In [2]:
```
# Import Packages
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import xarray as xr
import cartopy.feature as cfeature
import cartopy.crs as ccrs
from matplotlib.axes import Axes
from cartopy.mpl.geoaxes import GeoAxes
import os
import re
```

```
---------------------------------------------------------------------------
ModuleNotFoundError                       Traceback (most recent call last)
<ipython-input-2-2e70742018cb> in <module>()
      3 import numpy as np
      4 import matplotlib.pyplot as plt
----> 5 import xarray as xr
      6 import cartopy.feature as cfeature
      7 import cartopy.crs as ccrs

ModuleNotFoundError: No module named 'xarray'
```

In [5]:
```
### Purple Air Data
# Regular Expressions to get correct files, and information about the si
tes
re_files = re.compile(".*\(outside\).*Primary.*")
re_lat = re.compile("(?<= \()\d{2}\.\d*")
re_lon = re.compile("(?<=\d )-\d{3}\.\d*")
re_site_name = re.compile(".*(?= \(outside)")
obs_data_files = list(filter(re_files.match, os.listdir('/import/home/nj
une1_ua/WRFChemEval/PurpleAirData')))
obs_data = {}
for file in obs_data_files:
    obs_site = pd.read_csv('/import/home/njune1_ua/WRFChemEval/PurpleAir
Data/'+file)
    site_name = re_site_name.match(file).group()
    site_lat = re_lat.search(file).group()
    site_lon = re_lon.search(file).group()
    obs_site['site_name'] = site_name
    obs_site['LAT'] = float(site_lat)
    obs_site['LON'] = float(site_lon)
    obs_data[site_name] = obs_site
```

```
-----------------------------------------------------------------------
----
NameError                                 Traceback (most recent call l
ast)
<ipython-input-5-3c9227d0b20c> in <module>()
      1 ### Purple Air Data
      2 # Regular Expressions to get correct files, and information abo
ut the sites
----> 3 re_files = re.compile(".*\(outside\).*Primary.*")
      4 re_lat = re.compile("(?<= \()\d{2}\.\d*")
      5 re_lon = re.compile("(?<=\d )-\d{3}\.\d*")

NameError: name 're' is not defined
```

In [4]:
```
obs_data
```

```
-----------------------------------------------------------------------
----
NameError                                 Traceback (most recent call l
ast)
<ipython-input-4-0f15bac3a2b2> in <module>()
----> 1 obs_data

NameError: name 'obs_data' is not defined
```

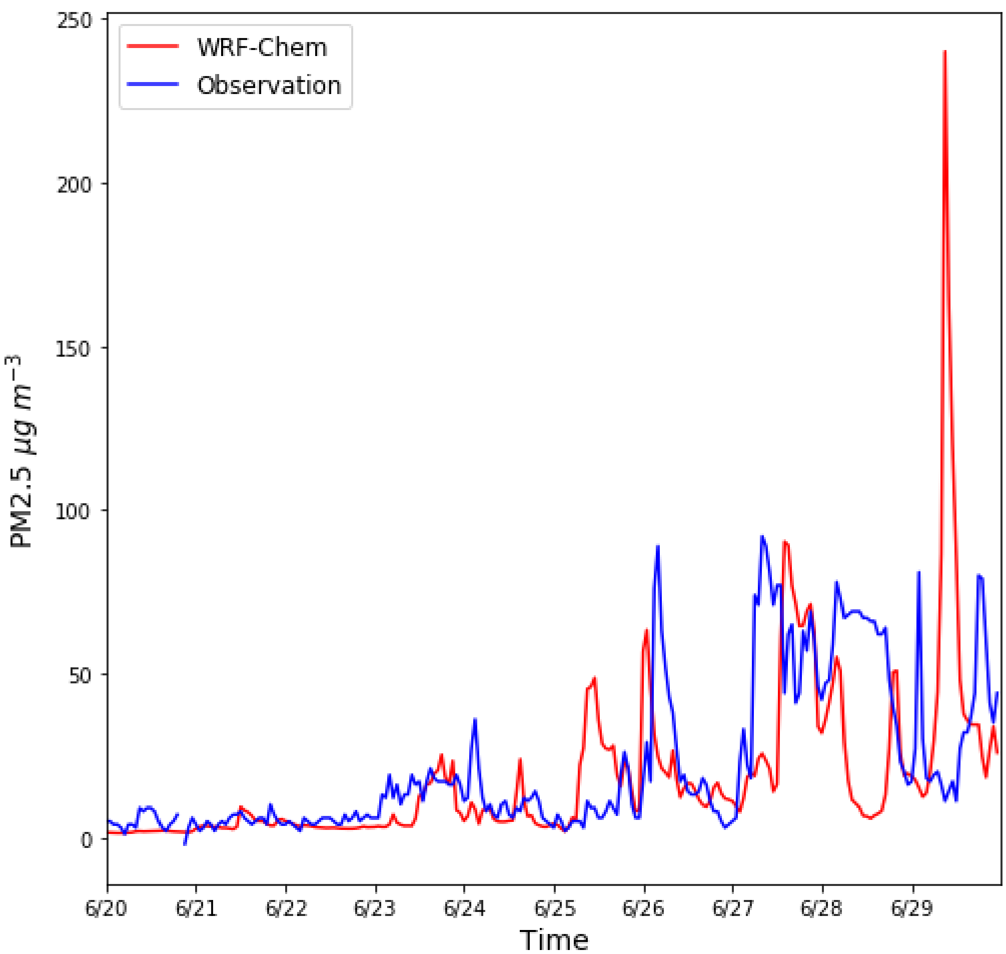
In [2]:
```
obs_data_DEC = pd.read_csv('/import/home/njune1_ua/WRFChemEval/DEC_May_J
une_2019.csv',index_col=False)
obs_data_DEC = obs_data.set_index('date_gmt')
```

