Challenges in simulating high air pollution concentrations during persistent cold air pool events

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Motivation: pollution in valleys

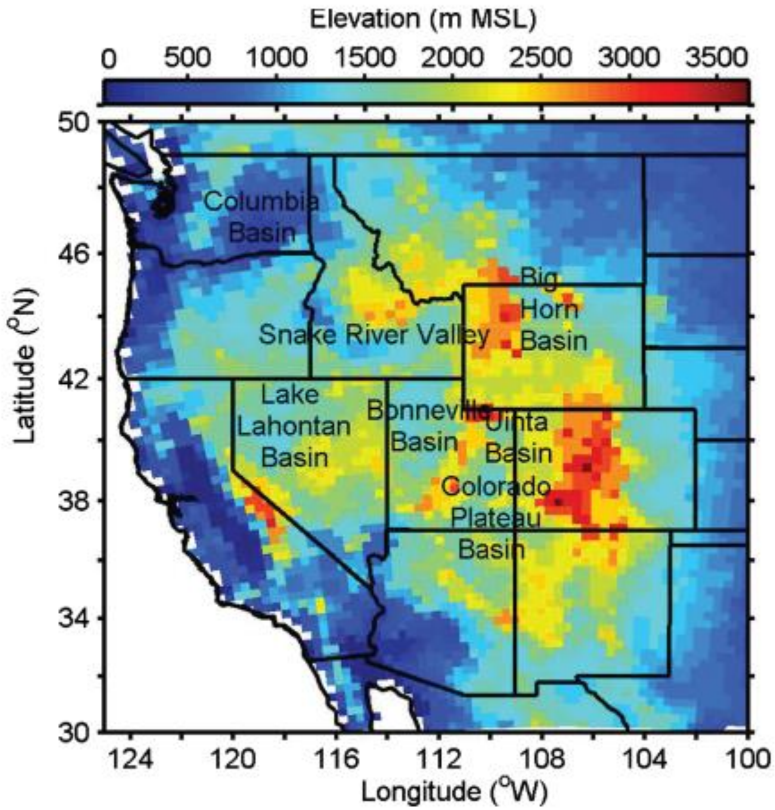
Cold air pool

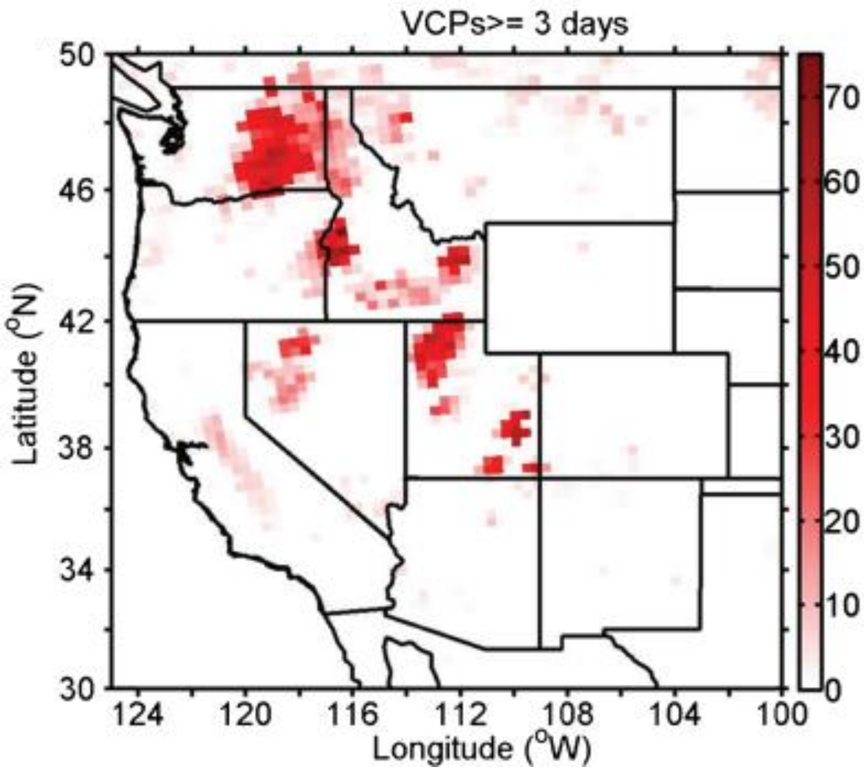
- Topographic depression with cold air
- During wintertime in mountain areas

Stratified layer of pollution during a "**cold pool**" event near Salt Lake City, Utah. Erik Crosman (photographed December 19, 2009) *(Baker et al. 2011)*

Persistent Cold Air Pools (PCAPs)

Total number of the occurrences of PCAPs ≥3 days during 1979 to 2012





(Yu et al. 2016)

Valley Heat Deficit

$$H22 = c_p \int_{sfc}^{2200} \rho(z)\,[\theta_{2200m} - \theta(z)]\,dz$$

- Bulk measure of atmospheric stability
- Energy per unit area (J m^{-2}) required to warm a column of air to the potential temperature at height z.

c_p: specific heat capacity of air;

ρ: air density

θ: potential temperature;

z: altitude

The Persistent Cold Air Pool Study

(Utah, 2010-2011, PIs: C. David Whiteman et al.)

