

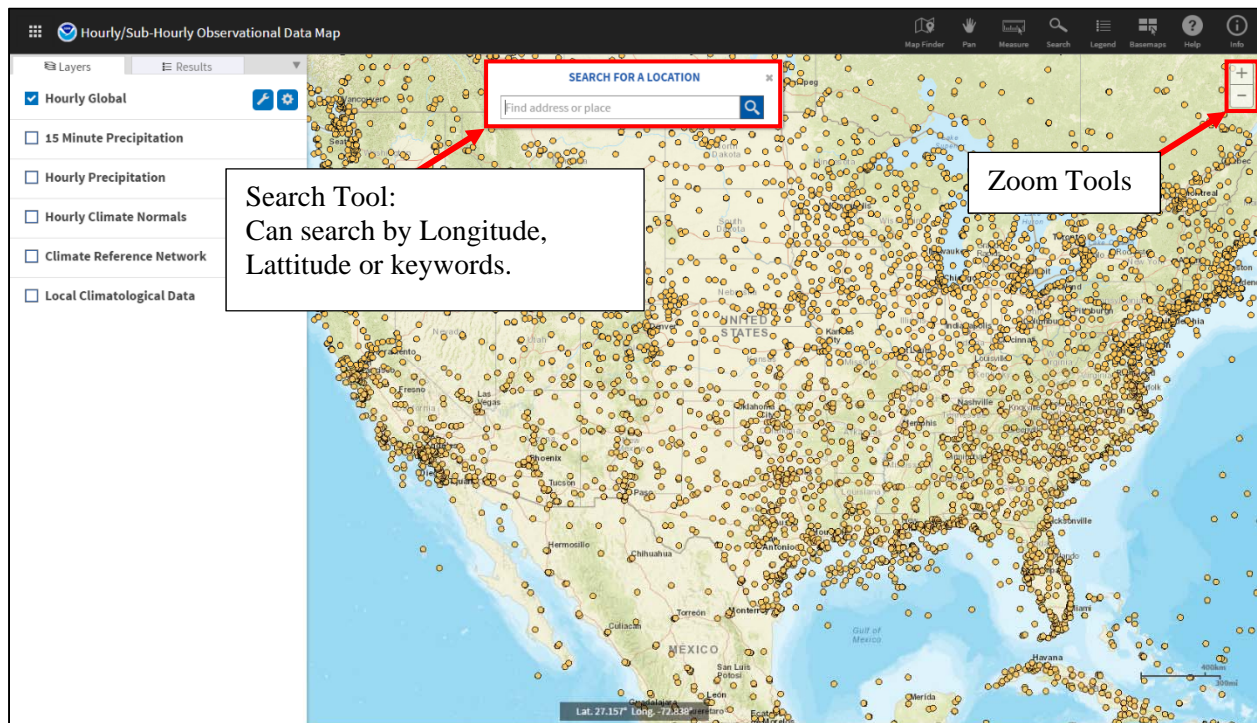
Steps to Run Effective Volume Model:

Note: This file has been updated from a previous version produced for Herkert et. al. (2016).¹