In [3]:
```
# Observation Data for Each day
obs_data_jun= obs_data.loc[['2019-06-20','2019-06-21','2019-06-22','2019
-06-23','2019-06-24','2019-06-25','2019-06-26','2019-06-27','2019-06-28'
,'2019-06-29']]
obs_data_jun = obs_data_jun.reset_index()
PM25_jun = obs_data_jun[obs_data_jun['parameter']=='PM2.5 Raw Data']
PM25_obs = np.array(PM25_jun['sample_measurement'])
```

In [4]:
```
# Model Data
lat_site = obs_data['latitude'][0]
lon_site = obs_data['longitude'][0]
dates = ['2019-06-20','2019-06-21','2019-06-22','2019-06-23','2019-06-2
4','2019-06-25','2019-06-26','2019-06-27','2019-06-28','2019-06-29']
PM25_mod = []
for date in dates:
    file = '/import/archive/GREENING/mstuefer/uafsmoke_wrfout/'+date[0:4
]+date[5:7]+date[8:10]+'00/wrfout_d01_'+date+'_00:00:00'
    data = xr.open_dataset(file)
    lon = data['XLONG'][0,:,:]
    lat = data['XLAT'][0,:,:]
    PM25_mod_date = []
    for time in range(0,24):
        PM25_MOD = np.array(data['PM2_5_DRY'].values[time,0,:,:])
        site_index = np.unravel_index(np.argmin(abs(lat-lat_site)+abs(lo
n-lon_site)),lat.shape)
        PM25_site = PM25_MOD[site_index]
        PM25_mod_date.append(PM25_site)
    PM25_mod.append(PM25_mod_date)
PM25_mod = np.reshape(PM25_mod,(240,))
PM25_obs = np.reshape(PM25_obs,(240,))
```