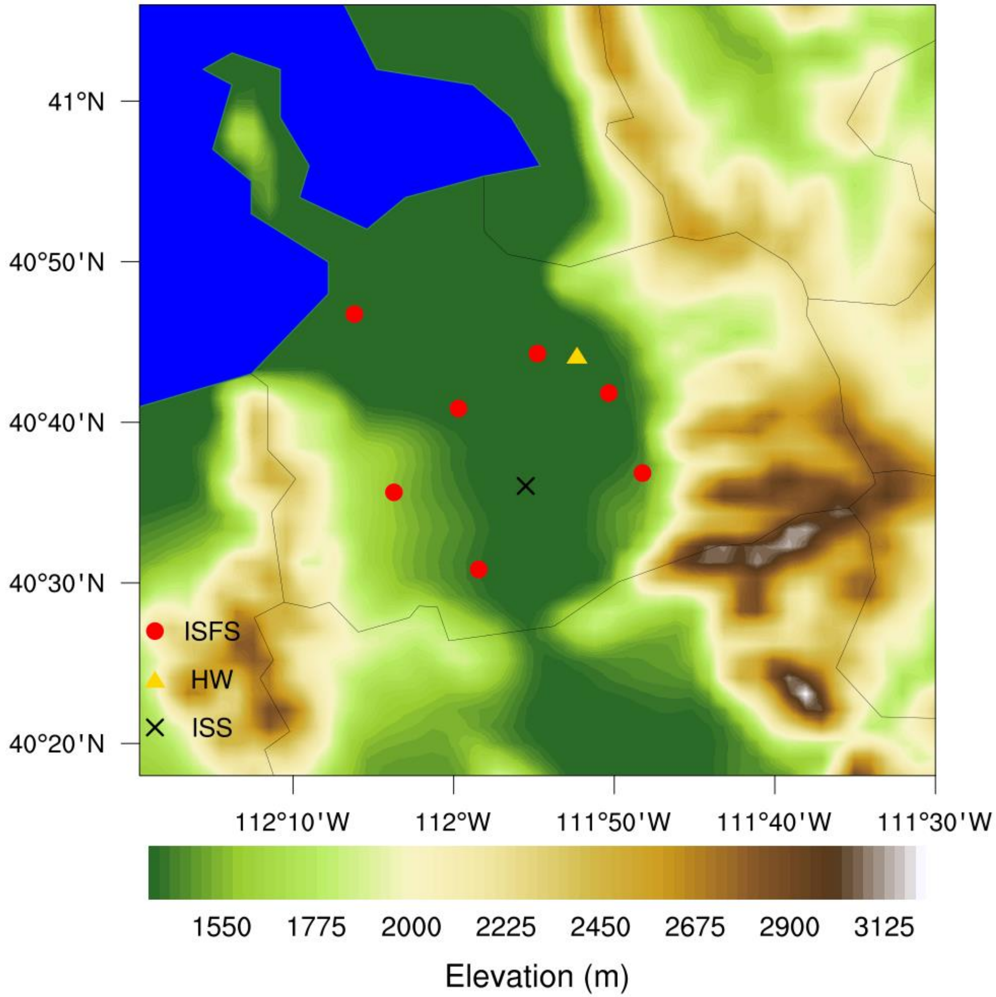


Figure 1 Topography map of SLV and measurement sites

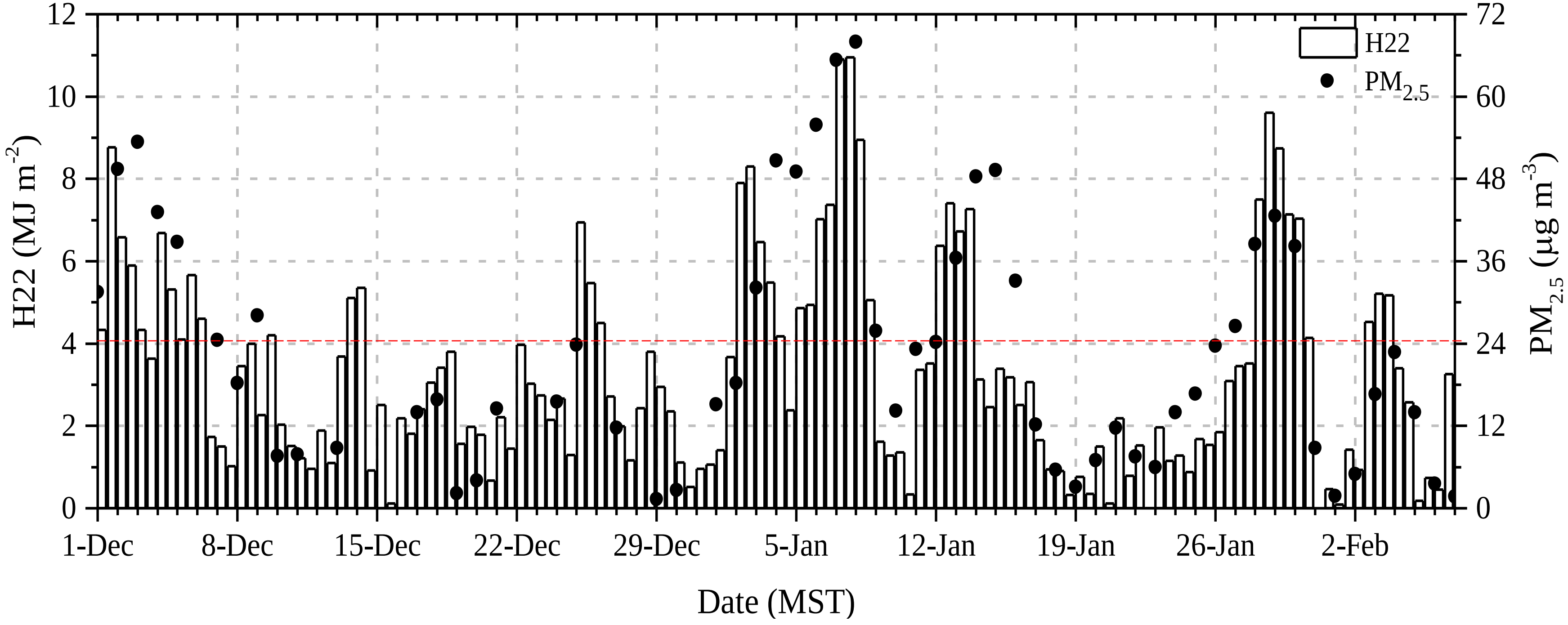
Focusing on meteorology

ISFS: surface energy balance
HW: routine air quality site
ISS: sounding site

(Sun et al. 2019)

The Persistent Cold Air Pool Study

PCAP: H22 > 4.04 MJ m^{-2} lasting for more than one day *(Whiteman 2014)*



Valley heat deficit: $H22 = c_p \int_{sfc}^{2200} \rho(z)\,[\theta_{2200m} - \theta(z)]\,dz$

CAPs are accompanied by high PM$_{2.5}$ *(Sun et al. 2019)*

WRF Model Configurations (v3.7)

- Microphysics: Thompson scheme
- Longwave radiation: RRTM
- Shortwave radiation: Dudhia
- Convective precipitation: Kain-Fritsch 2
- Lage-scale forcing dataset: NAM reanalysis with 3-hr forecasting
- Observational nudging: Outer domain

Experiment	Surface Layer Scheme	Land Surface Model	Planetary Boundary Layer Scheme
NAM_ACM2	Pleim-Xiu (Pleim 2006)	Pleim-Xiu (Pleim and Xiu 1995)	ACM2 (Pleim 2007)
NAM_YSU	Revised MM5 (Jiménez et al. 2012)	Noah (Ek et al. 2003)	YSU (Hong et al. 2006)
NAM_MYJ	Eta similarity (Janić 2001)	Noah	MYJ (Janić 2001)
NAM_MYNN	MYNN (Nakanish 2001)	Noah	MYNN (Nakanishi and Niino 2004)

CMAQ Model Configurations (v 5.2)

The Community Multiscale Air Quality Modeling System, (U.S. EPA)

- **Resolution:** d01: 12km, d02: 4km, 41 vertical layers
- **Emissions:** 2011 National Emissions Inventory (Kirk Baker, U.S. EPA)
- **Mechanism:**