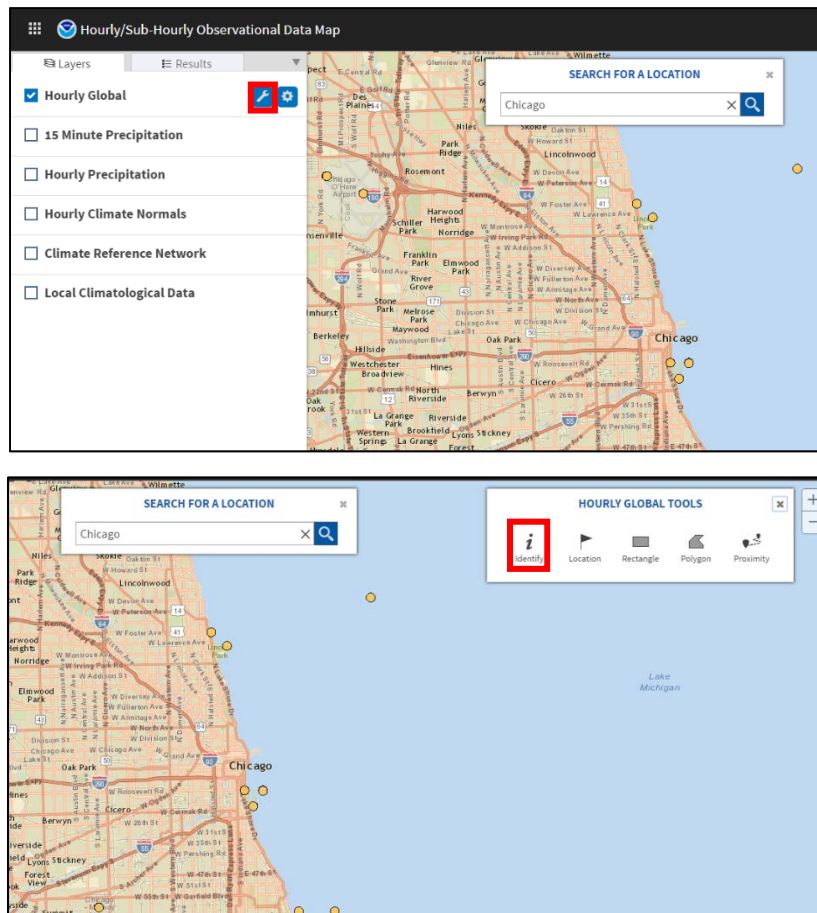
1. Identify the Site ID of the NOAA Integrated Surface Dataset that corresponds to the spatial location of your study using the Map Tool provided on the NOAA website
 - a. Go to → <https://gis.ncdc.noaa.gov/map/viewer/>
 - b. Click on Hourly/Sub-Hourly under the Time-Related Maps tab on the map GUI



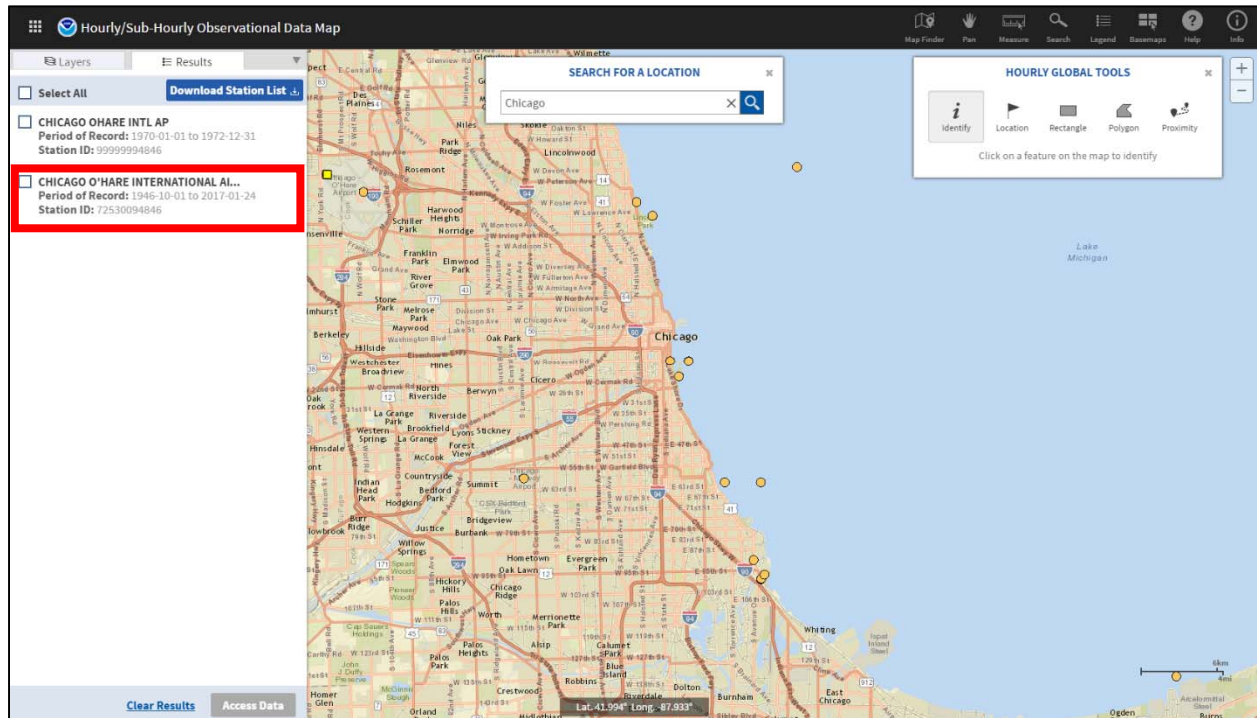
- c. Use the Map to zoom into the spatial location of your sampling location or search for your location.



