A New BCON Processor for AIRPACT5

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Topics to cover:

- AIRPACT5 system overview
- Previous BCON processing thru end of Dec 2017
- Default BCON processing since January 2018
- WACCM model
- WACCM processing for BCON for AIRPACT5, version 0
- BCON results using WACCM and possible spatial issues
- CMAQ results using new BCON
- WACCM processing for BCON for AIRPACT5, version 1.0?

AIRPACT5 system overview
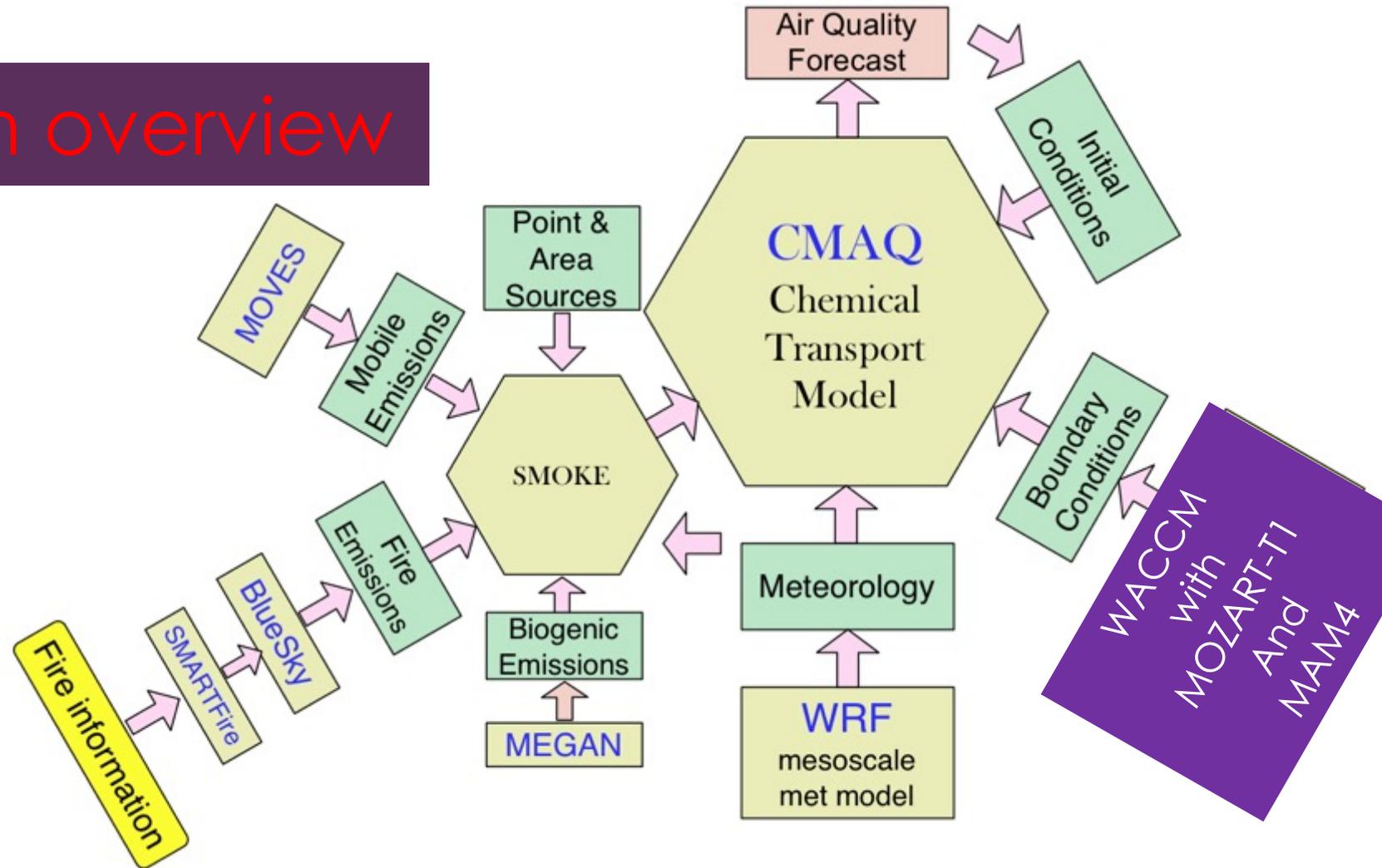
- WRF version 3.7.1
- SMOKE v3.5.1
- MEGAN v2.10
- SMARTFIRE2
- BLUESKY v 3.5.1
- CMAQ version 5.0.2
- Since MOZART4 operations ceased ~ Jan. 2018, Boundary Conditions have come from Monthly Average MOZART4 results from 2015.

Previous BCON processing using MOZART4 thru 12/2017

- Cron job does wget for MOZART4 data:

  - #00   19 *   *   *   . ~airpact5/.bash_profile;
    ~airpact5/AIRHOME/run_ap5_day1/bcon/get_mozart4file4bcon.pl >
    ~airpact5/AIRHOME/run_ap5_day1/logs4crontab/crontab_getmozart4.txt

- And for failsafe, script can do: wget -N -nv --no-check-certificate
  http://www.acom.ucar.edu/acresp/AMADEUS/mz4_output/chemfcst/${mz4file}

- Three executables from FORTRAN codes by Jeremy Avise with updates by Serena Chung and JKV.

  - # convert MOZART-4 output file to CMAQ BCON-formatted file

  - # convert units

  - # mechanism conversion

- lat = 33.158, 35.053, 36.947, 38.842, 40.737, 42.632, 44.526,

-      46.421, 48.316, 50.211, 52.105, 54, 55.895 ;   Delta Lat = 1.8497 degrees

- lon = 225, 227.5, 230, 232.5, 235, 237.5, 240, 242.5, 245, 247.5, 250,

-       252.5, 255 ;   Delta Lon = 2.5 degrees

- MOZART4 data files had 57 layers and hourly time steps.