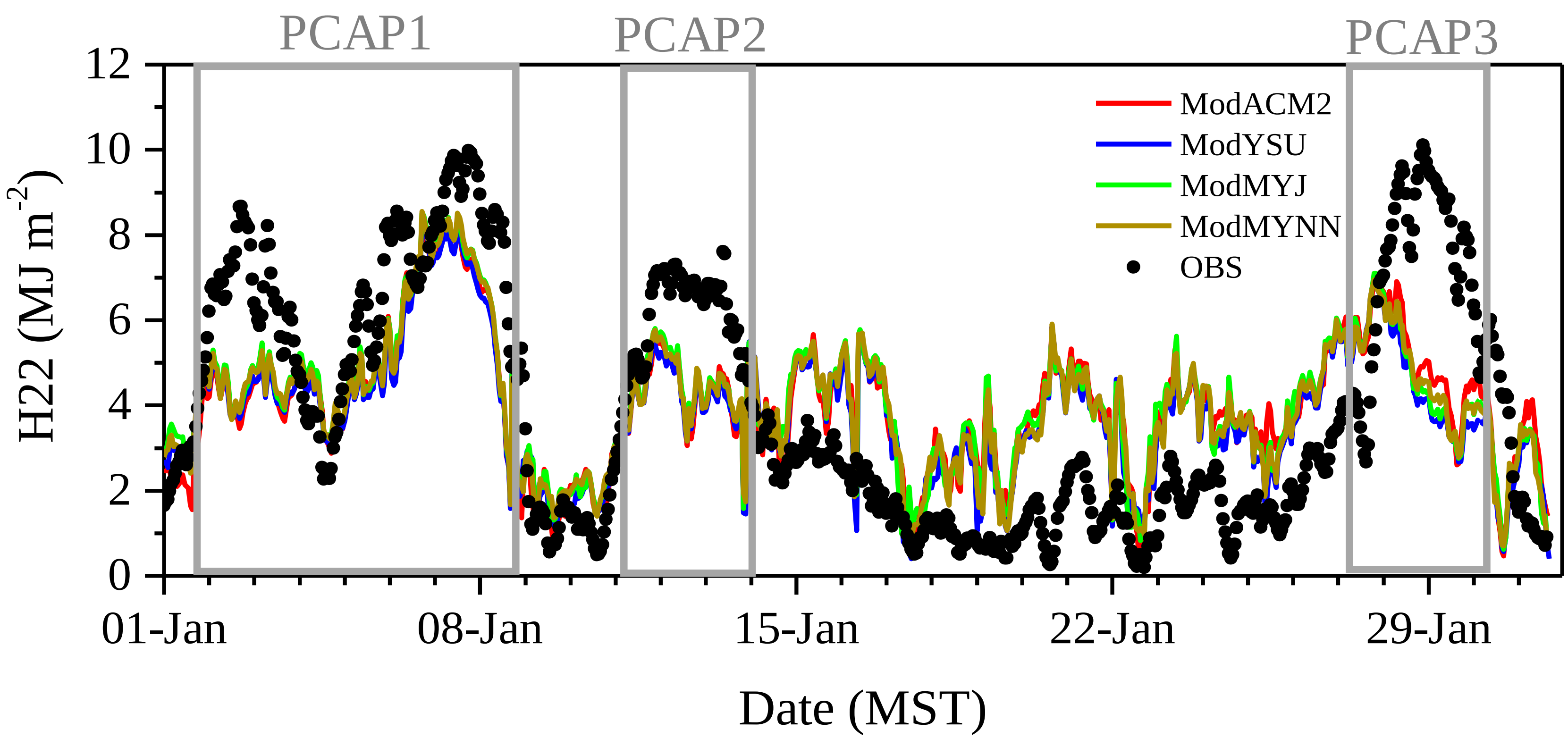
  --Carbon bond 6 (CB6), revision 3 gas-phase mechanism