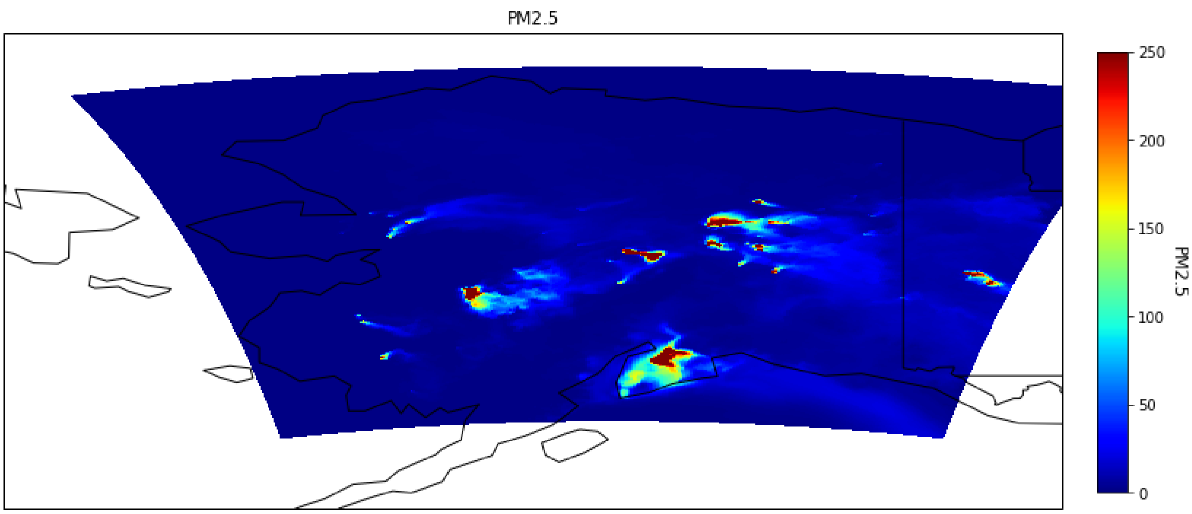
In [5]:
```
# WRF Chem and Observation Line Graph
time = np.arange(0,240)
plt.figure(figsize=(8,8))
plt.plot(time,PM25_mod,'r',time,PM25_obs,'b')
plt.legend(['WRF-Chem','Observation'],fontsize=12)
plt.xlabel('Time',fontsize=14)
plt.ylabel('PM2.5 $\mu g$ $m^{-3}$',fontsize=14)
plt.xlim(0,240)
ax = plt.gca()
ax.set_xticks([0,24,48,72,96,120,144,168,192,216])
ax.set_xticklabels(['6/20','6/21','6/22','6/23','6/24','6/25','6/26','6/
27','6/28','6/29'])
```

Out[5]:
```
[Text(0, 0, '6/20'),
 Text(0, 0, '6/21'),
 Text(0, 0, '6/22'),
 Text(0, 0, '6/23'),
 Text(0, 0, '6/24'),
 Text(0, 0, '6/25'),
 Text(0, 0, '6/26'),
 Text(0, 0, '6/27'),
 Text(0, 0, '6/28'),
 Text(0, 0, '6/29')]
```



In [6]:
```
T2 = data['PM2_5_DRY'][12,0,:,:]
c = 'jet'
e = 'k'
extent = [-175, -135, 55, 73]
plt.figure(figsize=(15, 6))
ax = plt.subplot(1,1,1,projection=ccrs.PlateCarree())
ax.set_extent(extent,ccrs.PlateCarree())
cb = ax.pcolormesh(lon,lat,T2,transform=ccrs.PlateCarree(),cmap=c,vmin=0
,vmax=250)
ax = plt.gca()
ax.coastlines(color='k')
ax.add_feature(cfeature.NaturalEarthFeature('cultural', 'admin_1_states_
provinces_lines', '50m',edgecolor='k', facecolor='none'))
ax.add_feature(cfeature.NaturalEarthFeature('cultural', 'admin_0_boundar
y_lines_land', '50m',edgecolor='k', facecolor='none'))
ax.set_title('PM2.5')
fig = plt.gcf()
fig.subplots_adjust(right=0.8,hspace=0.05,wspace=0.05)
cbar_ax = fig.add_axes([0.82, 0.15, 0.02, 0.7])
cbar = plt.colorbar(cb,cbar_ax)
cbar.ax.get_yaxis().labelpad = 15
cbar.ax.set_ylabel('PM2.5', rotation=270,fontsize=12)
```

