Data Dictionary for EPA data used in “Modeling attainment in Fairbanks, Alaska for wintertime PM2.5 24-hour non-attainment area using the CMAQ (Community Multi-Scale Air Quality) model”

# Summary

Fairbanks, Alaska, is a serious nonattainment area for the 24-hour PM2.5\*\* National Ambient Air Quality Standard (NAAQS). Violations of the NAAQS typically occur in winter when cold conditions are associated with strong temperature inversions and air stagnation that trap particulate pollution at the surface. There remain many uncertainties surrounding the processes that drive this pollution, including emissions characterization, meteorology, and the active chemistry occurring under these cold and dark conditions. To address some of these knowledge gaps, the Alaskan Layered Pollution and Chemical Analysis (ALPACA) study took place January 17 – February 25, 2022, and was a multipronged, intensive field campaign focused on better understanding emissions, meteorology, and atmospheric chemistry in Fairbanks during the wintertime. The CMAQ code used here was evaluated with routine and ALPACA field study observations for January-February 2022.

The paper with which these data are associated describes modeling performed by the Alaska Department of Environmental Conservation (AK DEC) for late 2019-early 2020. This dataset includes the EPA-provided CMAQ model code with heterogeneous sulfur chemistry and extended sulfur tracking method and a description of the EPA-provided CMAQ-ready meteorological inputs for the ADEC modeling domain (Figure 1) and time period.

The following sections describe the data provided by the EPA for this manuscript as well as their file names or, if very large files, their location on the archival file system, /asm, for EPA’s atmos high-performance computing platform.

\*\*PM2.5 refers to particulate matter 2.5 micrometers or less in diameter



**Figure 1:** US EPA domain configuration with 4 km outer domain (WRF) and a 1.33 km nested domain (WRF, CMAQ) centered over Fairbanks, AK. CMAQ modeling is performed over the inner domain **(**199 rows × 199 columns × 38 layers)

# CMAQ Model-Ready Inputs for Fairbanks (0133\_AK domain)

**Table 1: Location of CMAQ input files**

|  |  |  |
| --- | --- | --- |
| **Data description** | **File type\*** | **Location on asm** |
| CMAQ-ready meteorology inputs for Dec. 2019-Feb. 2020 (~240 GB) | netCDF | /asm/grc/FAIRBANKS/ALPACA/mcip\_20192020/USEPA\_FINAL\_RUN |

\*Note that netCDF files contain metadata describing the variables in each file and their units

# CMAQ code

**Table 2**

|  |  |  |
| --- | --- | --- |
| **Data description** | **File type** | **File name** |
| CMAQ Build directory – updated heterogeneous chemistry and sulfur tracking, v1  | ASCII (Fortran code) | CMAQ\_BLD\_AK\_v1.tar |
| CMAQ Build directory – updated heterogeneous chemistry and sulfur tracking, v2 (with bug fix for ionic strength effect factor applied to SO2 Henry’s law coefficient) | ASCII (Fortran code) | CMAQ\_BLD\_AK\_v2.tar |
| Example CMAQ Emissions control file | ASCII | EmissCtrl\_Fbks\_example.nml.txt |