  --sixth-generation CMAQ aerosol mechanism with sea salt and speciated PM other

  --aqueous phase chemistry

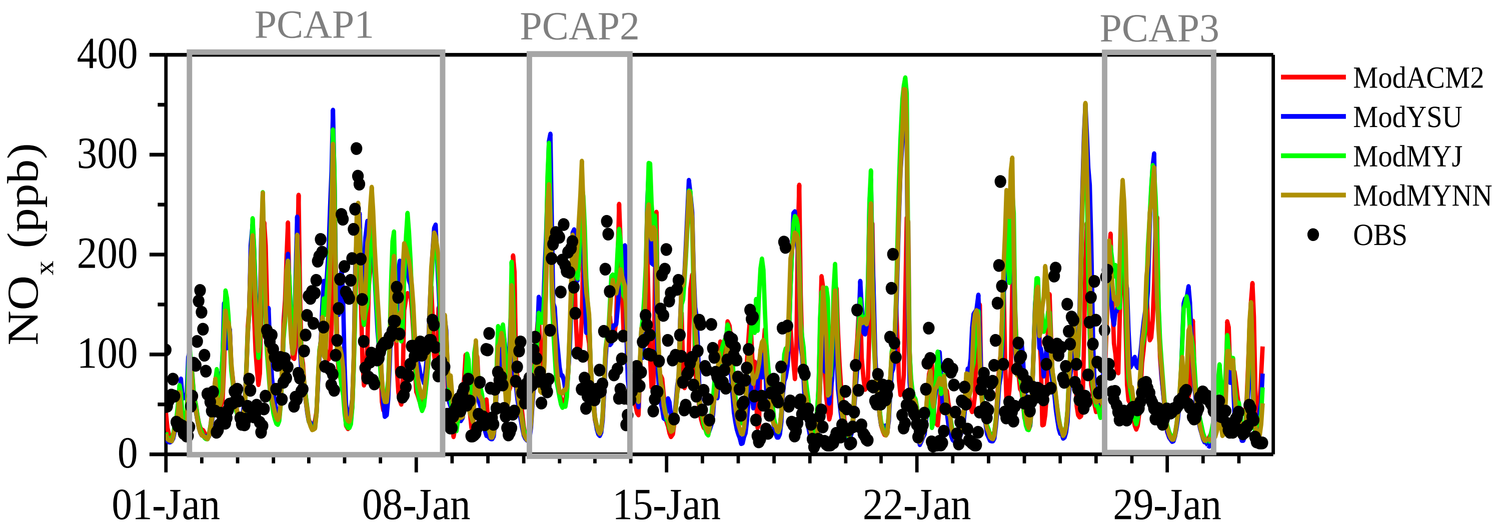
Valley heat deficit (H22) in Jan 2011

PCAP: H22 > 4.04 MJ m^{-2} lasting for more than one day *(Whiteman 2014)*

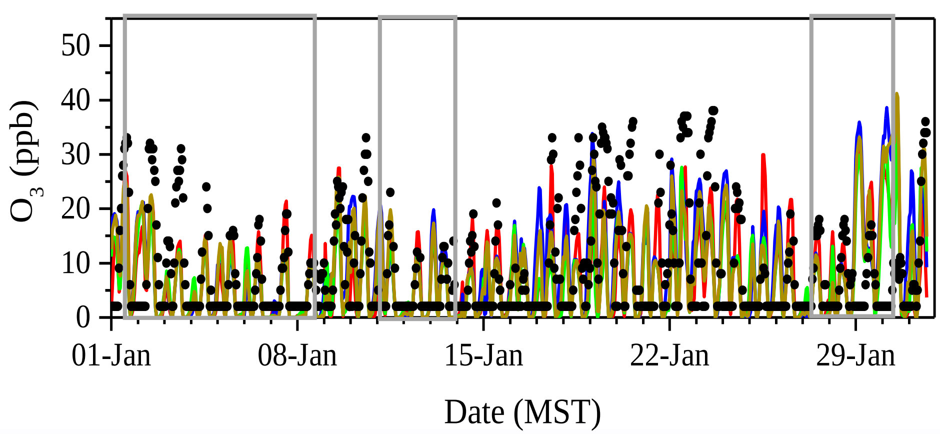


Gaseous Pollutants

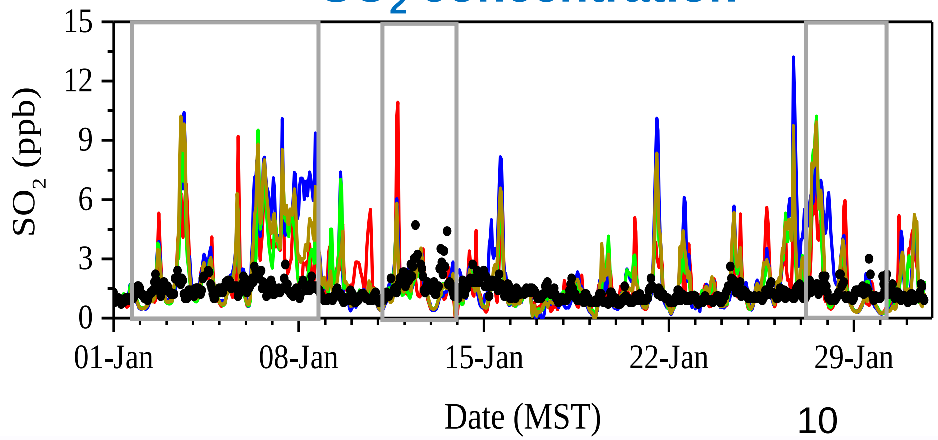
NOx concentration



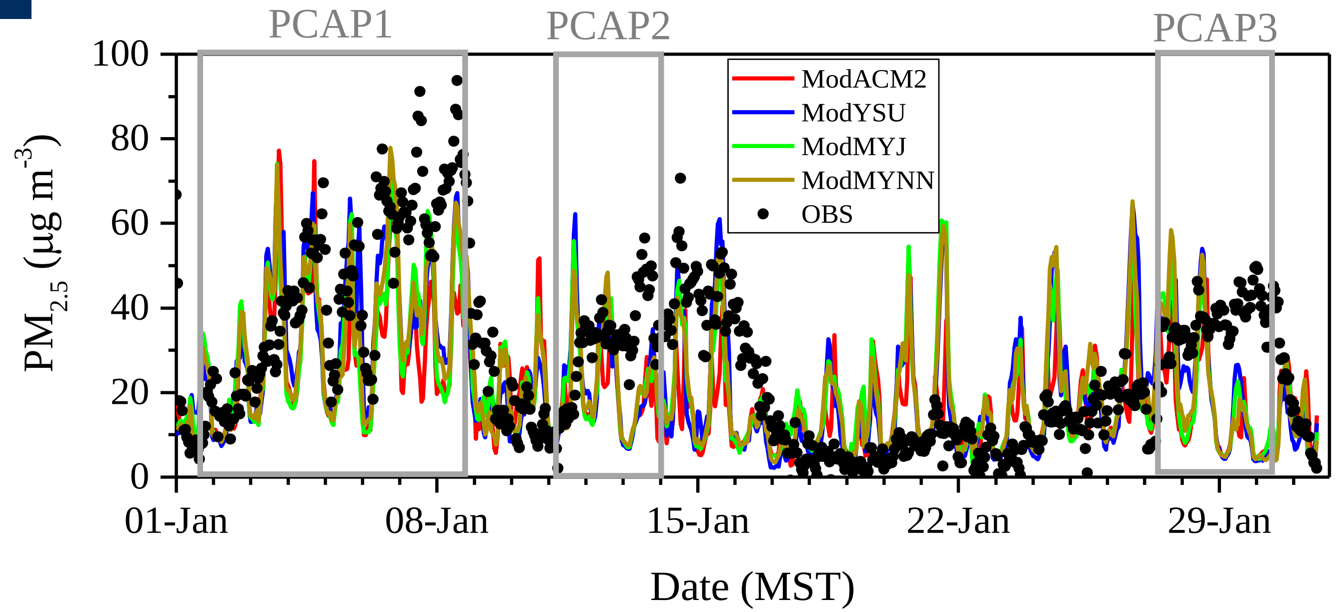
Ozone concentration



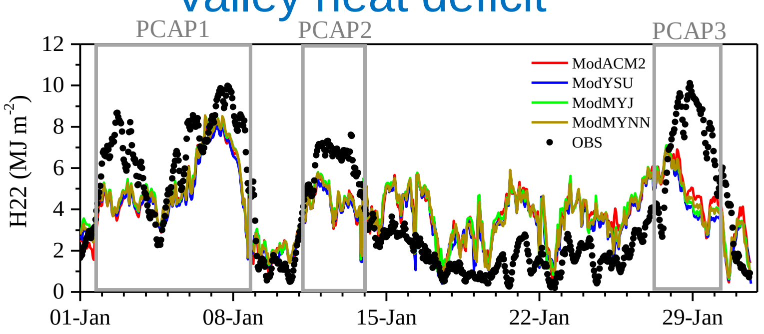
SO_2 concentration



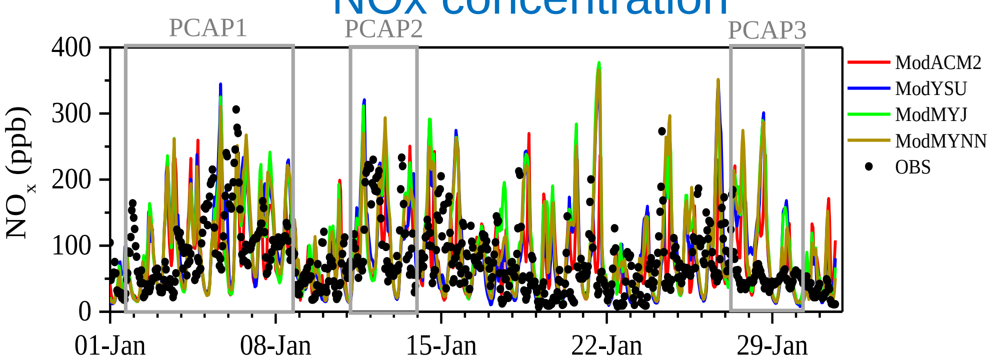
$PM_{2.5}$ mass concentration



Valley heat deficit



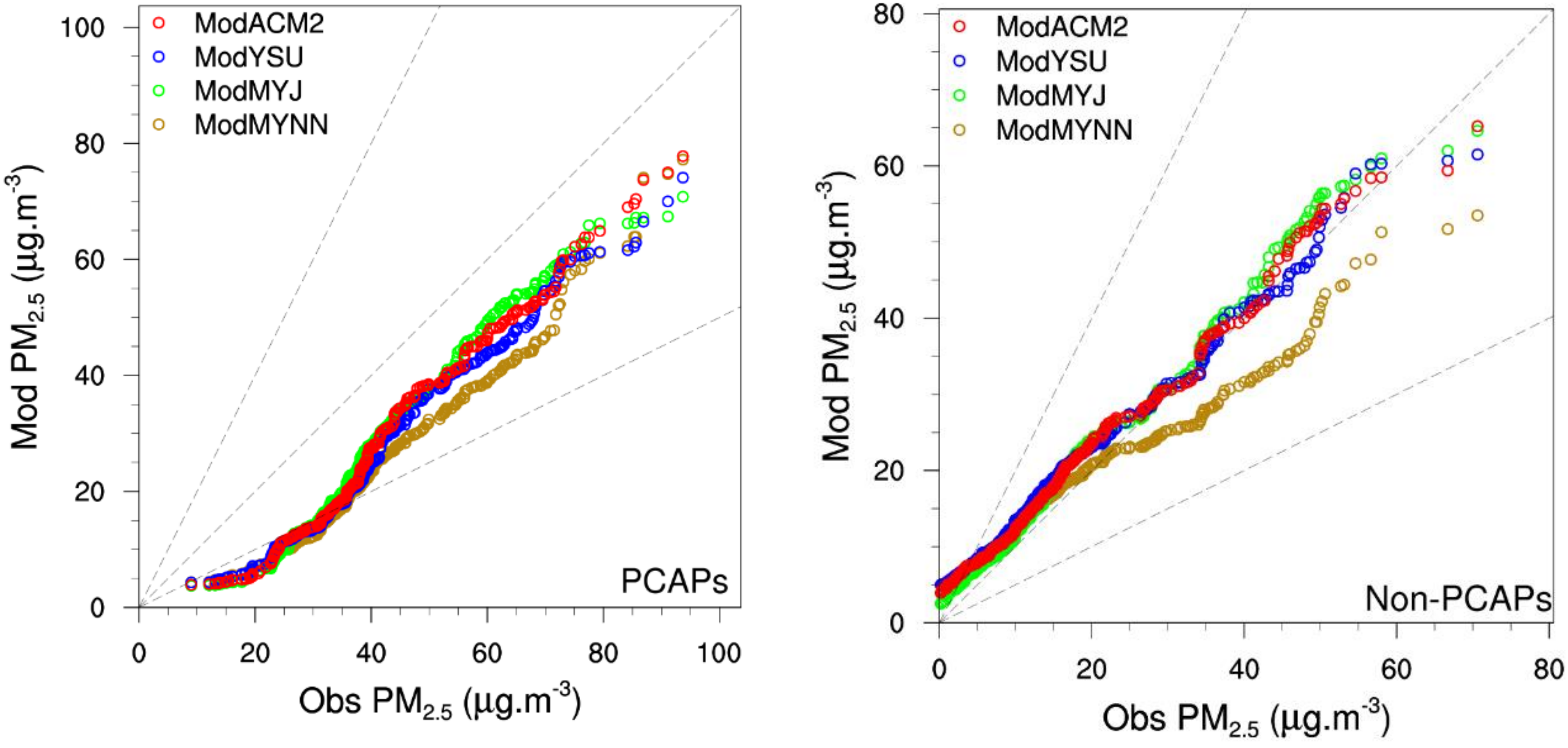
NOx concentration



- Overestimated NOx and H22 contribute to overestimated $PM_{2.5}$ during non-PCAPs
- High $PM_{2.5}$ during PCAP3 was attributed to high H22