Out[6]:
```
Text(0, 0.5, 'PM2.5')
```



In [7]:
```
def smafit(X0,Y0,W0=None,cl=0.95,intercept=True,robust=False,rmethod='Fa
stMCD'):
    """Standard Major-Axis (SMA) line fitting

    Calculate standard major axis, aka reduced major axis, fit to
    data X and Y. The main advantage of this over ordinary least squares
is
    that the best fit of Y to X will be the same as the best fit of X to
Y.

    The fit equations and confidence intervals are implemented following
    Warton et al. (2006). Robust fits use the FastMCD covariance estimat
e
    from Rousseeuw and Van Driessen (1999). While there are many alterna
tive
    robust covariance estimators (e.g. other papers by D.I. Warton using
M-estimators),
    the FastMCD algorithm is default in Matlab. When the standard error
 or
    uncertainty of each point is known, then weighted SMA may be preferr
able to
    robust SMA. The conventional choice of weights for each point i is
    W_i = 1 / ( var(X_i) + var(Y_i) ), where var() is the variance
    (squared standard error).

    References
    Warton, D. I., Wright, I. J., Falster, D. S. and Westoby, M.:
        Bivariate line-fitting methods for allometry, Biol. Rev., 81(0
2), 259,
        doi:10.1017/S1464793106007007, 2006.
    Rousseeuw, P. J. and Van Driessen, K.: A Fast Algorithm for the Mini
mum
        Covariance Determinant Estimator, Technometrics, 41(3), 1999.
    Parameters
    ----------
    X, Y : array_like
        Input values, Must have same length.
    W    : optional array of weights for each X-Y point, typically W_i =
1/(var(X_i)+var(Y_i))
    cl   : float (default = 0.95)
        Desired confidence level for output.
    intercept : boolean (default=True)
        Specify if the fitted model should include a non-zero intercept.
        The model will be forced through the origin (0,0) if intercept=F
alse.
    robust : boolean (default=False)
        Use statistical methods that are robust to the presence of outli
ers
    rmethod: string (default='FastMCD')
        Method for calculating robust variance and covariance. Options:
        'MCD' or 'FastMCD' for Fast MCD
        'Huber' for Huber's T: reduce, not eliminate, influence of outli
ers
        'Biweight' for Tukey's Biweight: reduces then eliminates influen
ce of outliers
```

```
    Returns
    -------
    Slope     : float
        Slope or Gradient of Y vs. X
    Intercept : float
        Y intercept.
    ste_grad : float
        Standard error of gradient estimate
    ste_int : float
        standard error of intercept estimate
    ci_grad : [float, float]
        confidence interval for gradient at confidence level cl
    ci_int : [float, float]
        confidence interval for intercept at confidence level cl
    """

    import numpy as np
    import scipy.stats as stats
    from sklearn.covariance import MinCovDet
    import statsmodels.formula.api as smf
    import statsmodels.robust.norms as norms

    # Make sure arrays have the same length
    assert ( len(X0) == len(Y0) ), 'Arrays X and Y must have the same le
ngth'
    if (W0 != None ):
        assert ( len(W0) == len(X0) ), 'Array W must have the same lengt
h as X and Y'

    # Make sure cl is within the range 0-1
    assert (cl < 1), 'cl must be less than 1'
    assert (cl > 0), 'cl must be greater than 0'

    if (W0==None):
        W0 = np.zeros_like(X0) + 1

    # Drop any NaN elements of X or Y
    # Infinite values are allowed but will make the result undefined
    idx = ~np.logical_or( np.isnan(X0), np.isnan(Y0) )

    X = X0[idx]
    Y = Y0[idx]
    W = W0[idx]

    # Number of observations
    N = len(X)

    # Degrees of freedom for the model
    if (intercept):
        dfmod = 2
    else:
        dfmod = 1


    # Choose whether to use methods robust to outliers
    if (robust):
```