Default BCON processing since January 2018

- Used old monthly-average MOZART4 BCON
- Single timestep for profile for entire month.

WACCM model

- Whole Atmosphere Community Climate Model at NCAR

- The chemical mechanism in WACCM includes comprehensive tropospheric, stratospheric and mesospheric chemistry. **The tropospheric chemistry mechanism has been significantly updated from MOZART-4 and is called MOZART-T1**. A preliminary version of this mechanism is described in Knote et al. (2014) and a complete description of the chemistry in CESM2 is being prepared. The most important change for users of the model output for regional model boundary conditions is the new treatment of aromatics: the previous lumped aromatic (confusingly called 'TOLUENE') has been replaced with the specific species BENZENE, TOLUENE and XYLENES. The lumped monoterpene is now called MTERP, and a sesquiterpene, BCARY, has been added. This document gives the full list of species. **The aerosol scheme in WACCM is the MAM4 modal aerosol scheme**, which is described in Liu et al. (GMD, 2015). Please contact Louisa Emmons if you have further questions.

- **WACCM data files have 88 layers and 6-hr time steps: 00Z, 06Z, 12Z, 18Z.**

WACCM model (cont.)

▶ **WACCM data files have 88 layers and 6-hr time steps: 00Z, 06Z, 12Z, 18Z.**

▶ **WACCM lat = 39.12, 40.05, 40.99, 41.94, 42.88, 43.82, 44.76, 45.71, 46.65, 47.59, 48.53,**

▶ **49.48, 50.42;**   **Delta Lat = 0.9424 degrees**

▶ **WACCM lon = 233.75, 235, 236.25, 237.5, 238.75, 240, 241.25, 242.5, 243.75, 245,**

▶ **246.25, 247.5, 248.75, 250, 251.25; ;**   **Delta Lon = 1.25 degrees**

> western longitudes are valued 180 -- 360

WACCM processing for BCON for AIRPACT5, v0

BCON SPECIES =
```
"NR        PAR        IOLE       TERP       ETH       ETOH       ROOH       ETHA
OLE        AECJ       FORM       ALD2       MGLY      AACD       MEOH       MEPX
CH4        CO         CRES       DMS        ASOIL     ALDX       H2O2       HNO3
PNA        HO2        ISPD       ISOP       PANX      N2O5       NH3        ANO3J
ANH4J      NO2        NO         O3         APOCI     APOCJ      NTR        PAN
SO2        ASO4J      TOL        NO3        ANAJ      ACLJ       ANAK       ACLK
APNCOMI    APNCOMJ    ACLI       ANAI       NUMACC    NUMATKN    NUMCOR     ASO4I
ASO4K      AOLGAJ     AOLGBJ            " ;
```

▶ **Time shift of BCON Template file to current period for DAY1 and DAY2 of AIRPACT5**

▶ **Python code called to read WACCM file, MCIP BDY files, and rewrite to re-dated BCON file (from the template file).**

Python 2 code:
(mapping of WACCM cells to BCON cells)

▶ **Reads MCIP BCON GRIDBDY2D and METBDY3D files for Lat, Lon and Pressure**

▶ **Reads WACCM file for Lat and Lon.**

▶ **Finds for each of 1090 BCON cells (lat,lon) the nearest WACCM cell (lat, lon)**

▶ **WACCM:**

    ▶ **Delta Lat = 0.9424 degrees**

    ▶ **Delta Lon = 1.25 degrees**

▶ **BCON:**

    ▶ **Delta Lat: ~0.0369 Degrees**

    ▶ **Delta Lon: 0.0484 degrees on S to -0.0574 on N.**

▶ **RISK of grabbing results from a WACCM cell with a wildfire and that wildfire also being on interior of BCON and within AIRPACT5 domain. Danger of Double Counting?**
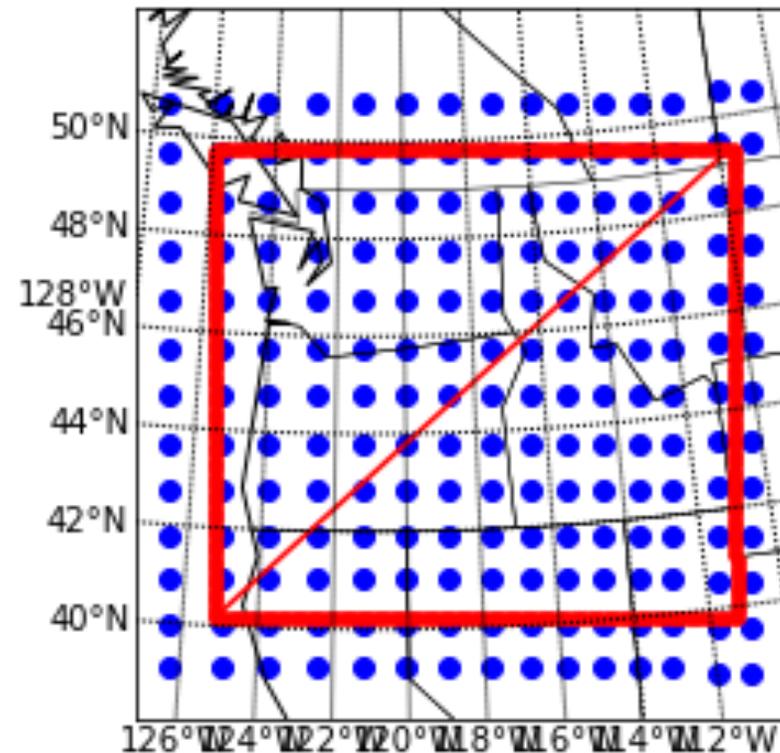
Python 2 code:
(mapping of WACCM layer to BCON layer)

▶ **WACCM: Use hybrid vertical structure formula to compute Pressure per layer:**

