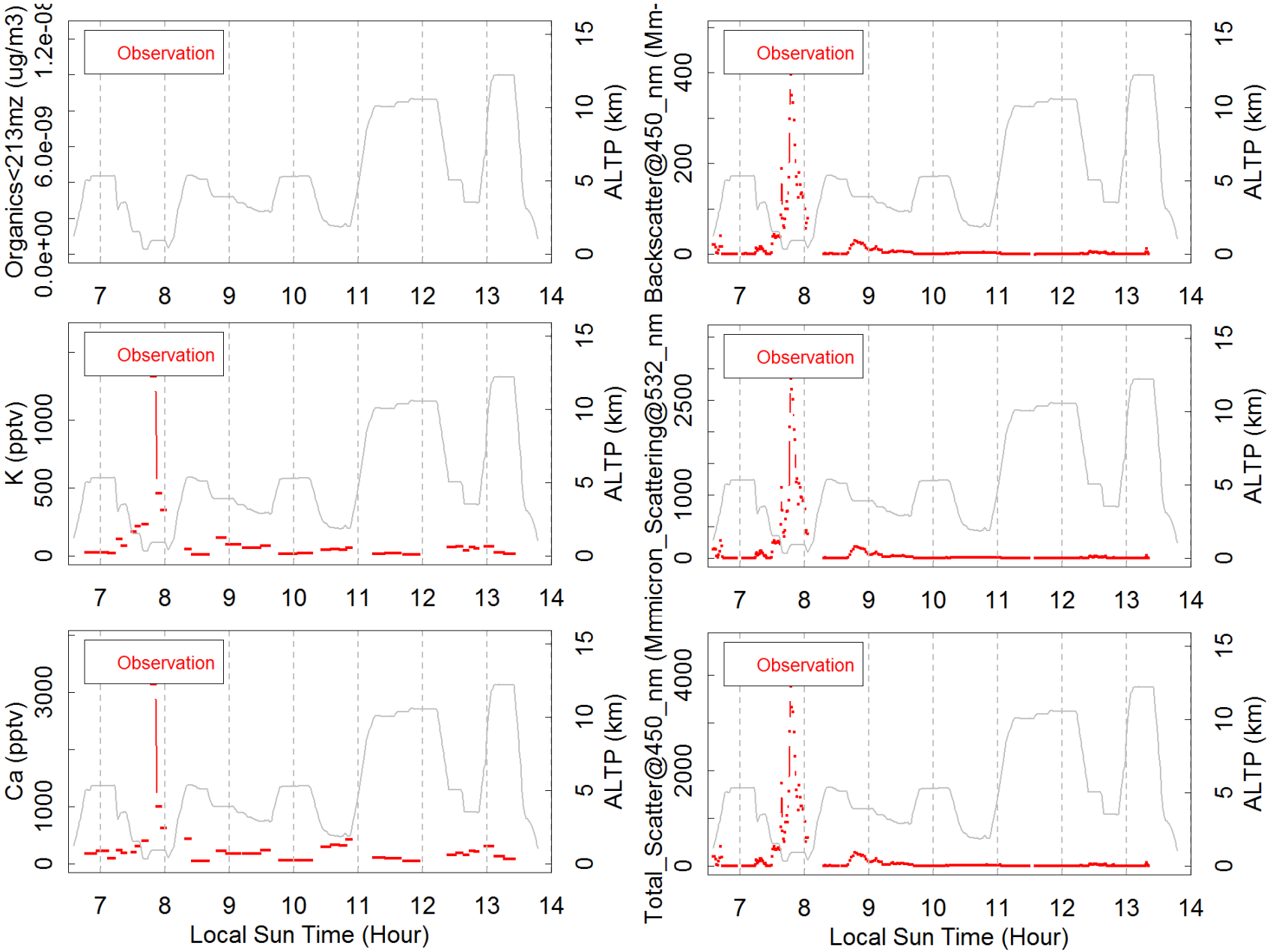
Terra/MODIS 18:30 UTC

Wildfire Signature

June 26, 2008



Wildfire Markers
June 26, 2008