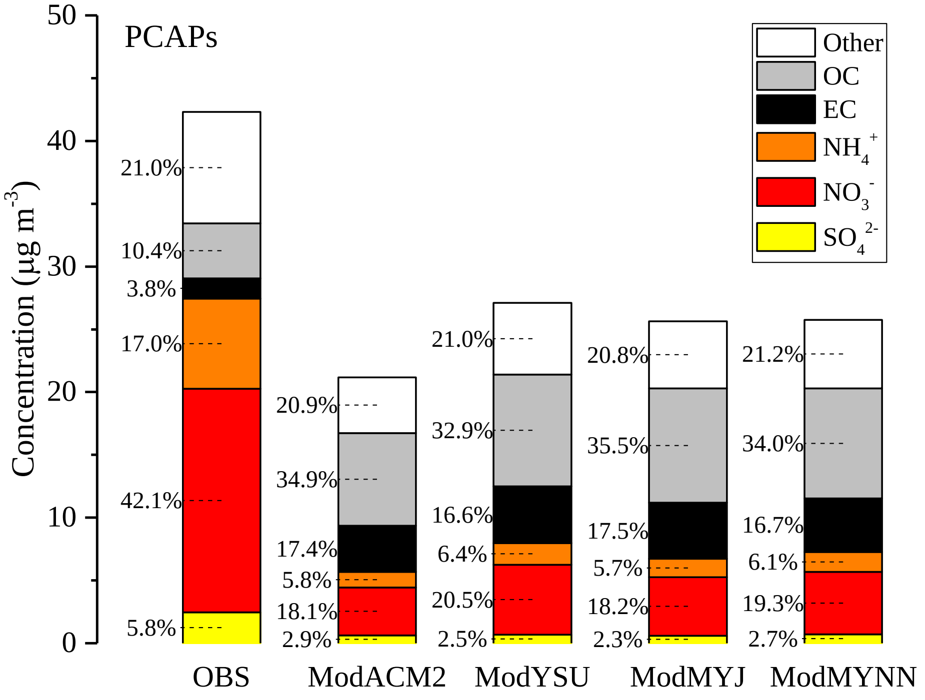
Quantile-Quantile plot (probability)

modeled vs observed $PM_{2.5}$ concentration

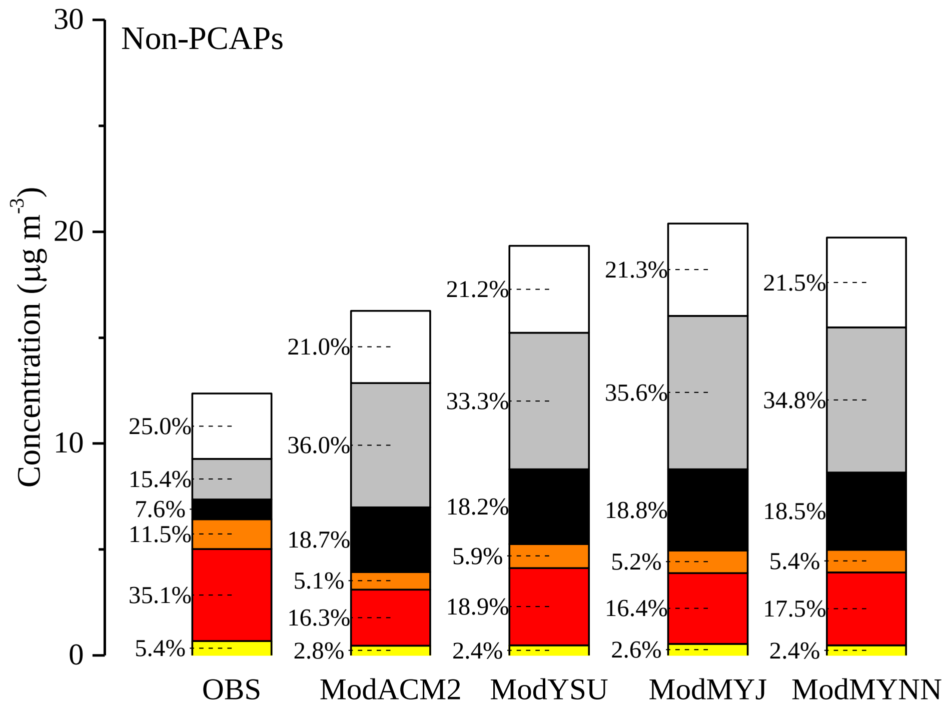


$PM_{2.5}$ chemical composition

PCAPs



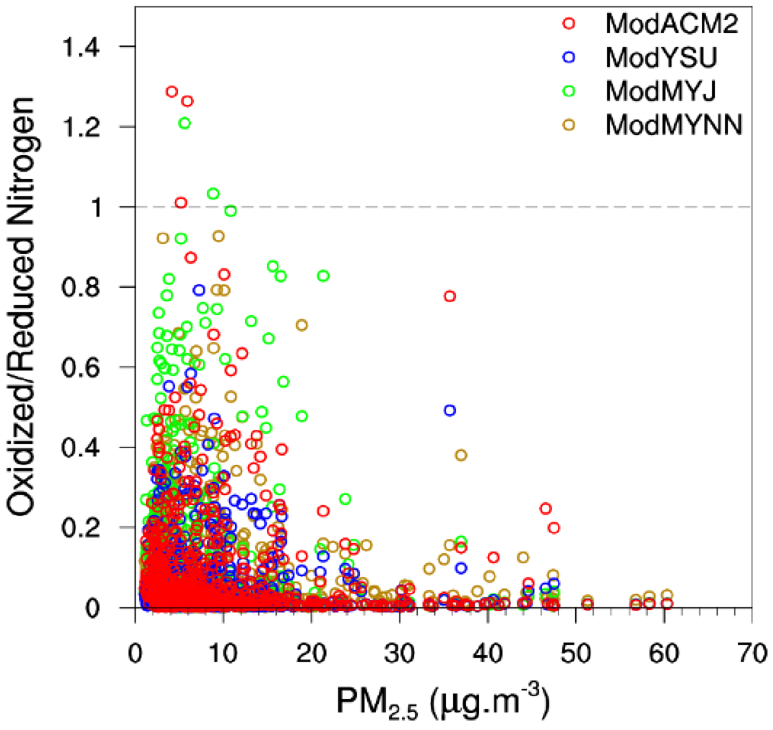
Non-PCAPs



During PCAPs:
Observed main component: nitrate, ammonium
Modeled main component: OC, nitrate