▶ **P_in_Z[tdx, levdx, latdx, londx] = waccm_hyam[levdx] * waccm_P0 + waccm_hybm[levdx] * waccm_PS[tdx, latdx, londx]**

▶ **Compute conversion factors:**

   ▶ **C_in_Z for conversion factors from [Kg/Kg] to [micrograms/cubic-meter]**

   ▶ **N_in_Z of conversion factors from [#/Kg] to [#/cubic-meter].**

   ▶ **Conversions in place for units, WACCM to BCON style.**

▶ **For each horizontal cell match from WACCM to BCON:**

   ▶ **Nearest layer identified by matching WACCM P_of_Z to BCON P**

   ▶ **Copy species WACCM to BCON doing needed combinations or allocations**

▶ **THIS IS NOT INTERPOLOATION BUT RATHER SAMPLING.**
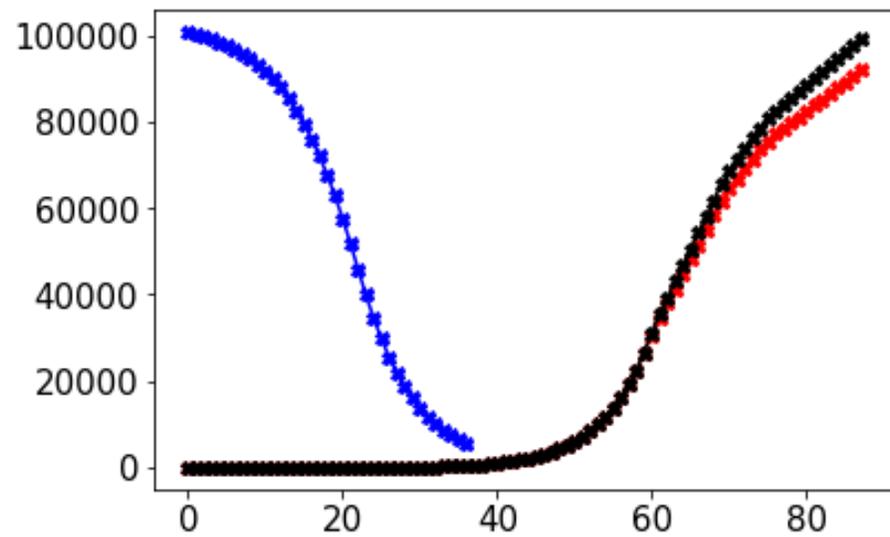
PRESSURES in Pascals. Black shows nominal pressure P, associated with level.

RED: WACCM P(Z) at SW corner, Z on X-axis (abscissa) is inverted, so ToA is far left, Sea Level on far right
BLUE: BCON P(Z) at SW corner, Z on X-axis (abscissa), so ToA is far right, Sea Level on far left
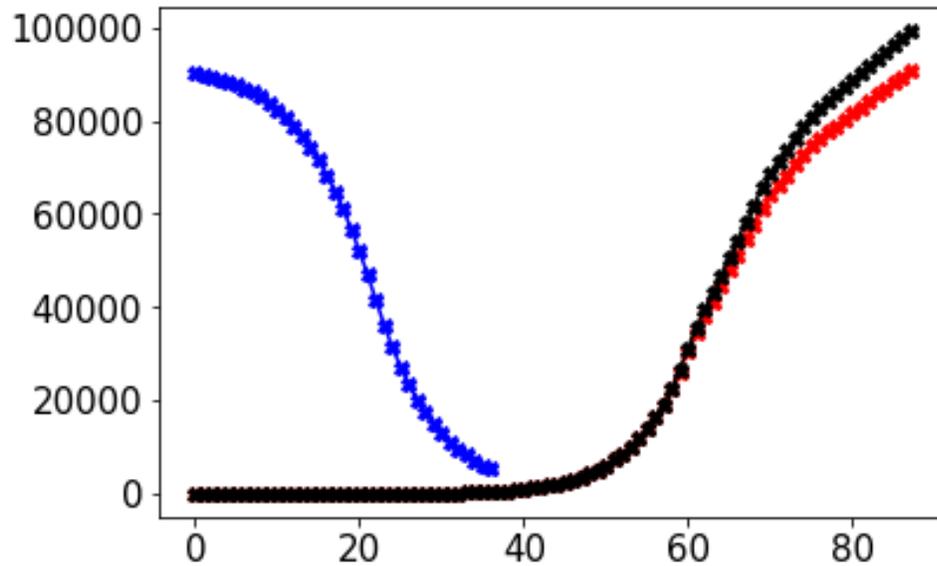
WACCM P(Z) at NE corner, Z on X-axis (abscissa) is inverted, so ToA is far left
BLUE: BCON P(Z) at NE corner, Z on X-axis (abscissa), so ToA is far right, Sea Level on far left

