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;
- \( \rho \): air density
- \( \theta \): potential temperature;
- \( z \): altitude
The Persistent Cold Air Pool Study
(Utah, 2010-2011, PIs: C. David Whiteman et al.)

Focusing on meteorology

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

(Sun et al. 2019)

Figure 1 Topography map of SLV and measurement sites
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

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Surface Layer Scheme</th>
<th>Land Surface Model</th>
<th>Planetary Boundary Layer Scheme</th>
</tr>
</thead>
<tbody>
<tr>
<td>NAM_YSU</td>
<td>Revised MM5 (<a href="#">Jiménez et al. 2012</a>)</td>
<td>Noah (<a href="#">Ek et al. 2003</a>)</td>
<td>YSU (<a href="#">Hong et al. 2006</a>)</td>
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<tr>
<td>NAM_MYJ</td>
<td>Eta similarity (<a href="#">Janić 2001</a>)</td>
<td>Noah</td>
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</tr>
<tr>
<td>NAM_MYNN</td>
<td>MYNN (<a href="#">Nakanish 2001</a>)</td>
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<td>MYNN (<a href="#">Nakanishi and Niino 2004</a>)</td>
</tr>
</tbody>
</table>
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**

- **PCAP1**
- **PCAP2**
- **PCAP3**

**Date (MST)**
- **ModACM2**
- **ModYSU**
- **ModMYJ**
- **ModMYNN**
- **OBS**

**NOx concentration**

- **Ozone concentration**

- **SO2 concentration**

**Date (MST)**
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

PCAPs

Non-PCAPs
PM$_{2.5}$ chemical composition

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

Nitrogen ratio variation with PM$_{2.5}$ concentrations

- NH$_4$NO$_3$ 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

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

Ratio $> 1$, NH$_3$ limited
Ratio $< 1$, HNO$_3$ limited

(Baasandorj, et al. 2018)
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)

Sensible heat flux

Date (MST)

NAM_ACM2
NAM_YSU
NAM_MYJ
NAM_MYNN
OBS

H (W m\(^{-2}\))

01-Jan 02-Jan 03-Jan 04-Jan 05-Jan 06-Jan 07-Jan 08-Jan 09-Jan

-60
-30
0
30
60
90
120
150
Surface exchange coefficient under stable conditions

Bulk transfer equation:

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

- \( \rho \): air density
- \( c_p \): specific heat capacity of air
- \( U_a \): air wind speed
- \( T_s \) and \( T_a \): 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