# Sulfur Tracking Method (STM) sulfate tags, definitions, and units

**Table 3. STM tags**

|  |  |  |
| --- | --- | --- |
| **Tag** | **Definition** | **Units** |
| ASO4GASx | Gas-phase sulfate production (x = I,J, and K modes) | Micrograms per cubic meter |
| ASO4EMISx | Primary sulfate emissions (x = I,J, and K modes) | Micrograms per cubic meter |
| ASO4ICBCx | Sulfate from initial/boundary conditions (x = I,J, and K modes) | Micrograms per cubic meter |
| ASO4AEH2O2J | Heterogeneous sulfate production from H2O2 in aerosol water | Micrograms per cubic meter |
| ASO4AEO3J | Heterogeneous sulfate production from O3 in aerosol water | Micrograms per cubic meter |
| ASO4AEFEMNJ | Heterogeneous sulfate production from O2 catalyzed by Fe3+ and Mn2+ in aerosol water | Micrograms per cubic meter |
| ASO4AEMHPJ | Heterogeneous sulfate production from methyl hydroperoxide in aerosol water | Micrograms per cubic meter |
| ASO4AEPAAJ | Heterogeneous sulfate production from peroxyacetic acid in aerosol water | Micrograms per cubic meter |
| ASO4AEHNO4J | Heterogeneous sulfate production from HNO4 in aerosol water | Micrograms per cubic meter |
| ASO4AENO2J | Heterogeneous sulfate production from NO2 in aerosol water | Micrograms per cubic meter |
| ASO4AQH2O2J | In-cloud sulfate production from H2O2 | Micrograms per cubic meter |
| ASO4AQO3J | In-cloud sulfate production from O3 | Micrograms per cubic meter |
| ASO4AQFEMNJ | In-cloud sulfate production from O2 catalyzed by Fe3+ and Mn2+ | Micrograms per cubic meter |
| ASO4AQMHPJ | In-cloud sulfate production from methyl hydroperoxide | Micrograms per cubic meter |
| ASO4AQPAAJ | In-cloud sulfate production from peroxyacetic acid | Micrograms per cubic meter |
| ASO4AQHNO4J | In-cloud sulfate production from HNO4 | Micrograms per cubic meter |
| ASO4AQNO2J | In-cloud sulfate production from NO2 | Micrograms per cubic meter |
| ASO4AQRADJ | In-cloud sulfate production from OH radical chain | Micrograms per cubic meter |
| ASO4AQNIIIJ | In-cloud sulfate production from N(III) | Micrograms per cubic meter |
| OSO4J | Inorganic sulfate loss to organosulfate | Micrograms per cubic meter |

# Meteorology variables names, descriptions, and units

**Table 4:** Meteorological input file types

|  |  |  |
| --- | --- | --- |
| **File name** | **File type\*** | **Description** |
| GRIDDESC | ASCII | Grid description file with coordinate and grid definition information |
| GRID\_BDY\_2D | netCDF | Time-independent 2-D boundary meteorology file |
| GRID\_CRO\_2D | netCDF | Time-independent 2-D cross-point meteorology file |
| GRID\_CRO\_3D | netCDF | Time-independent 3-D cross-point meteorology file |
| GRID\_DOT\_2D | netCDF | Time-independent 2-D dot-point meteorology file |
| LUFRAC\_CRO | netCDF | Time-independent fractional land use by category |
| MET\_BDY\_3D | netCDF | Time-varying 3-D boundary meteorology file |
| MET\_CRO\_2D | netCDF | Time-varying 2-D cross-point meteorology file |
| MET\_CRO\_3D | netCDF | Time-varying 3-D cross-point meteorology file |
| MET\_DOT\_3D | netCDF | Time-varying 3-D dot-point meteorology file |

\*Note that netCDF files contain metadata describing the variables in each file and their units