WACCM BCON plots for CO AIRPACT5 for 10/3/18 (time stamps are incorrect…)
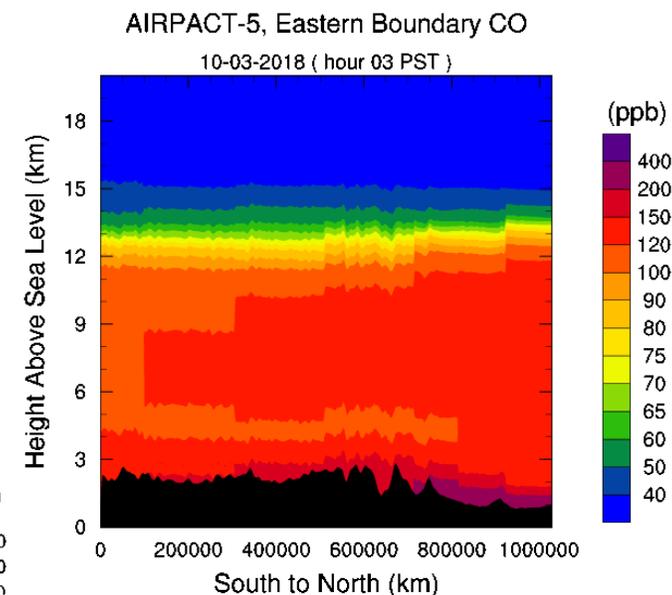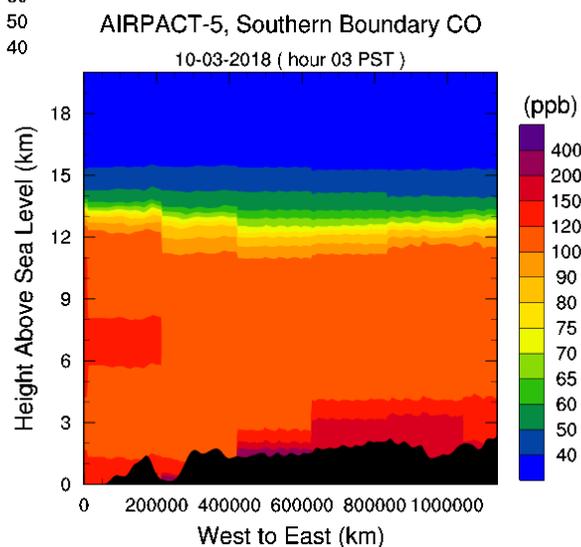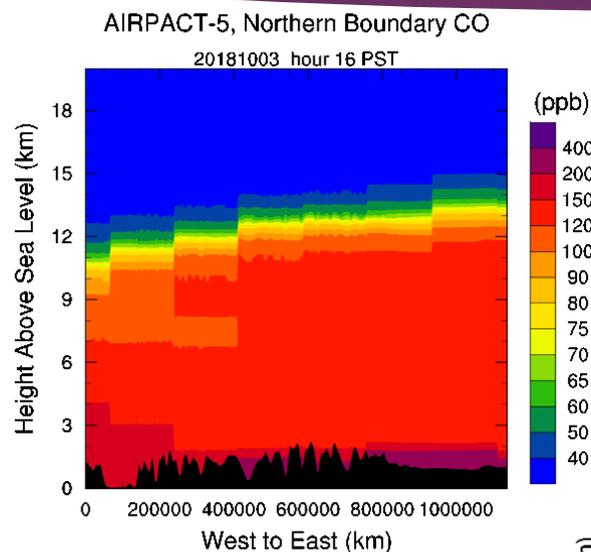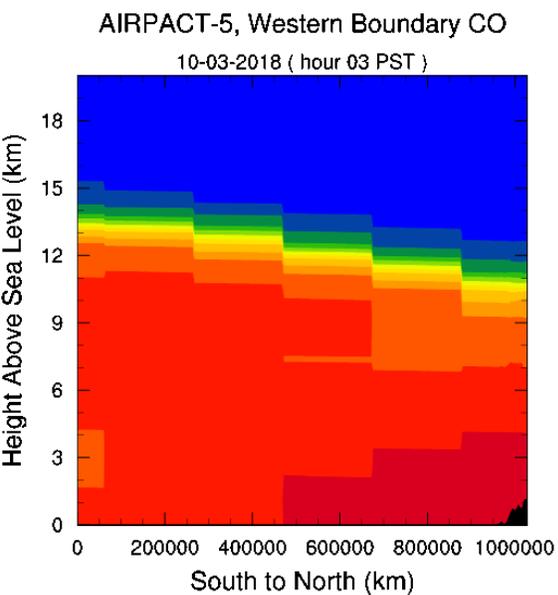
WACCM BCON plots for O3 AIRPACT5 for 10/3/18 (time stamps are incorrect...)

AIRPACT-5, Western Boundary O3
10-03-2018 (hour 03 PST)

AIRPACT-5, Northern Boundary O3
20181003 hour 16 PST
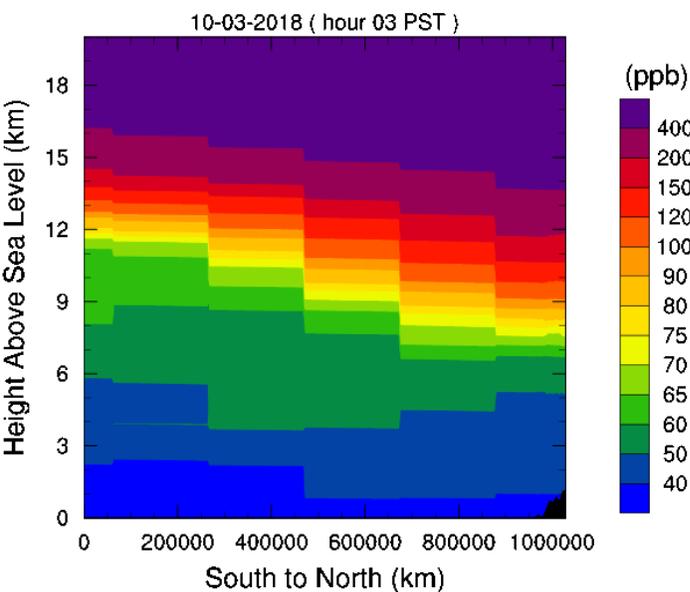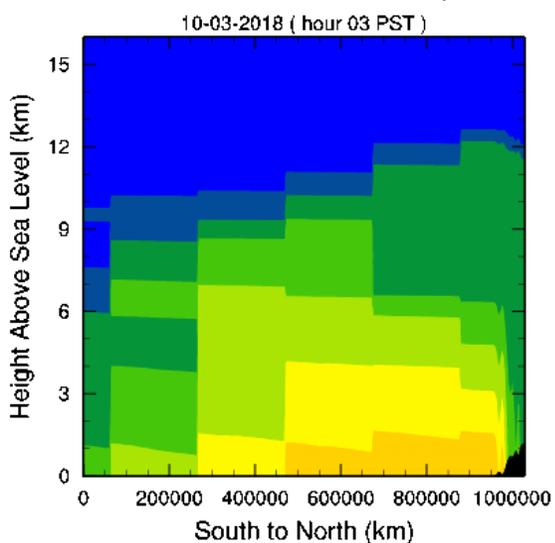
AIRPACT-5, Southern Boundary O3
10-03-2018 (hour 03 PST)