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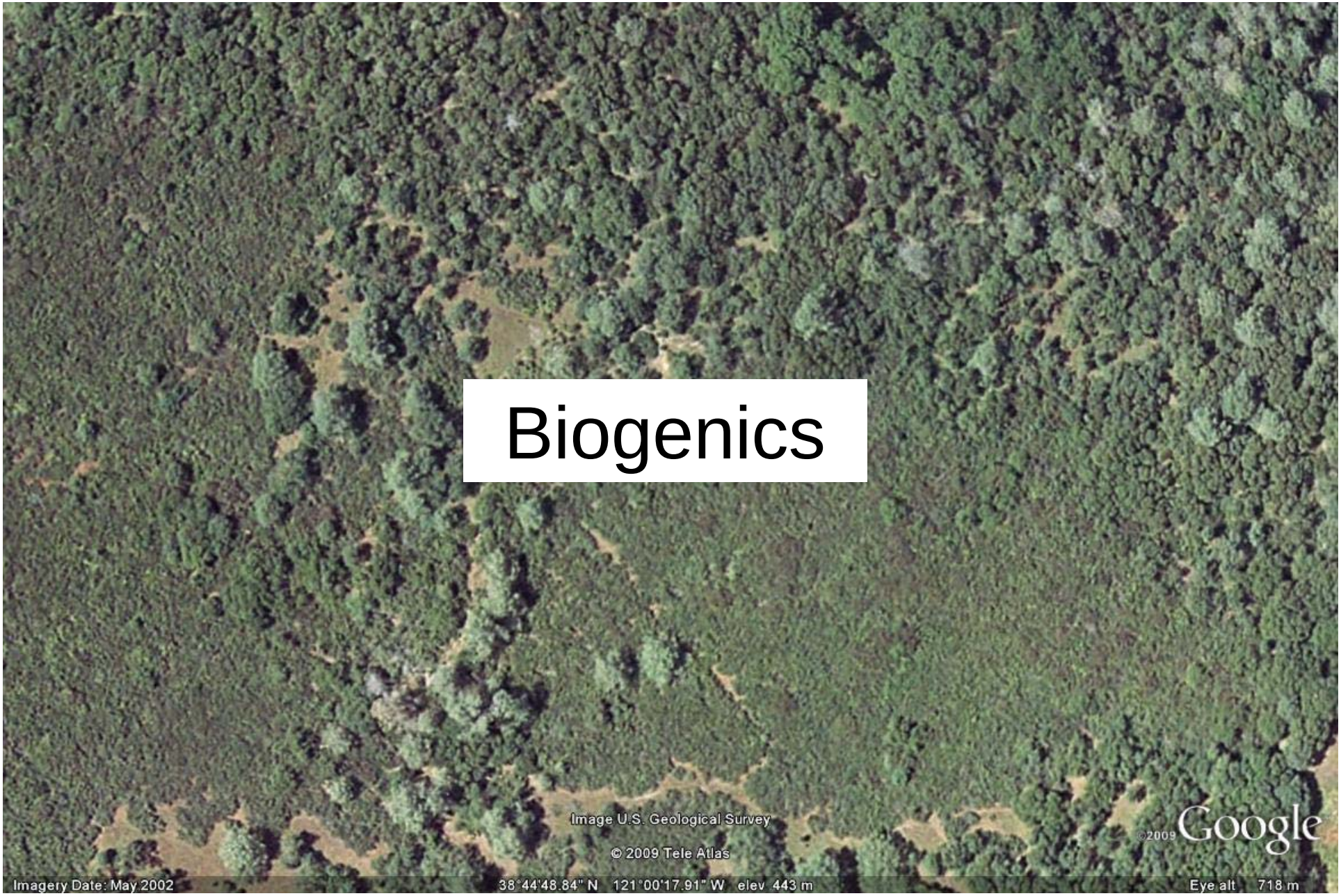
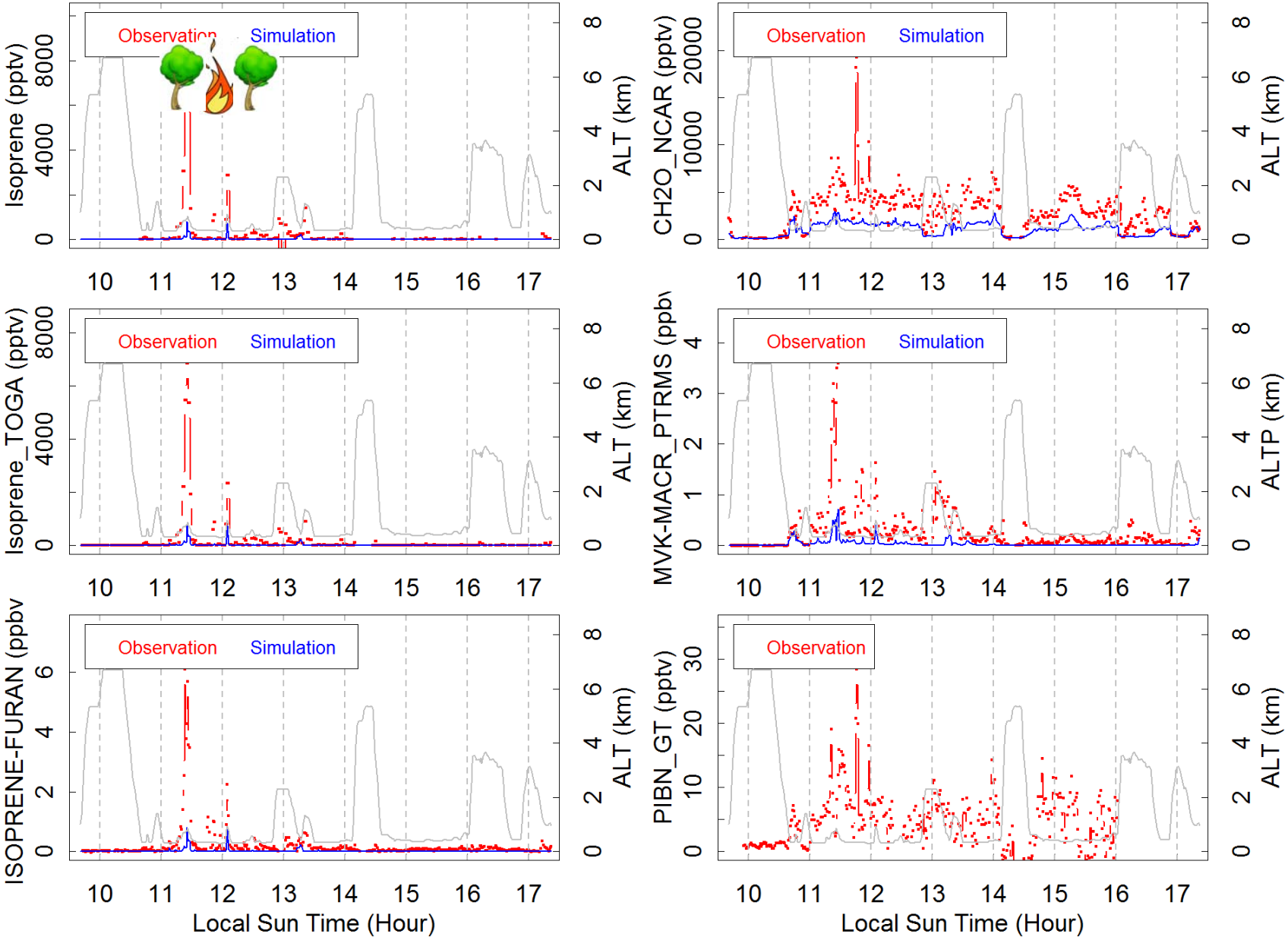
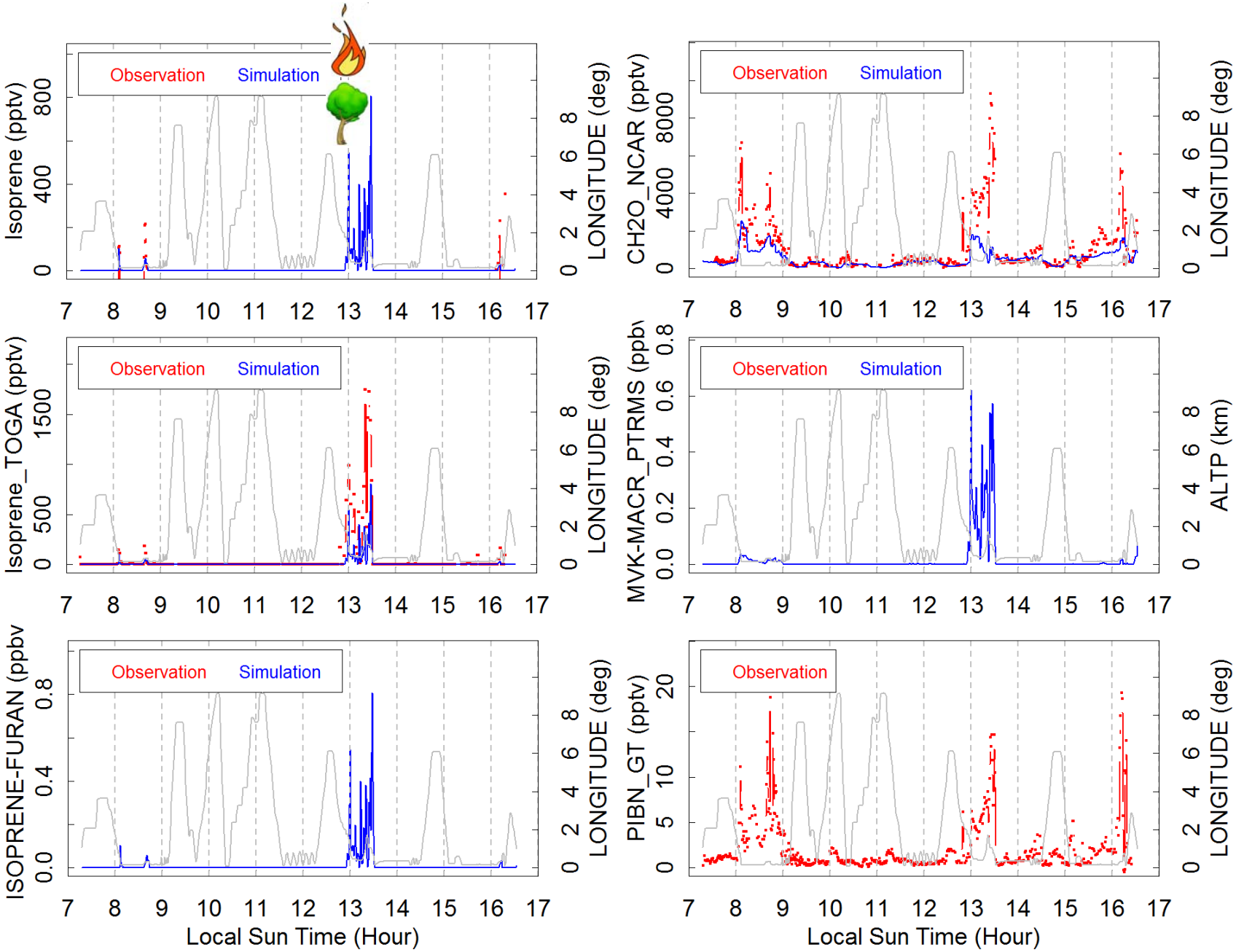