- d. Click on the information cursor option in the upper left hand corner of the screen



- e. Select a weather station that is spatially close to your sampling location and ensure the weather data spans the appropriate time to encapsulate your study. (From our experience the best data quality typically comes from Airport data and we recommend selecting airport data where possible.)



- f. If the weather station spans the appropriate time span, record the station id, for future reference (from above example 72530094846)

2. Obtain the Raw NOAA ISD Lite file for the given year/years of your study and download them into your MATLAB workspace

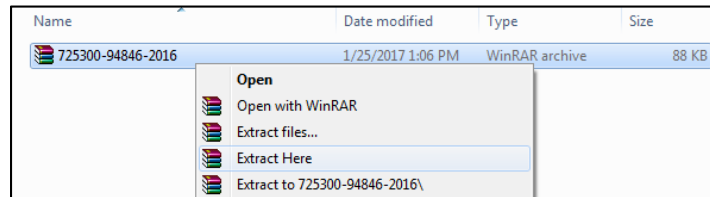
- a. Go to → <ftp://ftp.ncdc.noaa.gov/pub/data/noaa/isd-lite>
- b. Select the appropriate year for your study

| Index of /pub/data/noaa/isd-lite | | |
|----------------------------------|------|----------------------|
| Name | Size | Date Modified |
| [parent directory] | | |
| 1901/ | | 9/29/14, 12:00:00 AM |
| 1902/ | | 9/29/14, 12:00:00 AM |
| 1903/ | | 9/29/14, 12:00:00 AM |
| 1904/ | | 9/29/14, 12:00:00 AM |
| 1905/ | | 9/29/14, 12:00:00 AM |
| 1906/ | | 9/29/14, 12:00:00 AM |
| 1907/ | | 9/29/14, 12:00:00 AM |
| 1908/ | | 9/29/14, 12:00:00 AM |
| 1909/ | | 9/29/14, 12:00:00 AM |
| 1910/ | | 9/29/14, 12:00:00 AM |

- c. Locate the weather station ID previously recorded via the map tool (We recommend using the search function control-f)

| | | |
|----------------------|---------|---------------------|
| 725283-99999-2016.gz | 3.5 kB | 1/23/17, 4:25:00 PM |
| 725287-04724-2016.gz | 87.6 kB | 1/23/17, 4:25:00 PM |
| 725290-14768-2016.gz | 87.2 kB | 1/23/17, 4:25:00 PM |
| 725292-14976-2016.gz | 77.4 kB | 1/23/17, 4:25:00 PM |
| 725294-99999-2016.gz | 51.1 kB | 1/23/17, 4:25:00 PM |
| 725300-94846-2016.gz | 87.9 kB | 1/23/17, 4:25:00 PM |
| 725305-94892-2016.gz | 85.8 kB | 1/23/17, 4:25:00 PM |
| 725314-03960-2016.gz | 83.4 kB | 1/23/17, 4:25:00 PM |
| 725315-94870-2016.gz | 86.0 kB | 1/23/17, 4:25:00 PM |
| 725316-03887-2016.gz | 85.2 kB | 1/23/17, 4:25:00 PM |
| 725317-53802-2016.gz | 84.7 kB | 1/23/17, 4:25:00 PM |

- d. Download the appropriate file and extract the zip file.