AIRPACT-5, Eastern Boundary O3
10-03-2018 (hour 03 PST)

WACCM BCON plots for PM2.5 AIRPACT5 for 10/3/18 (time stamps are incorrect…)
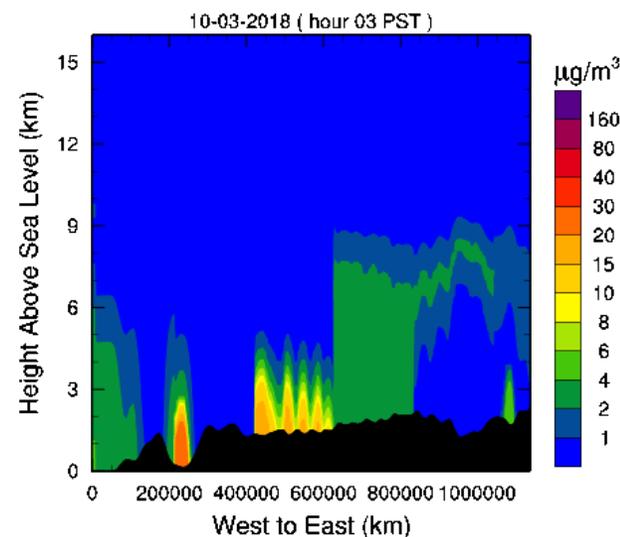
CMAQ PM2.5 Noon results from MOZART4 monthly avg BCON and from WACCM 6-hr BCON
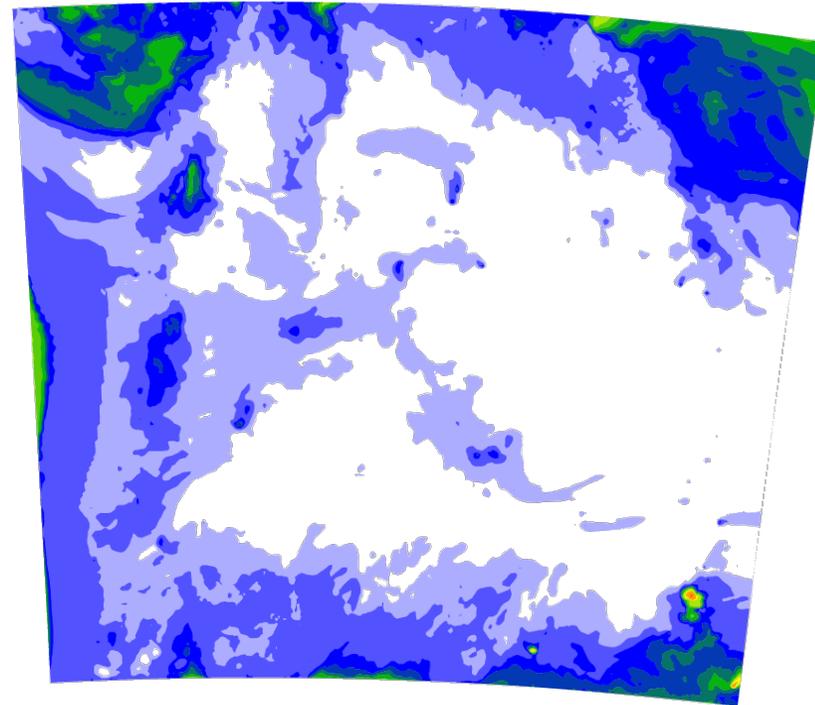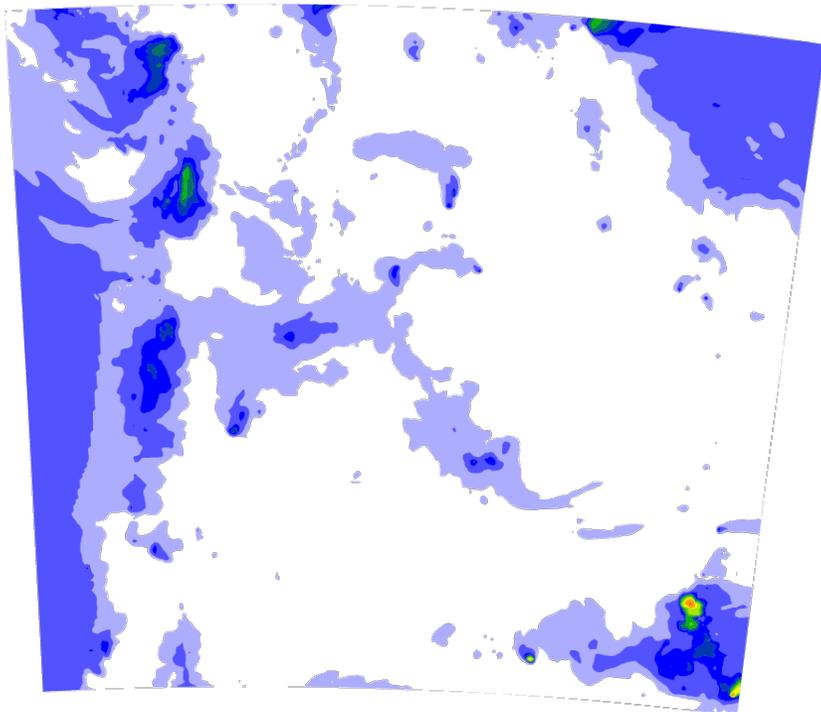