Biogenics
Image U.S. Geological Survey
© 2009 Tele Atlas
©2009 Google
Imagery Date: May 2002
38°44'48.84" N 121°00'17.91" W elev 443 m
Eye alt 718 m

Biogenics
June 20, 2008



Biogenics
June 22, 2008



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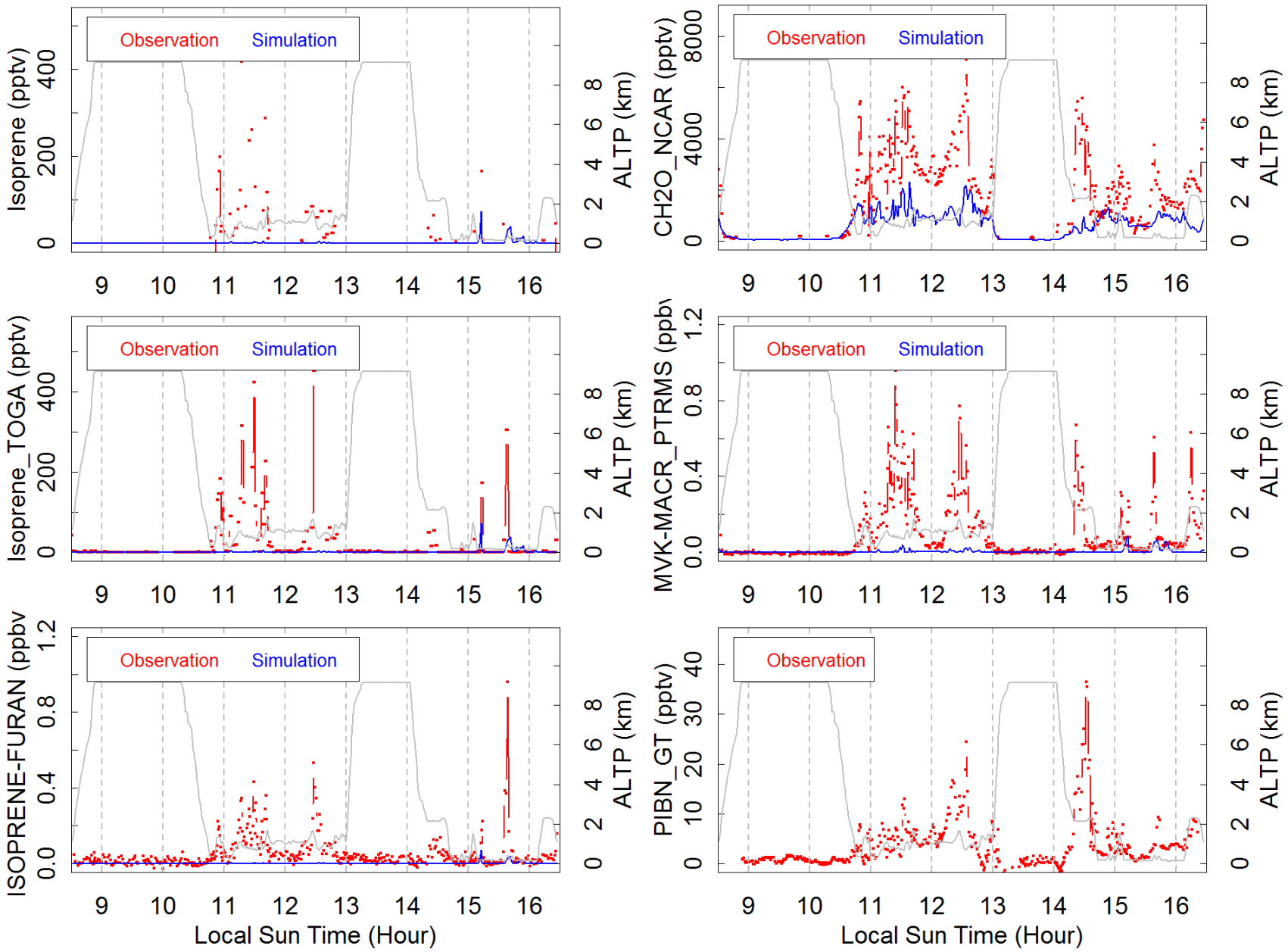