- e. Move the extracted file to the folder containing the **process_isd_metdatav2.m** script
- f. Repeat Steps B through E for each required year of meteorological data (if your study spans more than one year)

| Name | Date modified | Type | Size |
|------------------------------------|--------------------|----------------------|--------|
| 725300-94846-2014 | 1/15/2016 5:35 AM | File | 531 KB |
| 725300-94846-2015 | 3/21/2016 1:50 PM | File | 531 KB |
| 725300-94846-2016 | 1/23/2017 3:25 PM | File | 532 KB |
| Chemical_Descriptors | 1/12/2017 2:54 PM | Microsoft Excel C... | 14 KB |
| process_isd_metdatav2.m | 1/31/2017 11:26 AM | M File | 12 KB |
| PUF_PAS_Effective_Volume_Modelv2.m | 1/31/2017 12:46 PM | M File | 13 KB |

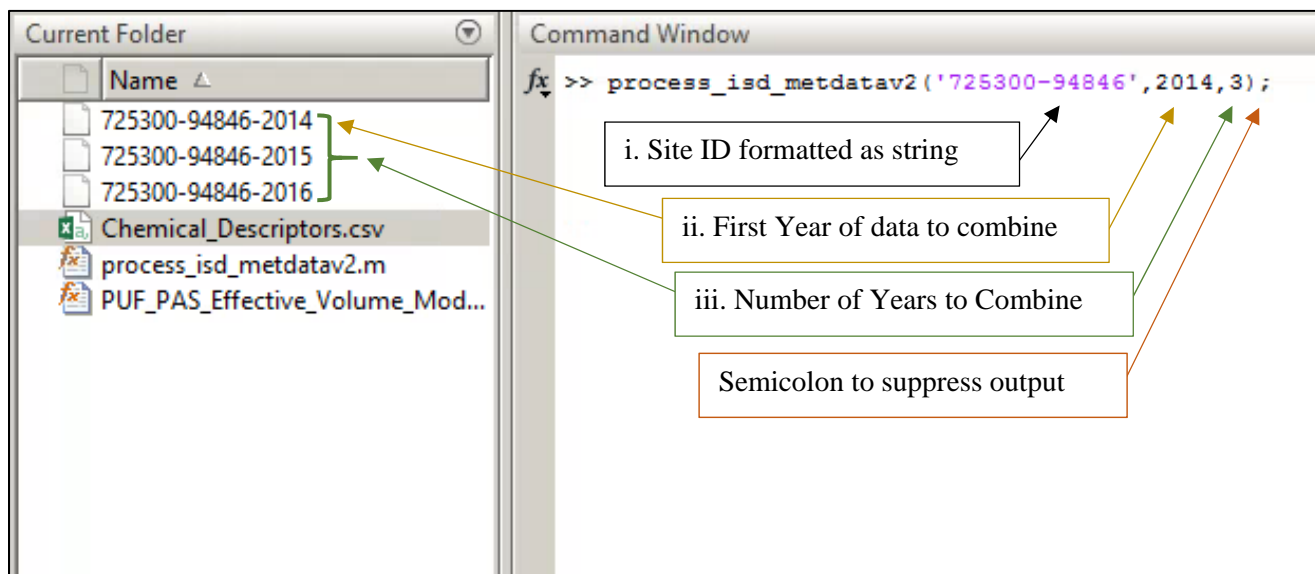
3. Check the data quality and convert the meteorological data to the required format of each individual year using the **process_isd_metdatav2.m** script.

a. The input should be in the form of

process_isd_metdatav2 ('XXXXXX-XXXXX',iYear, NumberYears);

where,

- 'XXXXXX-XXXXX' = the site ID to be combine formatted as a string (i.e. enclosed in apostrophes ' ').
- iYear = the first year of the data to be combined
- NumberYears = the number of years to be combined



- b. A final formatted csv file with the site ID will be created with a summary of the data quality for each year that will be both printed to the screen after the run and saved as a readme file to be accessed later. The readme file will overwrite any previous version of the file. The script will provide a summary of missing values for all 5 weather parameters and detect any gaps greater than 12 hours.
- c. Below is an example of a weather data station being run for 3 consecutive years and the resulting data quality summary.

Current Folder

- 725300-94846-2014
- 725300-94846-2014_ReadMe.txt
- 725300-94846-2015
- 725300-94846-2015_ReadMe.txt
- 725300-94846-2016
- 725300-94846-2016_ReadMe.txt
- 725300-94846.csv
- Chemical_Descriptors.csv
- process_isd_metdatav2.m
- PUF_PAS_Effective_Volume_Mod...