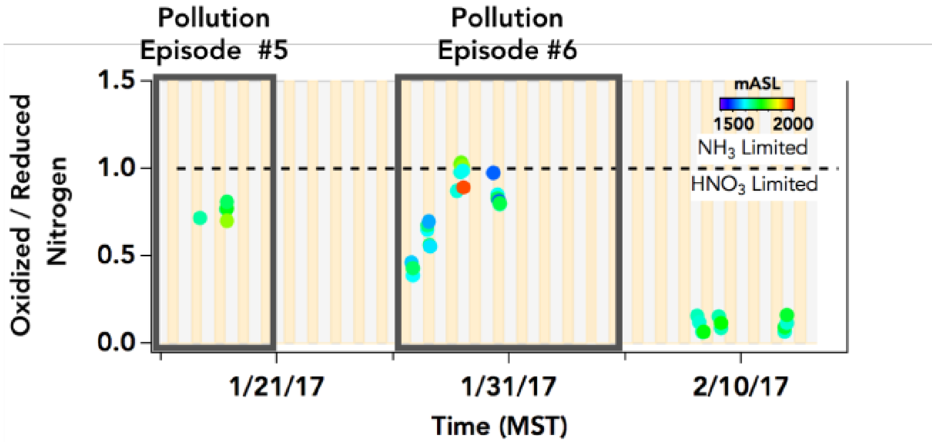
Modeled Nitrate formation

Nitrogen ratio variation with $PM_{2.5}$ concentrations



$$\text{Ratio} = \frac{HNO_3(g) + NO_3^-(p)}{NH_3(g) + NH_4^+(p)}$$

Ratio>1, NH_3 limited
Ratio<1, HNO_3 limited



(Baasandorj, et al. 2018)

- NH_4NO_3 formation in SLV during wintertime was mainly in excess of reduced nitrogen and limited by HNO_3(g).
- Reverse behavior of the variation of nitrogen ratio with increasing $PM_{2.5}$ concentrations

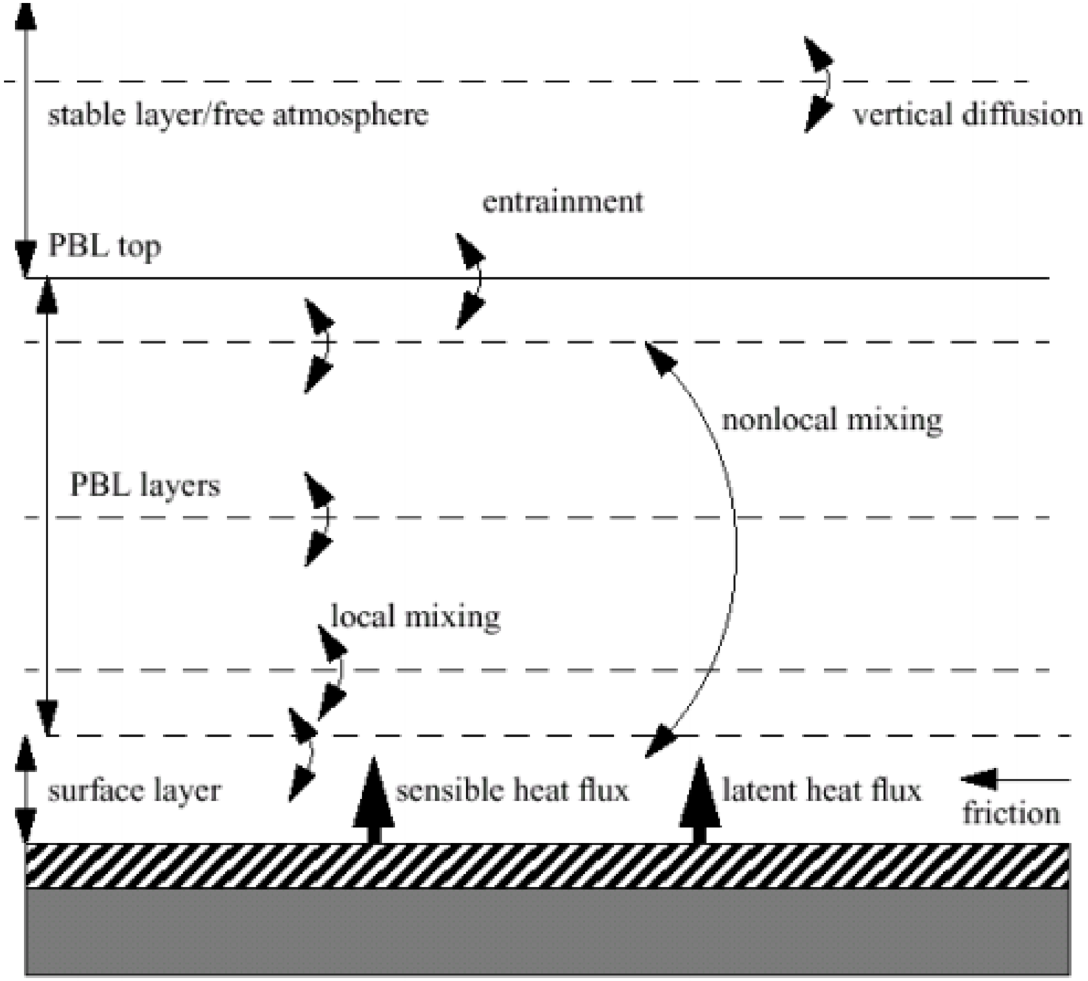
Summary

The CMAQ model simulated elevated $PM_{2.5}$ concentrations during PCAP events but underestimated the magnitude

- Emissions: The NO_x level was overestimated in the CMAQ model for both PCAP and non-PCAP scenarios using the 2011 NEI
- Meteorology: Less simulated PCAP strength contributes to the underestimated $PM_{2.5}$ concentration
- Chemistry: Underestimated ammonium nitrate formation contributes to the underestimated $PM_{2.5}$ concentration