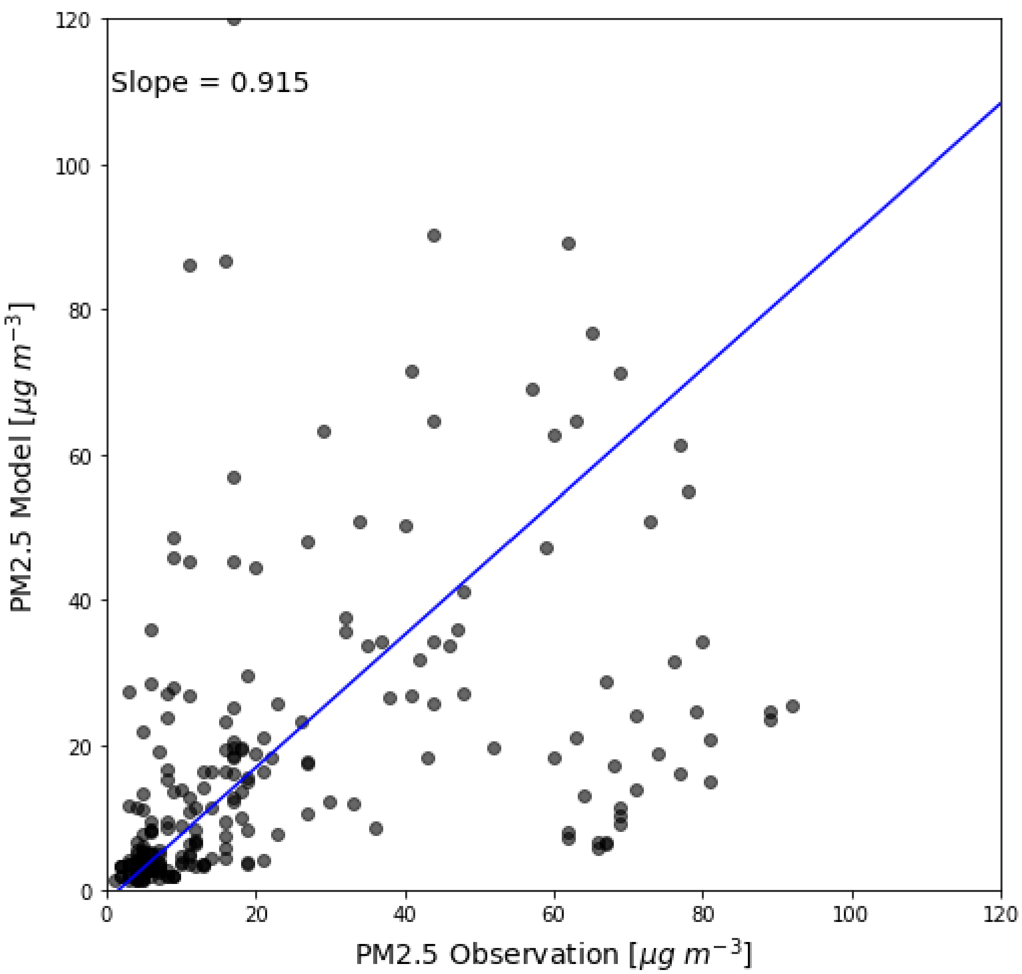
```
        # Choose the robust method
        if ((rmethod.lower() =='mcd') or (rmethod.lower() == 'fastmcd')
):
            # FAST MCD

            if (not intercept):
                # intercept=False could possibly be supported by calcula
ting
                # using mcd.support_ as weights in an explicit variance/
covariance calculation
                raise NotImplementedError('FastMCD method only supports
 SMA with intercept')

            # Fit robust model of mean and covariance
            mcd = MinCovDet().fit( np.array([X,Y]).T )

            # Robust mean
            Xmean = mcd.location_[0]
            Ymean = mcd.location_[1]

            # Robust variance of X, Y
            Vx    = mcd.covariance_[0,0]
            Vy    = mcd.covariance_[1,1]

            # Robust covariance
            Vxy   = mcd.covariance_[0,1]

            # Number of observations used in mean and covariance estimat
e
            # excludes observations marked as outliers
            N = mcd.support_.sum()

        elif ((rmethod.lower() =='biweight') or (rmethod.lower() == 'hub
er') ):

            # Tukey's Biweight and Huber's T
            if ( rmethod.lower() =='biweight'):
                norm = norms.TukeyBiweight()
            else:
                norm = norms.HuberT()

            # Get weights for downweighting outliers
            # Fitting a linear model the easiest way to get these
            # Options include "TukeyBiweight" (totally removes large dev
iates)
            # "HuberT" (linear, not squared weighting of large deviates)
            rweights = smf.rlm('y~x+1',{'x':X,'y':Y},M=norm).fit().weigh
ts

            # Sum of weight and weights squared, for convienience
            rsum  = np.sum( rweights )
            rsum2 = np.sum( rweights**2 )

            # Mean
            Xmean = np.sum( X * rweights ) / rsum
            Ymean = np.sum( Y * rweights ) / rsum
```

```
            # Force intercept through zero, if requested
            if (not intercept):
                Xmean = 0
                Ymean = 0

            # Variance & Covariance
            Vx    = np.sum( (X-Xmean)**2 * rweights**2 ) / rsum2
            Vy    = np.sum( (Y-Ymean)**2 * rweights**2 ) / rsum2
            Vxy   = np.sum( (X-Xmean) * (Y-Ymean) * rweights**2 ) / rsum
2

            # Effective number of observations
            N = rsum

        else:

            raise NotImplementedError("smafit.py hasn't implemented rmet
hod={:%s}".format(rmethod))
    else:

        if (intercept):

            wsum = np.sum(W)

            # Average values
            Xmean = np.sum(X * W) / wsum
            Ymean = np.sum(Y * W) / wsum

            # Covariance matrix
            cov = np.cov( X, Y, ddof=1, aweights=W**2 )

            # Variance
            Vx = cov[0,0]
            Vy = cov[1,1]