Command Window

```
>> process_isd_metdatav2('725300-94846',2014,3);
```

-----Data Quality Summary for the input site 725300-94846-2014-----

| | |
|--|-----------------|
| Total Missing Hours for Temperature | = 5 (0.057078%) |
| Total Missing Hours for Dew Point | = 5 (0.057078%) |
| Total Missing Hours for Pressure | = 158 (1.8037%) |
| Total Missing Hours for Wind Direction | = 99 (1.1301%) |
| Total Missing Hours for Wind Speed | = 5 (0.057078%) |

-----Data Quality Summary for the input site 725300-94846-2015-----

| | |
|--|-----------------|
| Total Missing Hours for Temperature | = 2 (0.022831%) |
| Total Missing Hours for Dew Point | = 2 (0.022831%) |
| Total Missing Hours for Pressure | = 116 (1.3242%) |
| Total Missing Hours for Wind Direction | = 101 (1.153%) |
| Total Missing Hours for Wind Speed | = 2 (0.022831%) |

-----Data Quality Summary for the input site 725300-94846-2016-----

| | |
|--|-----------------|
| Total Missing Hours for Temperature | = 3 (0.034153%) |
| Total Missing Hours for Dew Point | = 3 (0.034153%) |
| Total Missing Hours for Pressure | = 113 (1.2864%) |
| Total Missing Hours for Wind Direction | = 138 (1.571%) |
| Total Missing Hours for Wind Speed | = 3 (0.034153%) |

Annotations:

- Final combined formatted csv file:** Points to `725300-94846.csv` in the file explorer.
- Saved Data Quality Readme files:** Points to the `ReadMe.txt` files in the file explorer.
- Different years of the study:** Points to the three separate data quality summary blocks.
- # of missing values:** Points to the first number in the summary rows (e.g., 5, 2, 3).
- % of total hours:** Points to the percentage in parentheses (e.g., 0.057078%, 0.022831%, 0.034153%).

- d. The script will also detect if there are any gaps in data greater than 12 hours. This threshold can be change in **line 50** of the **process_isd_metdatav2.m** script if desired. In the example shown below there are several gaps greater than 12 hours for temperature, dew point, wind speed, and wind direction, while pressure is missing all measurements for the year. This data quality would be insufficient for the flowrate model since it does not contain any pressure measurements, and a different weather station would need to be selected (steps 1-2)

```

47
48     %Subfunction that logs any large gaps for all variable.
49
50 -     LargeGapThreshold = 12; %Threshold (in hours) for flagging consecutive missing values
51
52 -     TALargeGaps = findlargegaps(metdata(:,5),LargeGapThreshold);
53 -     TDLargeGaps = findlargegaps(metdata(:,6),LargeGapThreshold);
54 -     PrLargeGaps = findlargegaps(metdata(:,7),LargeGapThreshold);
55 -     WDLargeGaps = findlargegaps(metdata(:,8),LargeGapThreshold);
56 -     WSLargeGaps = findlargegaps(metdata(:,9),LargeGapThreshold);
57

```

Current Folder

- 725300-94846-2014
- 725300-94846-2014_ReadMe.txt
- 725300-94846-2015
- 725300-94846-2015_ReadMe.txt
- 725300-94846-2016
- 725300-94846-2016_ReadMe.txt
- 725300-94846.csv
- 997338-99999-2016
- 997338-99999-2016_ReadMe.txt
- 997338-99999.csv
- Chemical_Descriptors.csv
- process_isd_metdatav2.m
- PUF_PAS_Effective_Volume_Mod...