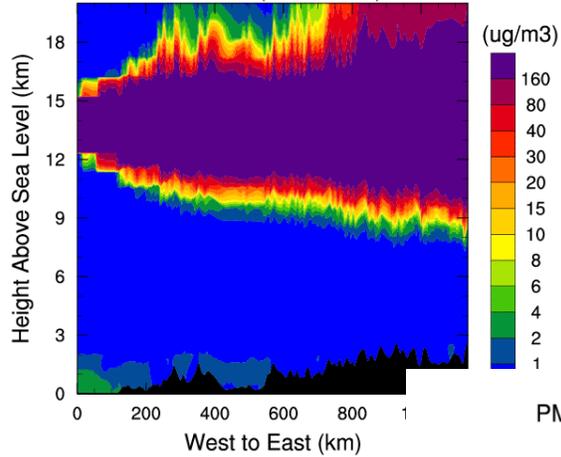CMAQ CO Noon results from MOZART4 monthly avg BCON and from WACCM 6-hr BCON
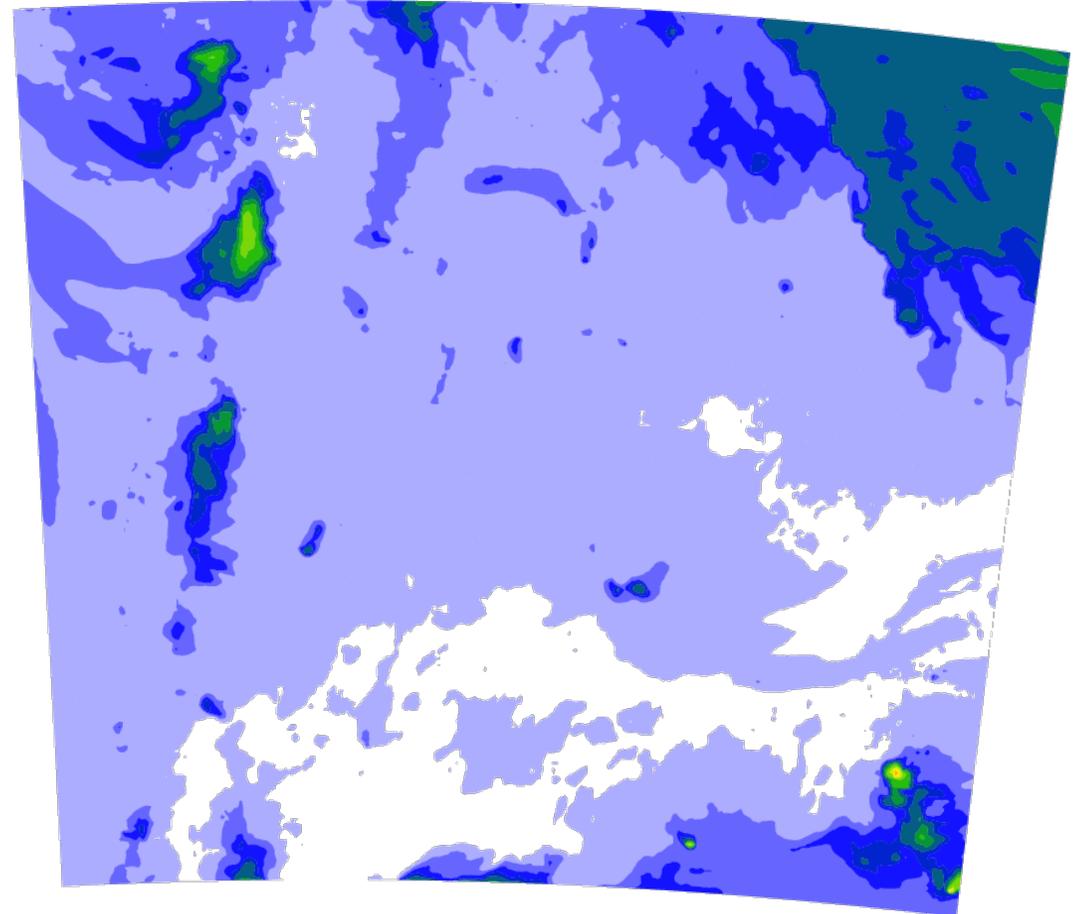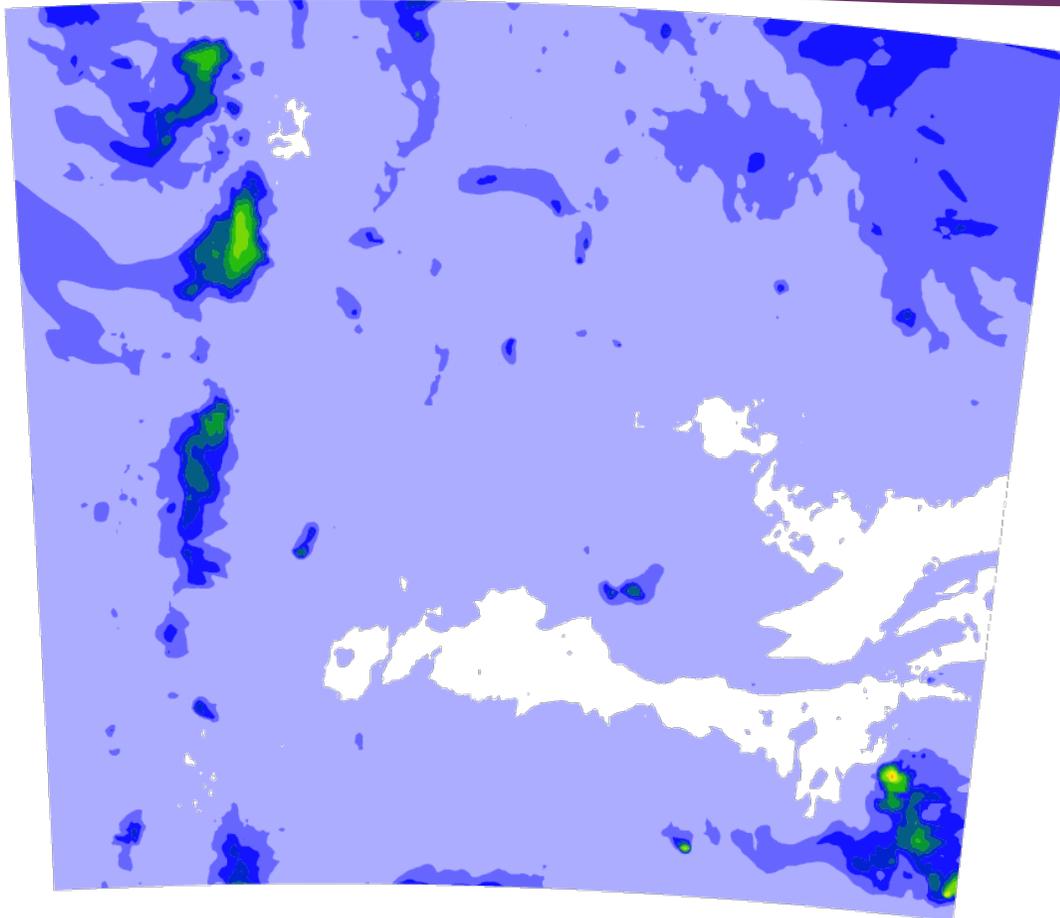
CMAQ O3 Noon results from MOZART4 monthly avg BCON and from WACCM 6-hr BCON