            # Covariance
            Vxy = cov[0,1]

        else:

            # Force the line to pass through origin by setting means to
 zero
            Xmean = 0
            Ymean = 0

            wsum = np.sum(W)

            # Sum of squares in place of variance and covariance
            Vx = np.sum( X**2 * W ) / wsum
            Vy = np.sum( Y**2 * W ) / wsum
            Vxy= np.sum( X*Y  * W ) / wsum

    # Standard deviation
    Sx = np.sqrt( Vx )
    Sy = np.sqrt( Vy )

    # Correlation coefficient (equivalent to np.corrcoef()[1,0] for non-
```

```
robust cases)
    R = Vxy / np.sqrt( Vx * Vy )

    #############
    # SLOPE

    Slope  = np.sign(R) * Sy / Sx

    # Standard error of slope estimate
    ste_slope = np.sqrt( 1/(N-dfmod) * Sy**2 / Sx**2 * (1-R**2) )

    # Confidence interval for Slope
    B = (1-R**2)/(N-dfmod) * stats.f.isf(1-cl,1,N-dfmod)
    ci_grad = Slope * ( np.sqrt( B+1 ) + np.sqrt(B)*np.array([-1,+1]) )

    #############
    # INTERCEPT

    if (intercept):
        Intercept = Ymean - Slope * Xmean

        # Standard deviation of residuals
        # New Method: Formula from smatr R package (Warton)
        # This formula avoids large residuals of outliers when using rob
ust=True
        Sr = np.sqrt((Vy - 2 * Slope * Vxy + Slope**2 *  Vx ) * (N-1) /
(N-dfmod) )

        # OLD METHOD
        # Standard deviation of residuals
        #resid = Y - (Intercept + Slope * X )
        # Population standard deviation of the residuals
        #Sr = np.std( resid, ddof=0 )

        # Standard error of the intercept estimate
        ste_int = np.sqrt( Sr**2/N + Xmean**2 * ste_slope**2  )

        # Confidence interval for Intercept
        tcrit = stats.t.isf((1-cl)/2,N-dfmod)
        ci_int = Intercept + ste_int * np.array([-tcrit,tcrit])

    else:

        # Set Intercept quantities to zero
        Intercept = 0
        ste_int   = 0
        ci_int    = np.array([0,0])


    return Slope, Intercept, ste_slope, ste_int, ci_grad, ci_int
```

In [10]:
```
# Scatter Plot With Linear Regression
from scipy import stats
# Create Linear Best Fit
PM25_mod = np.delete(PM25_mod,20)
PM25_obs = np.delete(PM25_obs,20)
slope, intercept, ste_slope, ste_int, ci_grad, ci_int = smafit(X0=PM25_o
bs,Y0=PM25_mod,W0=None,cl=0.95,intercept=True,robust=True,rmethod='FastM
CD')
b = str(round(intercept,4))
string = 'Slope = '+str(round(slope,3))
mod_for_linear   = np.arange(0,200,1)
obs_from_linear = mod_for_linear * slope + intercept
plt.figure(figsize=(8,8))
plt.scatter(PM25_obs,PM25_mod,c='k',alpha=0.6)
plt.plot(mod_for_linear,obs_from_linear, 'b')
plt.ylabel('PM2.5 Model [$\mu g$ $m^{-3}$]',fontsize=14)
plt.xlabel('PM2.5 Observation [$\mu g$ $m^{-3}$]',fontsize=14)
plt.text(0.5,110,string,fontsize=14)
plt.xlim(0,120)
plt.ylim(0,120)
```

Out[10]: (0, 120)



In [ ]:
```
np.argwhere(np.isnan(PM25_obs))
```