Biogenics
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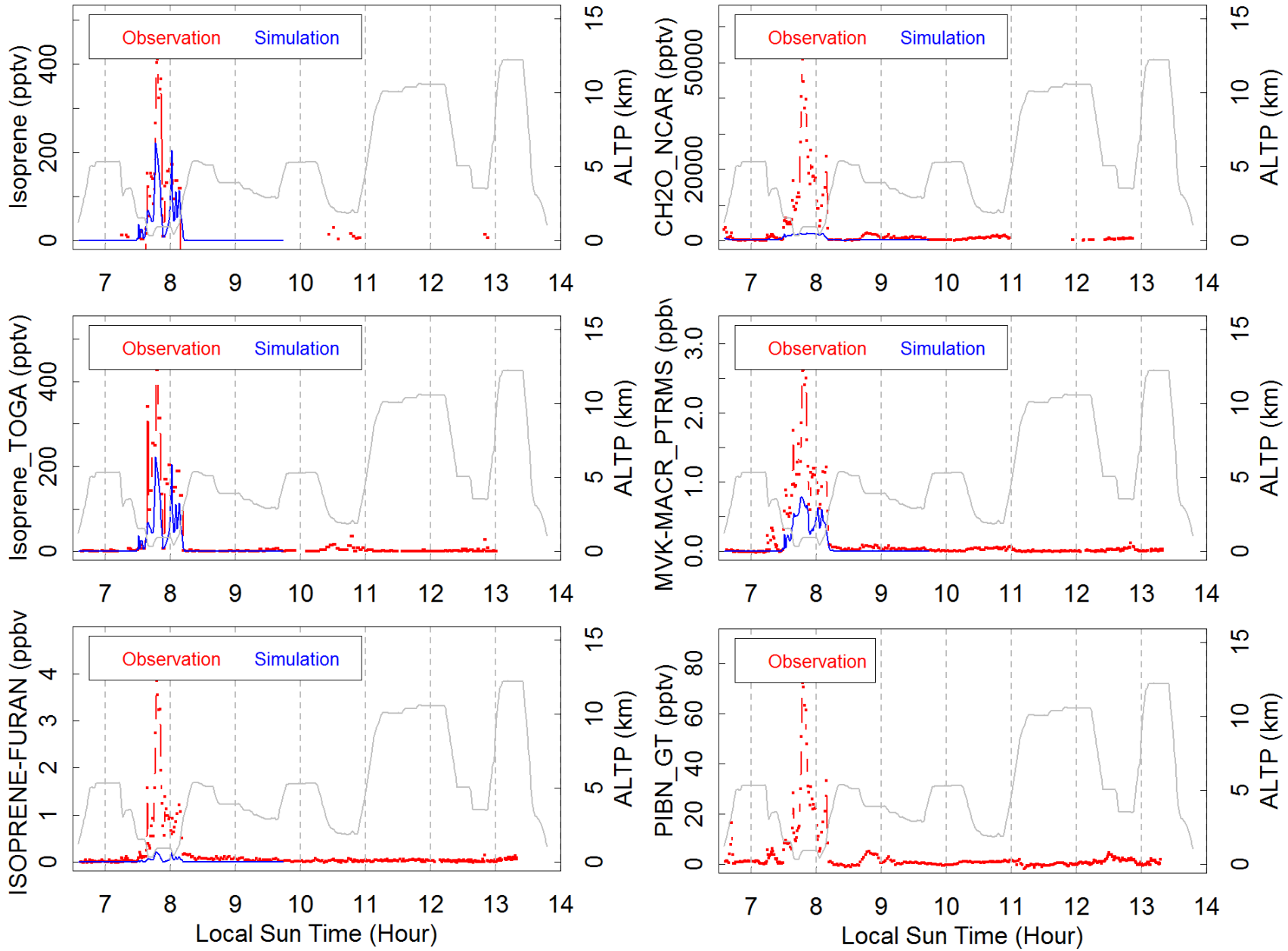
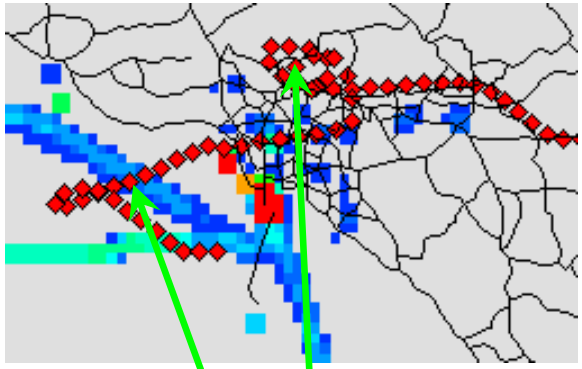
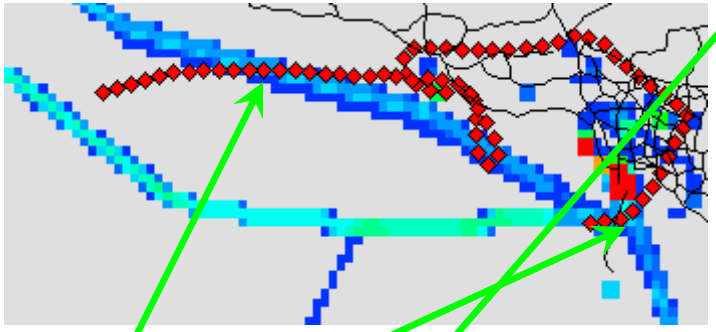