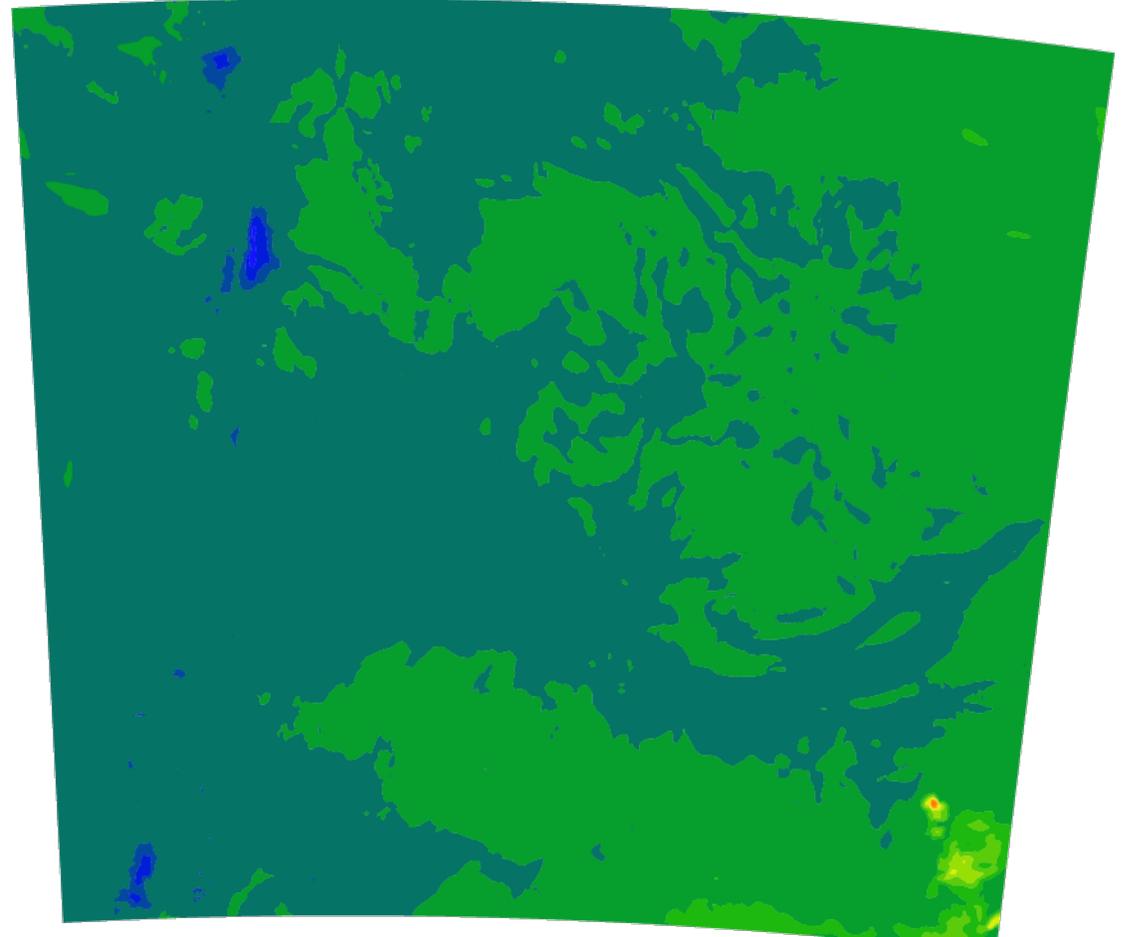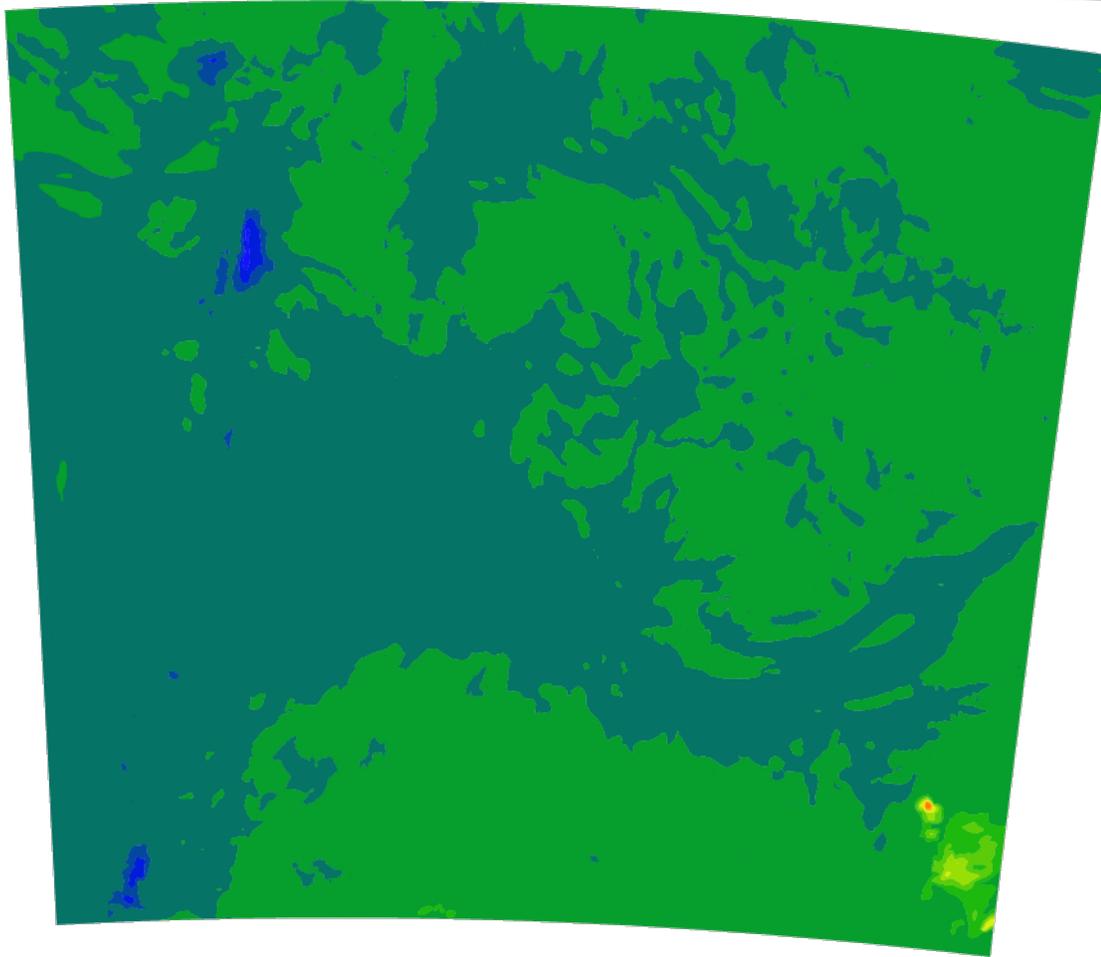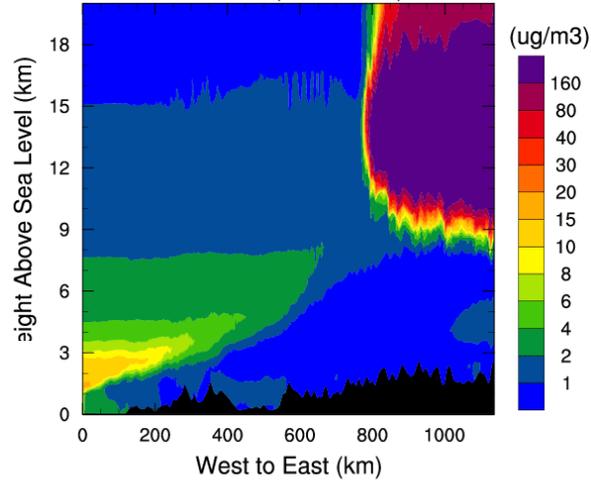
CMAQ PM2.5 Curtains Noon results from MOZART4 monthly avg BCON and from WACCM 6-hr BCON
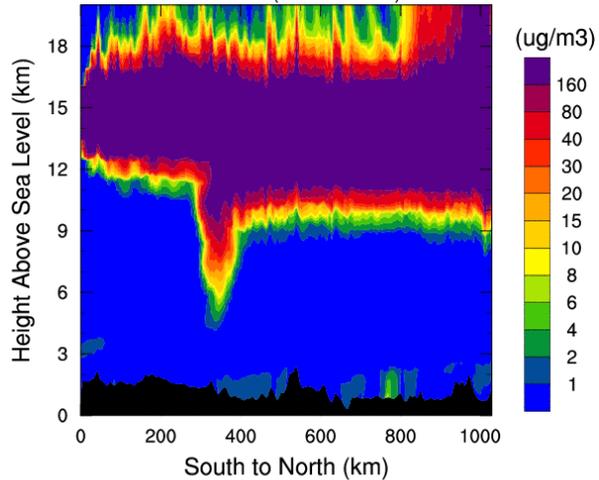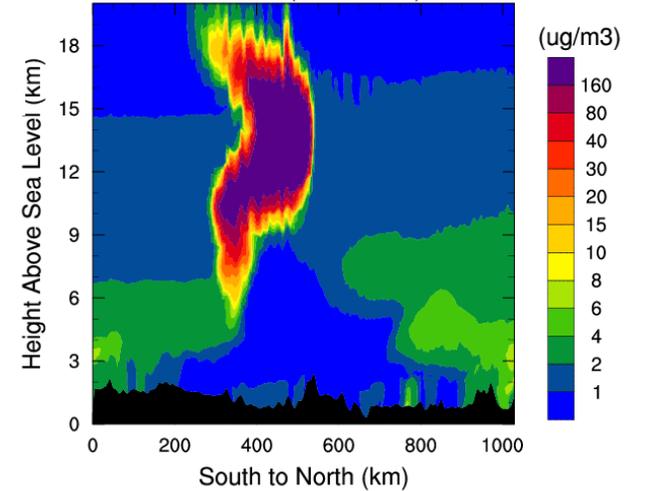
WACCM processing for BCON for AIRPACT5, version 1.0?

- Testing is needed for recent dates with lots of fires.

- Try to replace sampling with interpolation and compare results.

- Verify time step alignment in WACCM derived BCON file generation.

- Fix BCON graphics time step labeling

The End