Command Window

```

>> process_isd_metdatav2('997338-99999',2016,1);
-----Data Quality Summary for the input site 997338-99999-2016-----

Total Missing Hours for Temperature = 207(2.3566%)
Total Missing Hours for Dew Point = 250(2.8461%)
Total Missing Hours for Pressure = 8784(100%)
Total Missing Hours for Wind Direction = 201(2.2883%)
Total Missing Hours for Wind Speed = 201(2.2883%)

-----Gaps > 12 hours in Data for Temperature-----
Missing Data for 22 hours between 2016022814 and 2016022912
Missing Data for 24 hours between 2016111021 and 2016111121
Missing Data for 43 hours between 2016112917 and 2016120112
Missing Data for 40 hours between 2016120923 and 2016121115

-----Gaps > 12 hours in Data for Dew Point-----
Missing Data for 22 hours between 2016022814 and 2016022912
Missing Data for 24 hours between 2016111021 and 2016111121
Missing Data for 39 hours between 2016111822 and 2016112013
Missing Data for 43 hours between 2016112917 and 2016120112
Missing Data for 40 hours between 2016120923 and 2016121115

-----Gaps > 12 hours in Data for Pressure-----
Missing Data for 8784 hours between 2016010100 and 2016123123

-----Gaps > 12 hours in Data for Wind Speed-----
Missing Data for 22 hours between 2016022814 and 2016022912
Missing Data for 24 hours between 2016111021 and 2016111121
Missing Data for 43 hours between 2016112917 and 2016120112
Missing Data for 40 hours between 2016120923 and 2016121115

-----Gaps > 12 hours in Data for Wind Direction-----
Missing Data for 22 hours between 2016022814 and 2016022912
Missing Data for 24 hours between 2016111021 and 2016111121
Missing Data for 43 hours between 2016112917 and 2016120112
Missing Data for 40 hours between 2016120923 and 2016121115
fx >>

```

Summary Results

Missing all pressure

Gaps greater than large gap threshold listed here (12 hours is default)

4. After the met data has been converted use the **PUF_PAS_Effective_Volume_Modelv2.m** script to obtain congener and deployment specific effective sampling volumes and sampling rates [Note: ensure the accompanying SVOC physical-chemical and LFER descriptors properties CSV file (**Chemical_Descriptors.csv**) is in the same location as the **PUF_PAS_Effective_Volume_Modelv2.m** script].

- a. Prior to running the script a few modification at the beginning of the script may need to be made at the beginning of the script.

1. **Line 12:** Output file name (Use a name descriptive to the specific run)
2. **Line 17:** Select the method for determining the air/PUF partition coefficient
 - a. Method 1 is the empirical relationship (with temperature adjusted Koa) from Shoeib and Harner (2002)²
 - b. Method 2 is the temperature dependent linear free energy relationship for polyurethane foam from Sprunger et al. (2007)³
3. **Lines 21-24:** PUF Disk Parameters specific to the study.

Note: A screen shot of the beginning of the script where the above parameters can be adjusted is shown below.