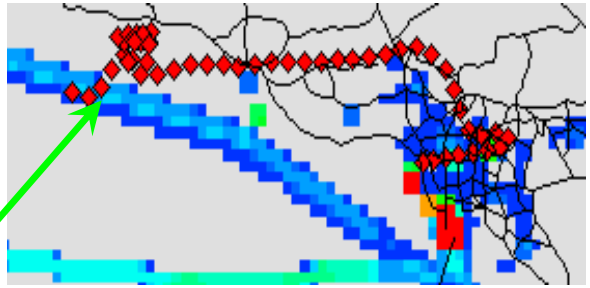
Sources of SO_2

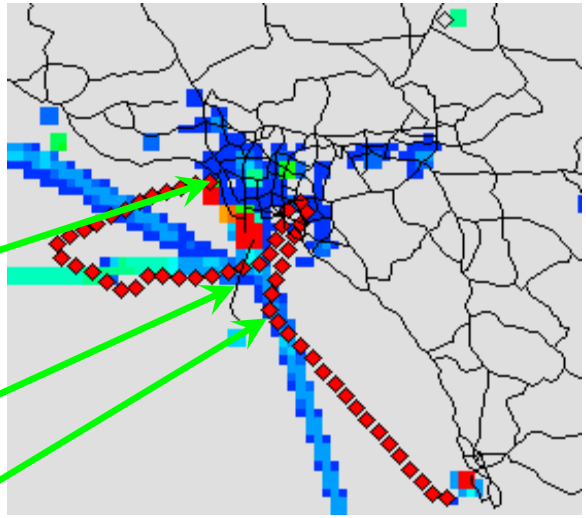
June 18, 2008

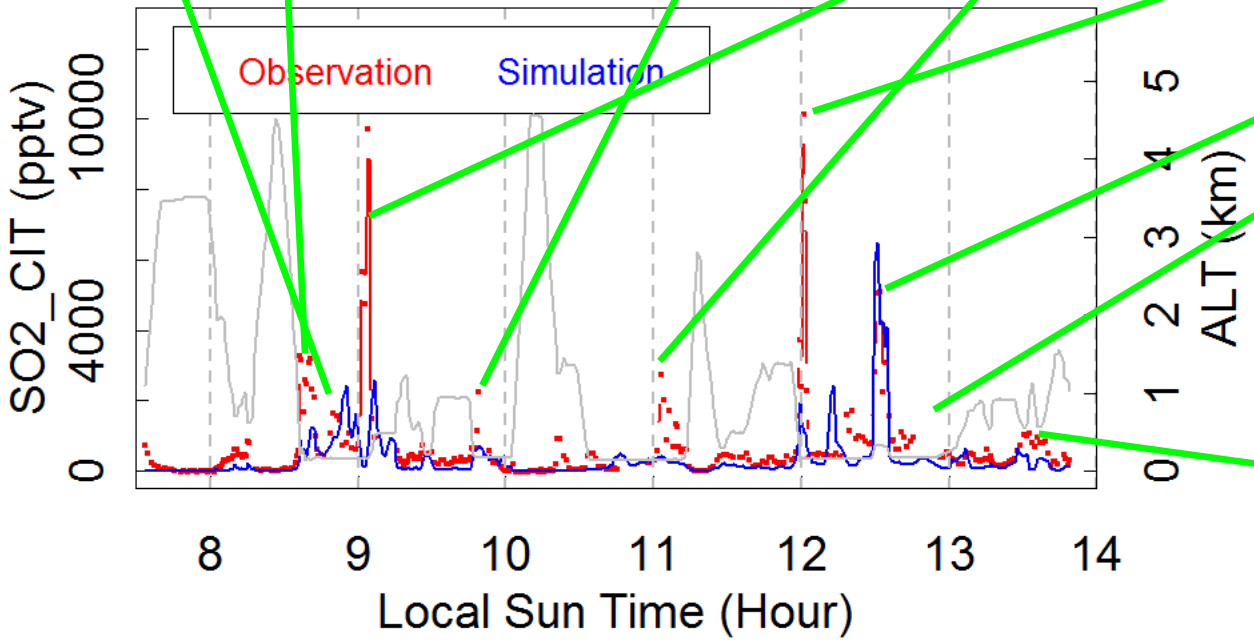
Sources of SO_2

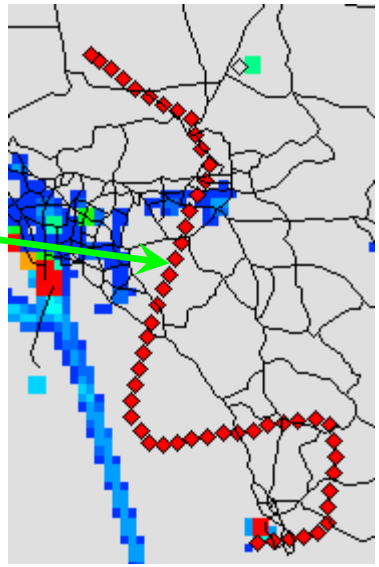




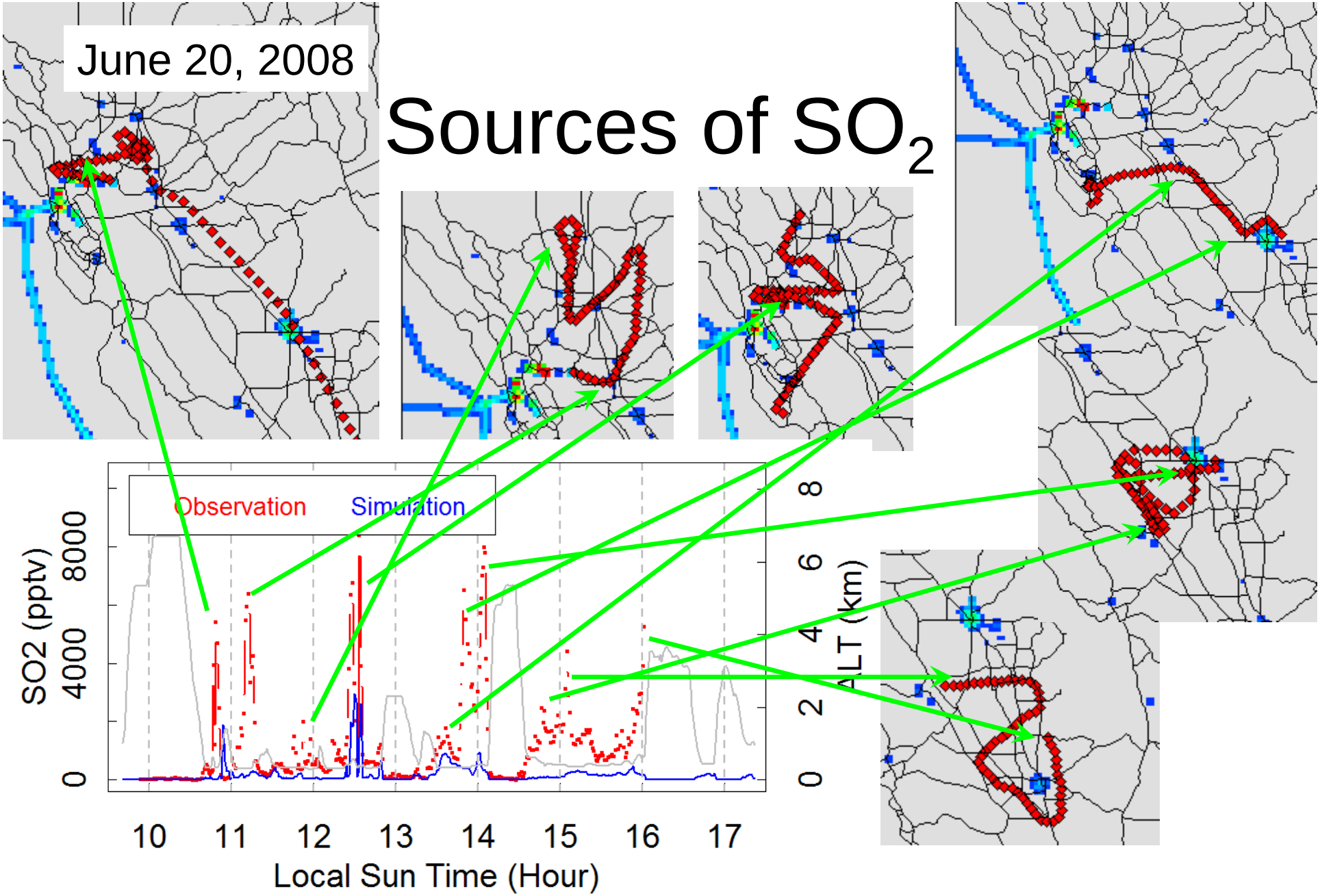








Sources of SO_2



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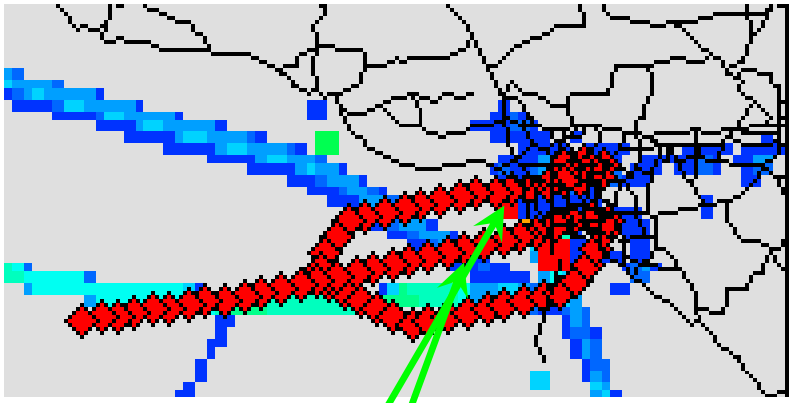
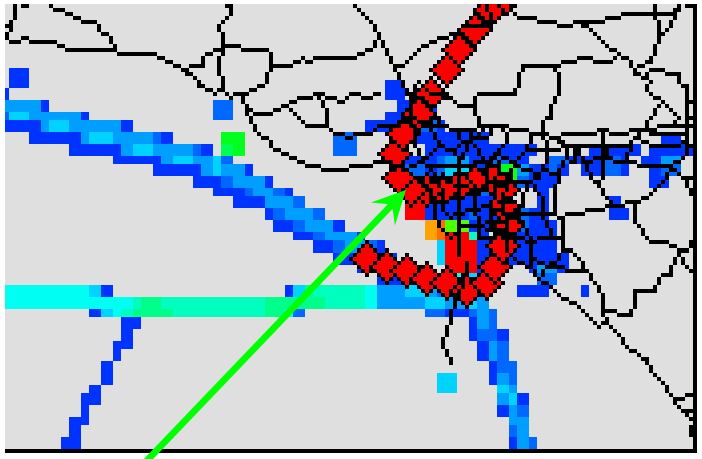
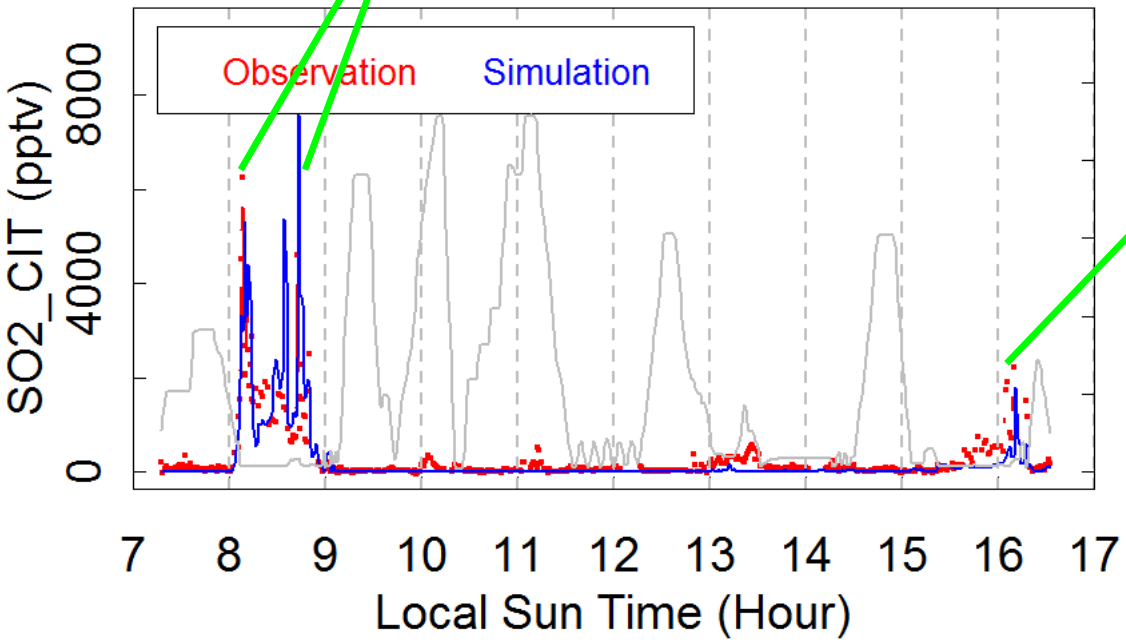
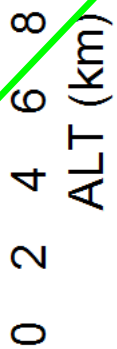
Sources of SO_2