Challenges in forecasting PCAP

Illustration of surface and PBL processes

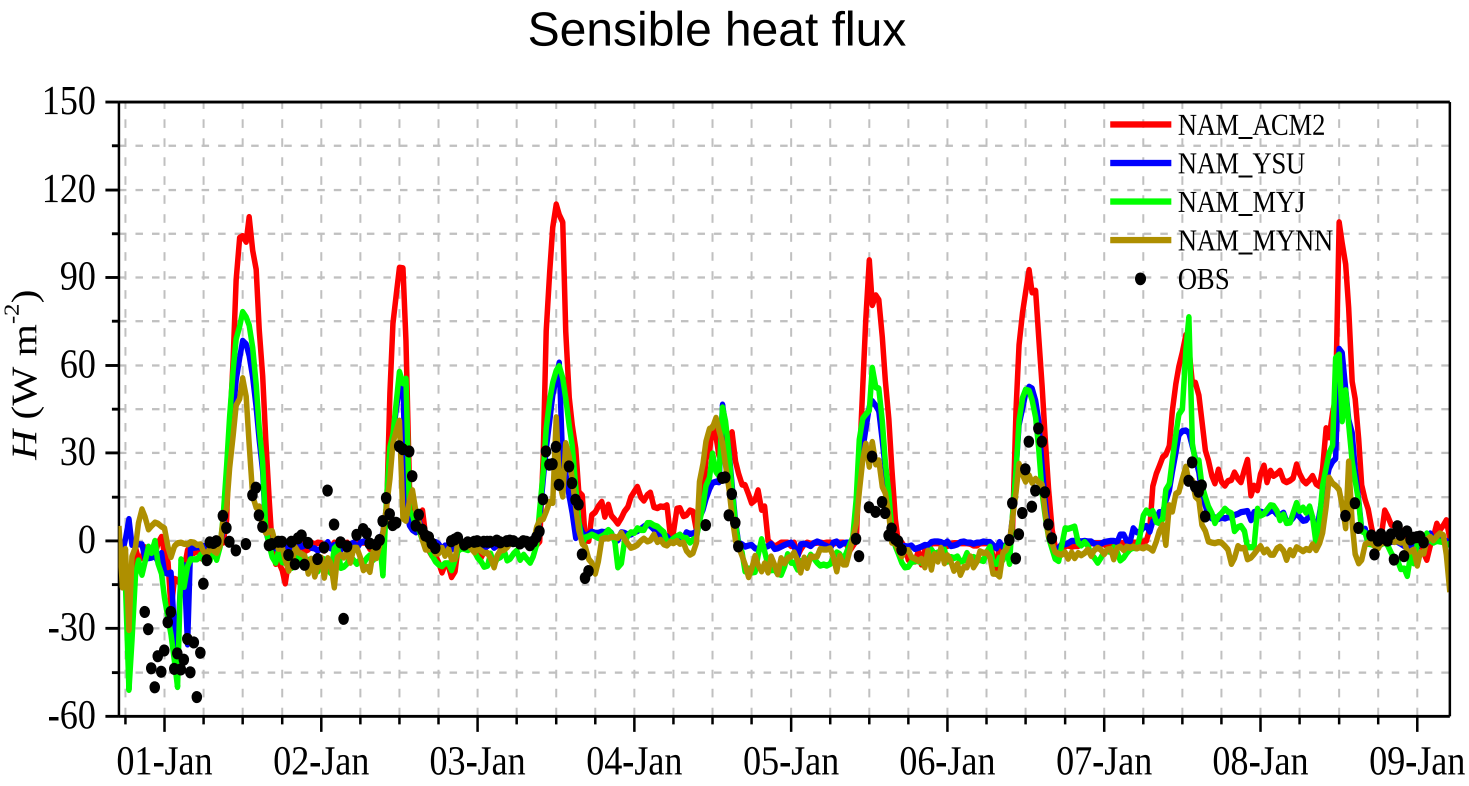


Model Challenges

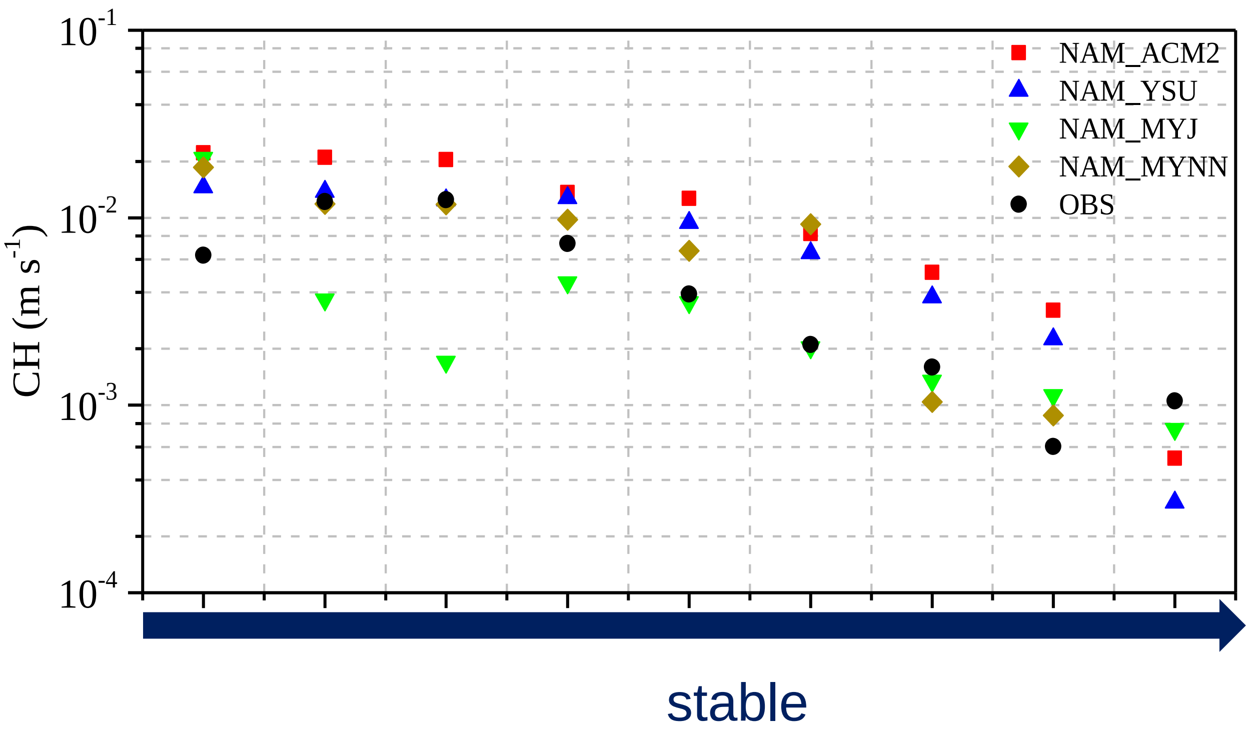
- Difficult to replicate the multiday stagnant conditions *(Baker et al. 2011)*
- Complex terrain
- ***Land-atmosphere exchange needs to be well addressed***

(Jimy Dudhia, NCAR)

Strong PCAP case (IOP5)



Surface exchange coefficient under stable conditions



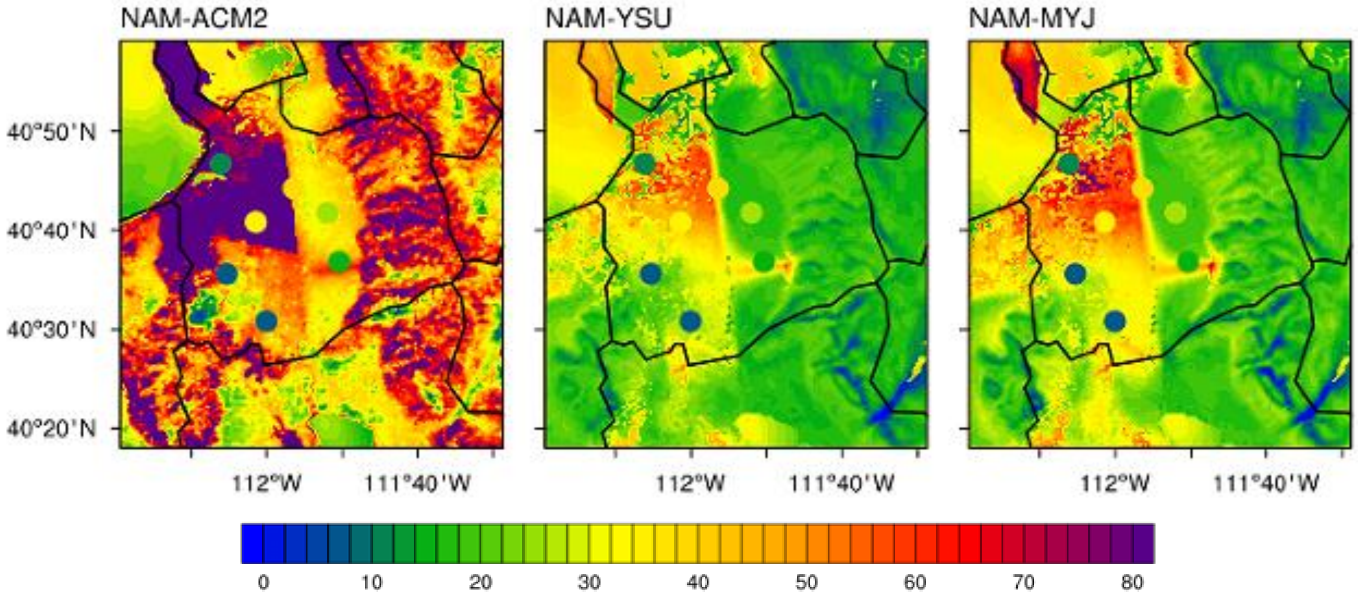
Bulk transfer equation:

$$H = \rho c_p C_h U_a (T_s - T_a)$$

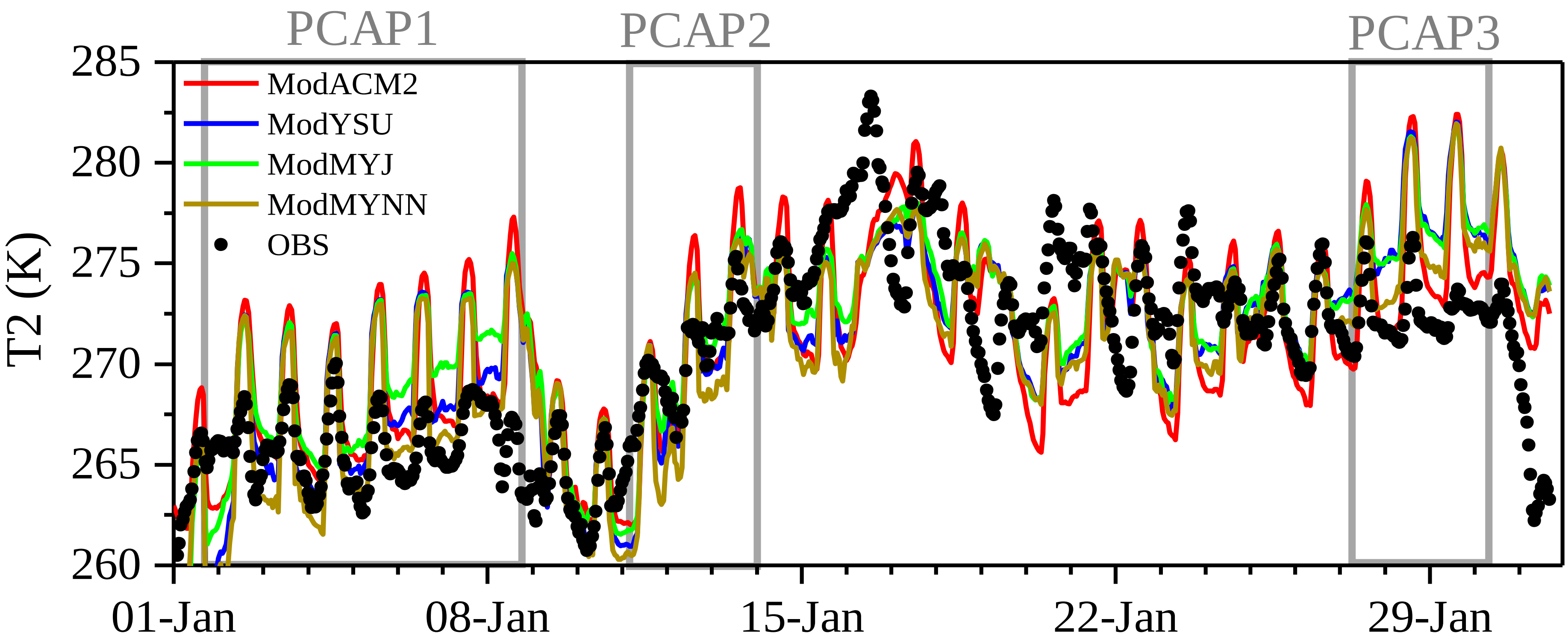
ρ: air density
cp: specific heat capacity of air
Ua: is air wind speed
Ts and Ta: surface and air temperature

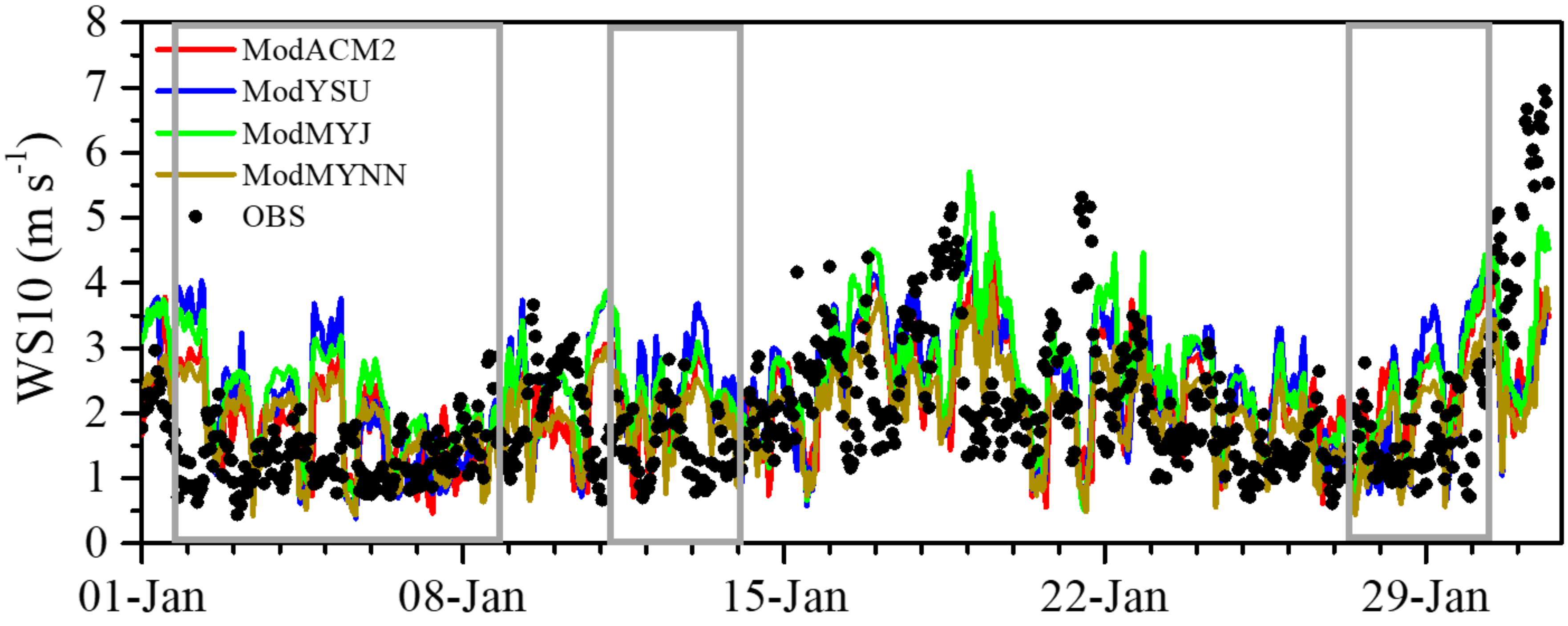
- All of the WRF scenarios generated an overestimation of *CH*, except for the NAM_MYJ case.

Thanks! Questions?



Simulated (contoured) and observed (dots) daytime surface sensible heat fluxes for IOP5


PCAP1
PCAP2
PCAP3
ModACM2
ModYSU
ModMYJ
ModMYNN
OBS
T2 (K)
285
280
275
270
265
260
01-Jan
08-Jan
15-Jan
22-Jan
29-Jan



8
7
6
5
4
3
2
1
0
WS10 (m s-1)
ModACM2
ModYSU
ModMYJ
ModMYNN
OBS
01-Jan
08-Jan
15-Jan
22-Jan
29-Jan