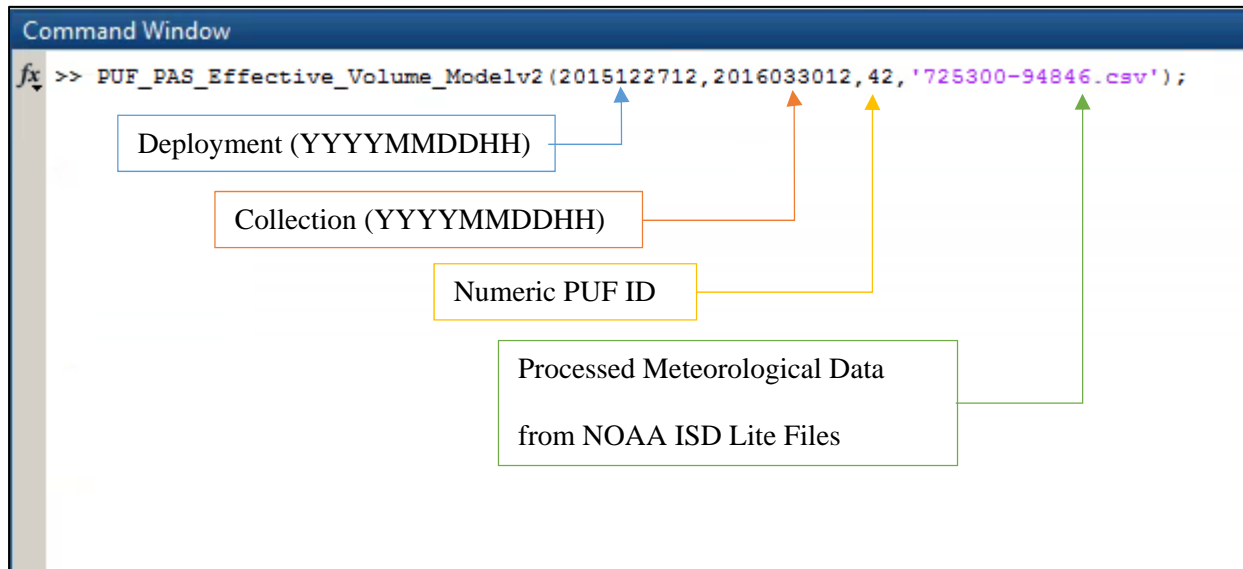
```
1 function(PAS_Array,DeploymentMetData) = PUF_PAS_Effective_Volume_Modelv2(Deployment,Collection,PUF_ID,MET_ID)
2 %This version of the model was published by Herkert et al. (2017) Environ. Sci. Technol.
3 %based upon a model first developed by Petrich et al. (2013) Environ. Sci. Technol. and Herkert et al. (2016) Environ. Sci. Technol.
4
5 %Input variable formats:
6 % Deployment = PUF Deployment Date formatted as YYYYMMDDHH
7 % Collection = PUF Collection Date formatted as YYYYMMDDHH
8 % PUF_ID = Numerical PUF ID for identification in output data set
9 % MET_ID = string of AWS site ID formatted as 'XXXXXX-XXXXX.csv' for the weather data to be used for the PUF deployment
10
11 %Specify output file name and location
12 outfilename = 'Generic_Output_File_Name.csv';
13
14 %Specify the method for determining KPUF.
15 % KOA = Empirical relationship with temperature adjusted Koa from Shoeib and Harner (2002) Environ. Sci. Technol.
16 % LFER = Temperature dependent linear free energy relationship for polyurethane foam from Sprunger et al. (2007) Anal. Chem.
17 KPUFmethod = 'KOA'; %KOA or LFER
18
19 %Declarations: Known variables about PUF disk parameters to be used
20 %The default parameters are for PUF from Tisch Environmental used by Herkert et al. (2017)
21 diameter = 0.1397; % Length of PUF disk (m)
22 thickness = 0.0127; % Thickness of PUF disk (m)
23 dpuf = 23630; % Density of PUF (g/m^3)
24 As = .0365; % Surface area of the PUF (m^2)
25
```


b. The input should be in the form

PUF_PAS_Effective_Volume_Modelv2(Deployment,Collection,PUF_ID,MET_ID);

where,

- i. Deployment = PUF Deployment Date formatted as YYYYMMDDHH
- ii. Collection = PUF Collection Date formatted as YYYYMMDDHH
- iii. PUF_ID = Numerical PUF ID for identification in output data
- iv. MET_ID = string of AWS site ID formatted as 'XXXXXX-XXXXX' for the weather data to be used for the PUF deployment



- c. The final output file will produce a comma delimited file that can be opened in Microsoft Excel.

| | A | B | C | D | E | F | G | H | I | J |
|----|----|------------|------------|------|---|----------|----------|----------|----------|----------|
| 1 | 42 | 2015122712 | 2016033012 | 2257 | 1 | 83.9329 | 146.3399 | 153.1927 | 184.3405 | 250.7427 |
| 2 | 42 | 2015122712 | 2016033012 | 2257 | 2 | 4.042036 | 4.042036 | 4.042036 | 3.822283 | 3.822283 |
| 3 | | | | | | | | | | |
| 4 | | | | | | | | | | |
| 5 | | | | | | | | | | |
| 6 | | | | | | | | | | |
| 7 | | | | | | | | | | |
| 8 | | | | | | | | | | |
| 9 | | | | | | | | | | |
| 10 | | | | | | | | | | |
| 11 | | | | | | | | | | |
| 12 | | | | | | | | | | |
| 13 | | | | | | | | | | |
| 14 | | | | | | | | | | |
| 15 | | | | | | | | | | |
| 16 | | | | | | | | | | |
| 17 | | | | | | | | | | |
| 18 | | | | | | | | | | |
| 19 | | | | | | | | | | |
| 20 | | | | | | | | | | |
| 21 | | | | | | | | | | |
| 22 | | | | | | | | | | |
| 23 | | | | | | | | | | |
| 24 | | | | | | | | | | |
| 25 | | | | | | | | | | |