June 24, 2008

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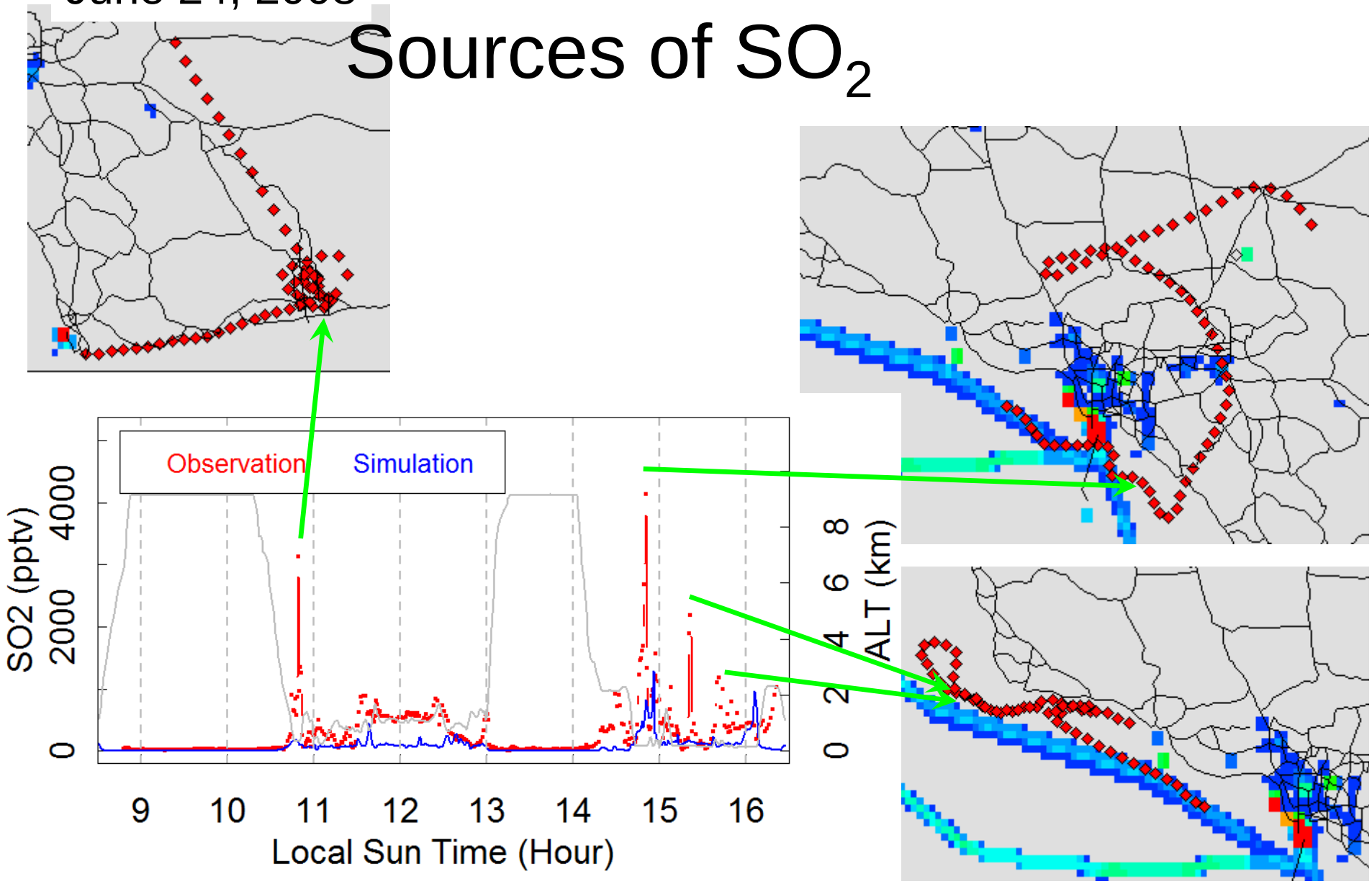