**Table 5:** Meteorological variables

|  |  |  |
| --- | --- | --- |
| **Variable** | **Definition** | **Units** |
| *GRIDBDY2D and GRIDCRO2D* |
| LAT  | latitude at cell centers | degrees\_north  |
| LON  | longitude at cell centers  | degrees east |
| MSFX2  | map-scale factor squared  | m2 m-2  |
| HT  | terrain elevation  | m |
| DLUSE  | dominant land use category USGS24  |  |
| LWMASK  | land-water mask (1=land, 0=water)  |  |
| PURB | urban percent of cell based on land  | percent |
| *LUFRAC* |
| LUFRAC  | Fractional land use |  |
| *GRIDDOT2D* |
| LATD  | latitude at cell corners  | degrees\_north  |
| LOND  | longitude at cell corners  | degrees\_east  |
| MSFD2  | squared map-scale factor at cell corners  | m2 m-2  |
| LATU  | latitude at cell U faces  | degrees\_north  |
| LONU  | longitude at cell U faces  | degrees\_east  |
| MSFU2  | squared map-scale factor at cell U faces  | m2 m-2  |
| LATV  | latitude at cell V faces  | degrees\_north  |
| LONV  | longitude at cell V faces  | degrees\_east  |
| MSFV2 | squared map-scale factor at cell V faces  | m2 m-2  |
| *METDOT3D* |
| UWINDC  | U-comp. of true wind at W-E faces  | m s-1  |
| VWINDC  | V-comp. of true wind at S-N faces  | m s-1  |
| UHAT\_JD  | (contravariant\_U\*Jacobian\*Density) at square pt  | kg m-1 s-1  |
| VHAT\_JD  | (contravariant\_V\*Jacobian\*Density) at triangle pt  | kg m-1 s-1  |
| UWIND  | U-comp. of true wind at dot point  | m s-1  |
| VWIND  | V-comp. of true wind at dot point  | m s-1  |
| *METCRO3D and METBDY3D* |
| JACOBF  | Jacobian at layer face scaled by MSFX2  | m |
| JACOBM  | Jacobian at layer middle scaled by MSFX2  | m  |
| DENSA\_J  | J-weighted air density (dry) scaled by MSFX2  | kg m-2  |
| WHAT\_JD  | J- and density weighted vert contravariant-W  | kg m-1 s-1  |
| TA  | Air temperature  | K |
| QV  | water vapor mixing ratio  | kg kg-1  |
| PRES  | pressure  | Pa  |
| DENS  | density of air (dry  | kg m-3 |
| ZH  | mid-layer height above ground  | m |
| ZF  | full-layer height above ground  | m |
| CFRAC\_3D  | 3D resolved cloud fraction  |  |
| QC  | cloud water mixing ratio  | kg kg-1  |
| QR  | rain water mixing ratio  | kg kg-1  |
| QI  | ice mixing ratio  | kg kg-1  |
| QS  | snow mixing ratio  | kg kg-1  |
| QG | graupel mixing ratio  | kg kg-1  |
| *METCRO2D* |
| PRSFC  | surface pressure  | Pa "  |
| USTAR  | cell averaged friction velocity  | m s-1  |
| WSTAR  | convective velocity scale  | m s-1  |
| PBL  | PBL height  | m  |
| ZRUF  | surface roughness length  | m  |
| MOLI  | inverse of Monin-Obukhov length  | m-1  |
| HFX  | sensible heat flux  | W m-2  |
| LH  | latent heat flux  | W m-2  |
| RADYNI  | inverse of aerodynamic resistance  | m s-1  |
| RSTOMI  | inverse of stomatic resistance  | m s-1  |
| TEMPG  | skin temperature at ground  | K  |
| TEMP2  | temperature at 2 m  | K  |
| Q2  | mixing ratio at 2 m  | kg kg-1  |
| WSPD10  | wind speed at 10 m  | m s-1  |
| WDIR10  | wind direction at 10 m  | degree  |
| GLW  | longwave radiation at ground  | W m-2  |
| GSW  | solar radiation absorbed at ground  | W m-2  |
| RGRND  | solar radiation reaching ground  | W m-2  |
| RN  | nonconvective precipitation in interval  | cm  |
| RC  | convective precipitation in interval  | cm |
| CFRAC  | total cloud fraction  |  |
| CLDT  | cloud top layer height  | m  |
| CLDB  | cloud bottom layer height  | m  |
| WBAR  | average liquid water content of cloud  | g m-3  |
| SNOCOV  | snow cover  |  |
| VEG  | vegetation coverage  |  |
| LAI  | leaf-area index  | m2 m-2  |
| SEAICE  | sea ice  |  |
| SNOWH  | snow height  | m  |
| WR  | canopy moisture content  | m  |
| SOIM1  | volumetric soil moisture in top cm  | m3 m-3  |
| SOIM2  | volumetric soil moisture in top m  | m3 m-3  |
| SOIT1  | soil temperature in top cm  | K  |
| SOIT2  | soil temperature in top m  | K  |
| SLTYP | soil texture type by USDA category  |  |