June 26, 2008

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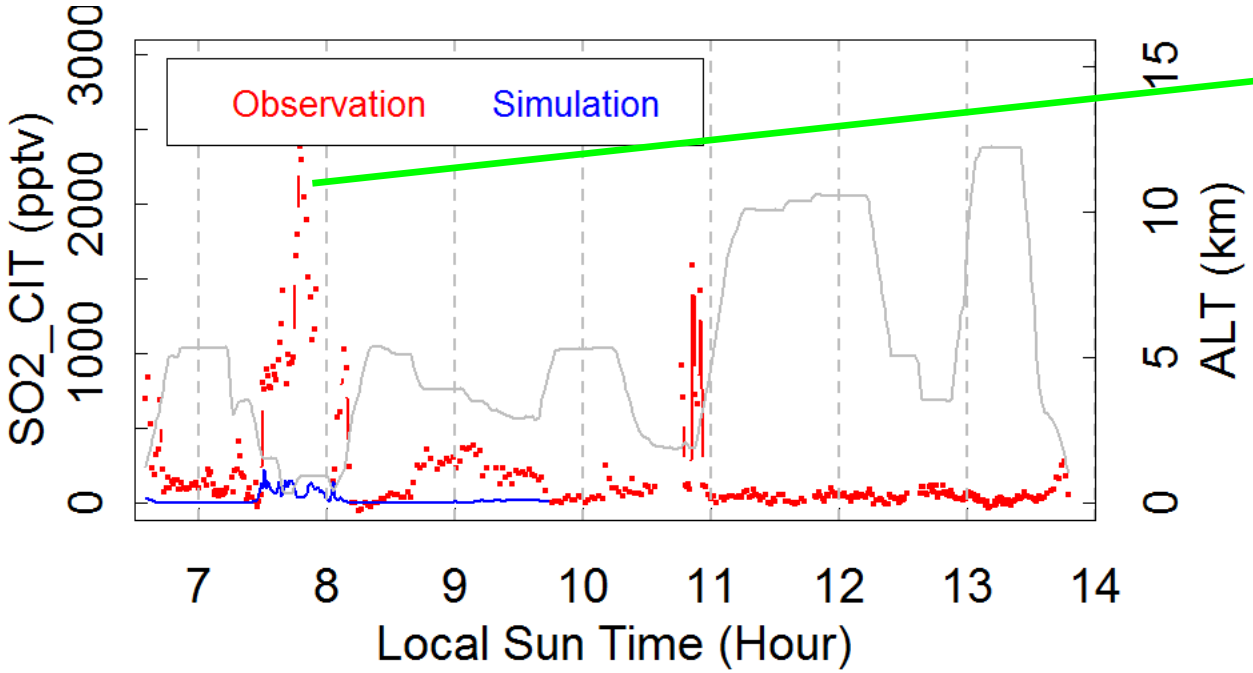
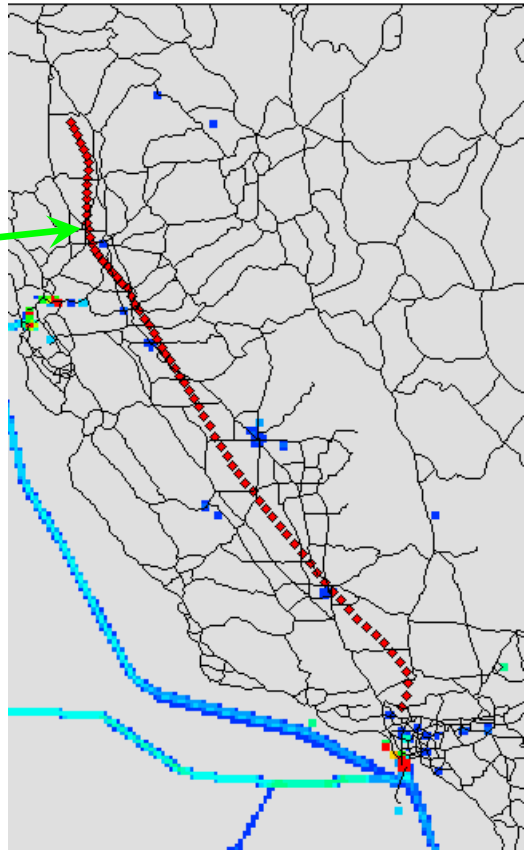
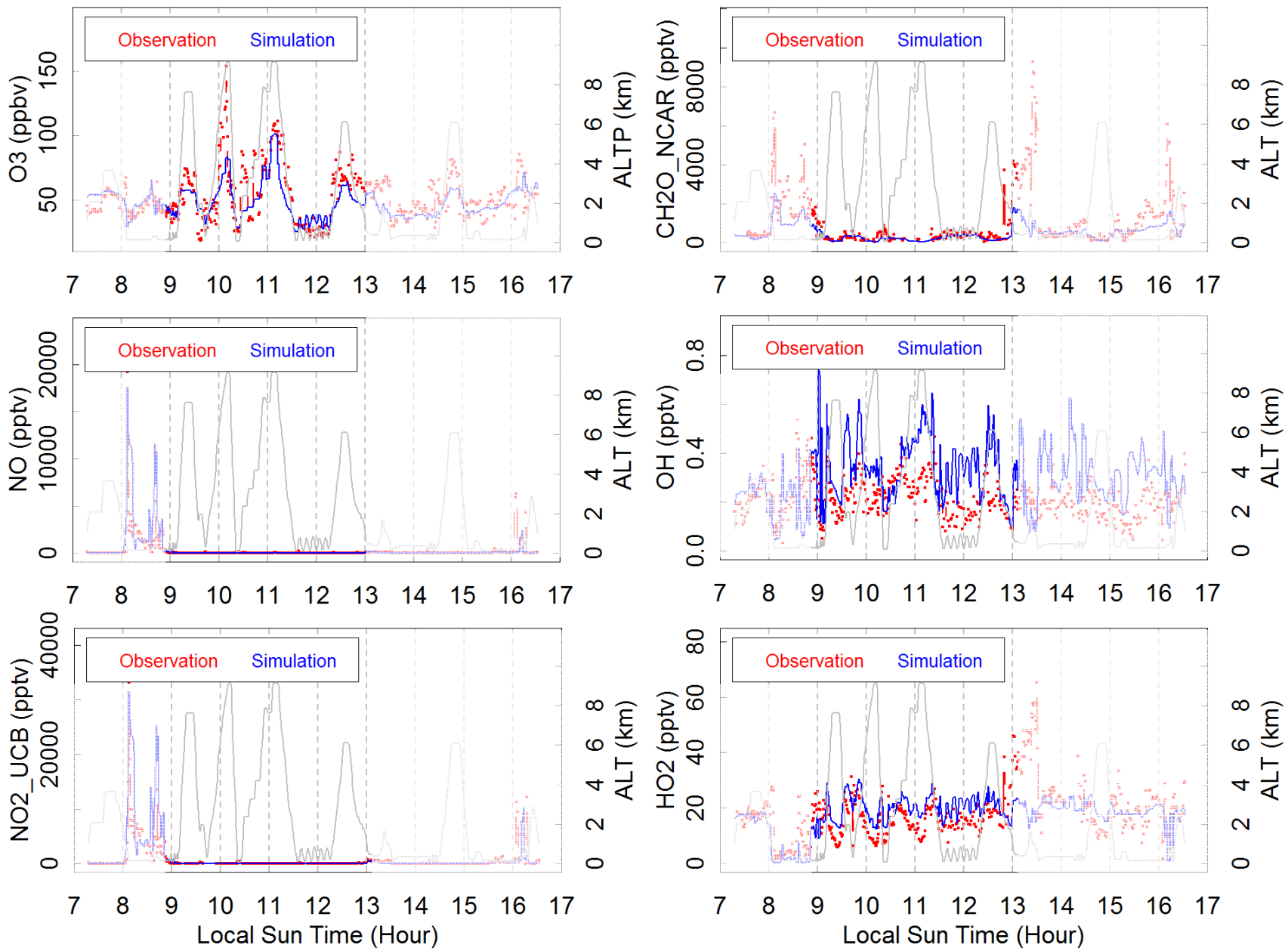




Boundary Conditions

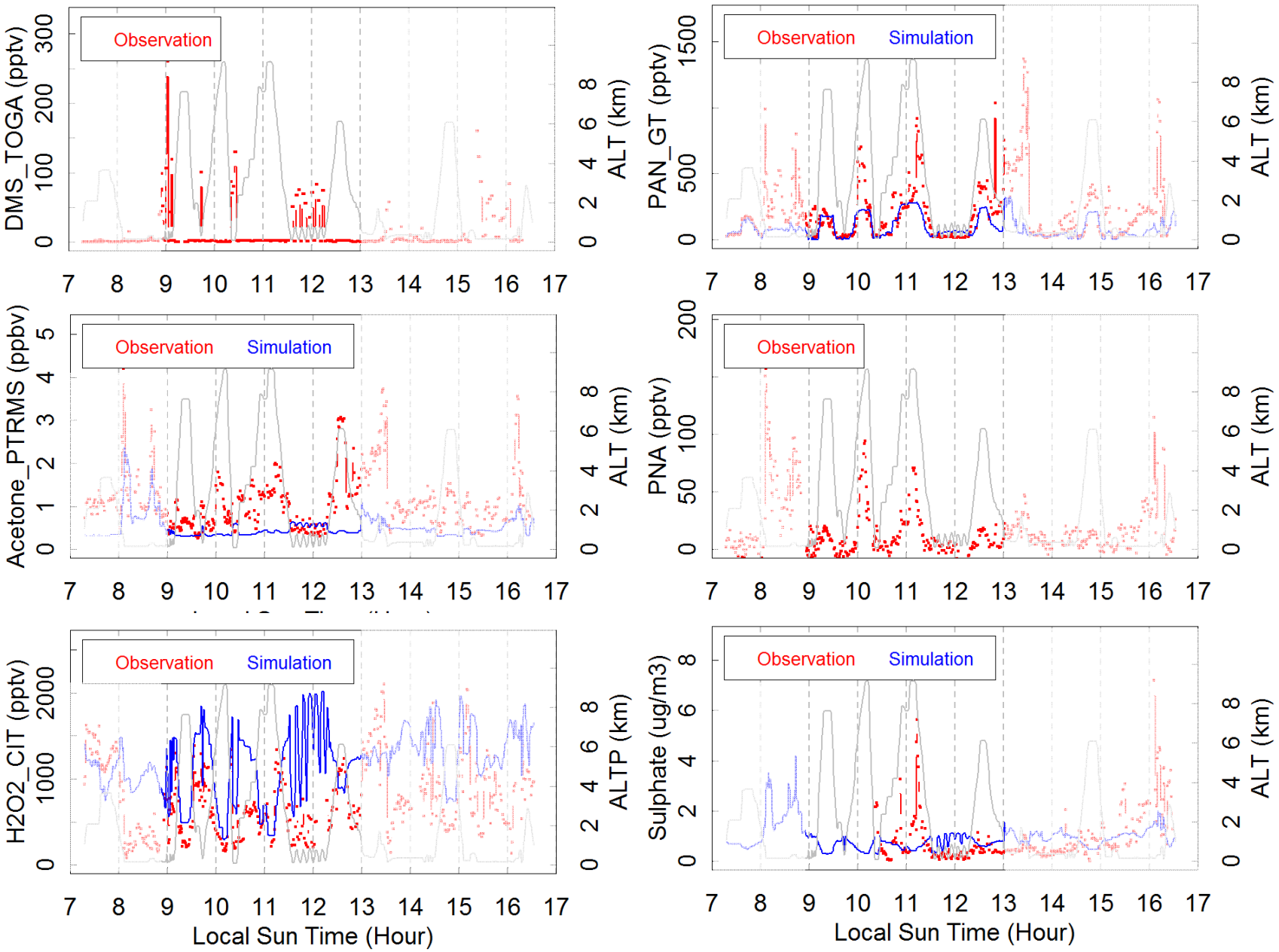
Boundary Conditions

June 22, 2008



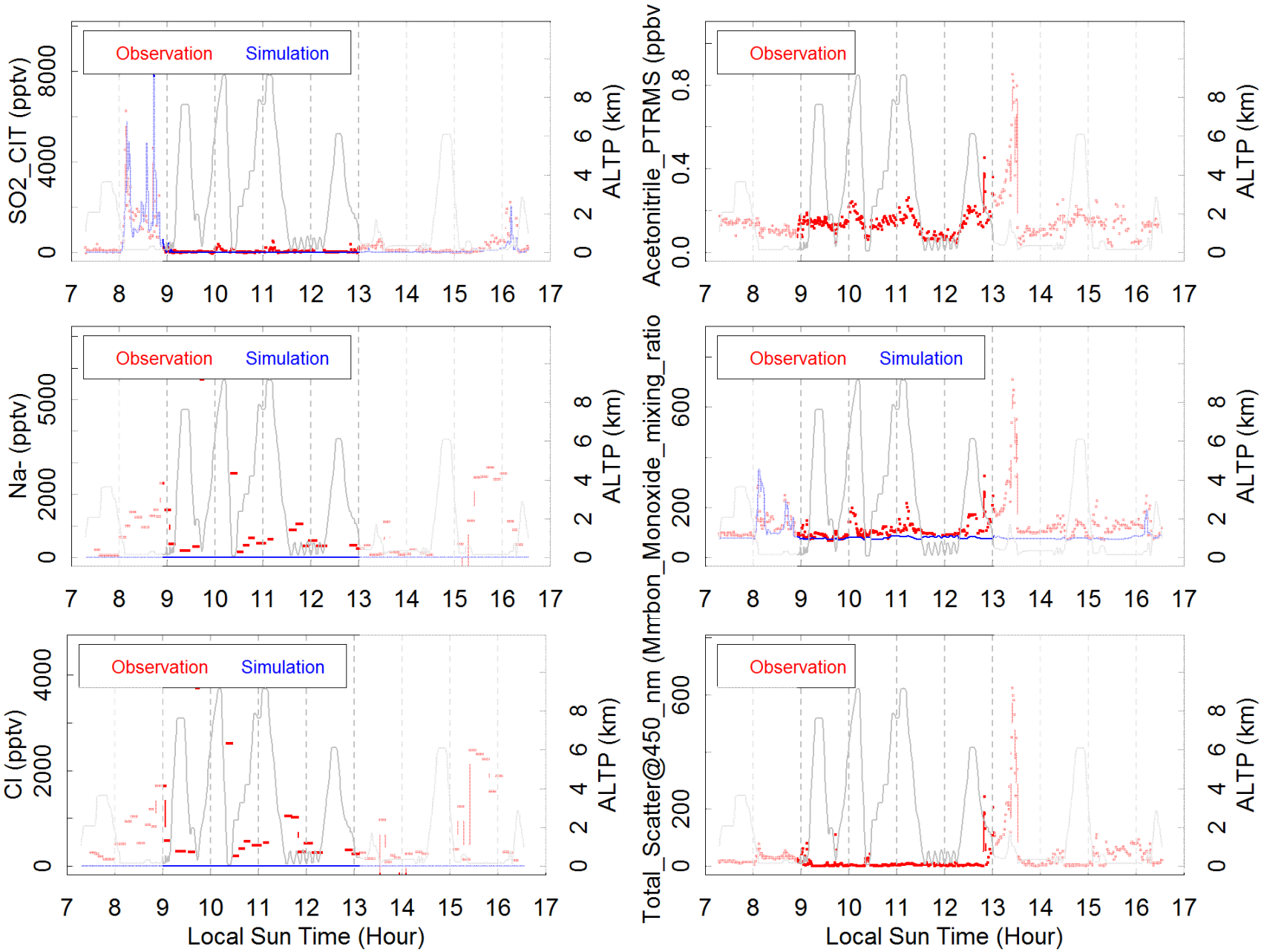
Boundary Conditions

June 22, 2008



Boundary Conditions

June 22, 2008



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What have We Learned?

- Aircraft measurements provide:
  - a way to evaluate 3-D spatial variations
  - indications of source locations and composition
  - possible ways to identify fire impacts on compliance monitors (useful in Exceptional Event Policy)
  - guidance on CalNex 2010 flight planning

Future Simulations

- MM5/WRF
  - analysis and observational nudging
- CMAQ
  - SAPRC99 with the additional chemical reactions to match observed species
- Emissions
  - Inclusion of fires
  - base year emissions for 2005 projected to 2008

Credits

- Fire cartoon: www.drawingcoach.com/cartoon-fire.html
- Wildfire: www.geog.umd.edu/.../wildfire_consumption.gif
- Terra/MODIS fire products: rapidfire.sci.gsfc.nasa.gov