Numerically Coded Output Variables;
 1 = Effective Sampling Volume (m³)
 2 = Sampling Rate (m³/d)

Deployment Length (hours)

Collection (YYYYMMDDHH)

Deployment (YYYYMMDDHH)

Numeric PUF ID

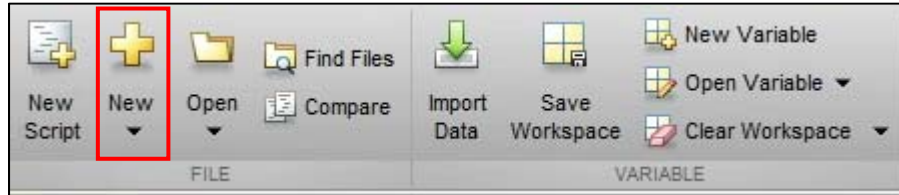
PCB 1

PCB 2

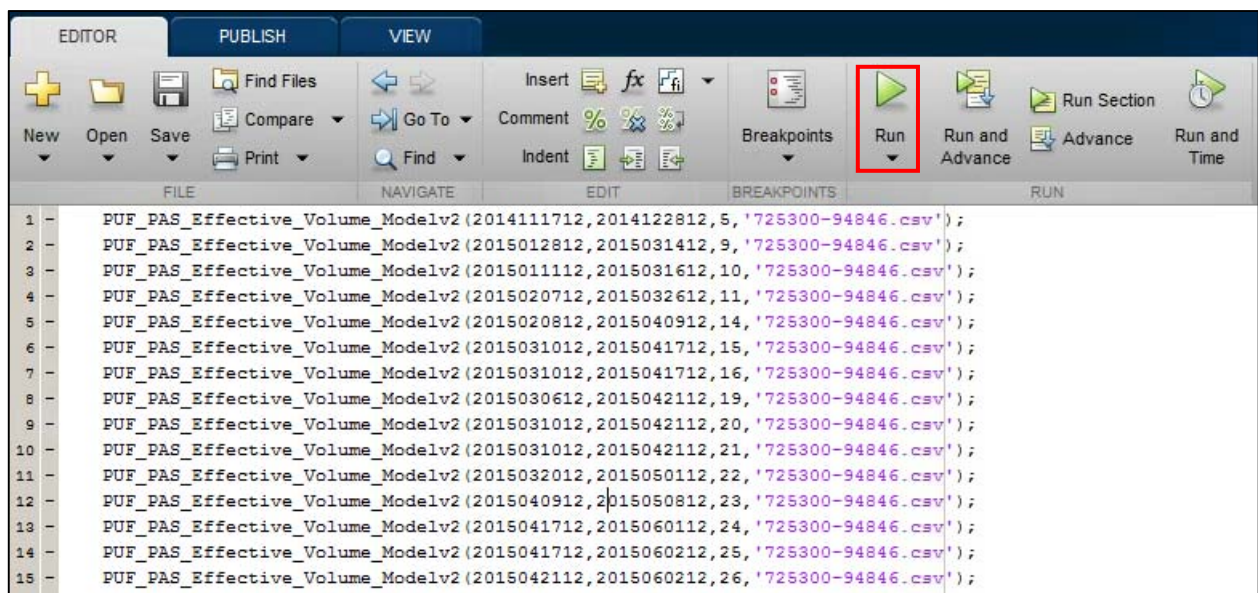
PCB 209

5. **(OPTIONAL)** If you want to run many samples in a row, a new script can be set up to run PUF consecutively.

- a. First open a new blank script by clicking “New Script” in the open left-hand corner of the MATLAB window.



- b. Then repeat the format from step 4B for as many PUF as needed and hit run (highlighted in red box)



- c. These run commands can also be created in excel using the concatenate function and pasted into the new script to speed up this process.

SUM

:

=CONCATENATE("PUF_PAS_Effective_Volume_Modelv2(",B11,"",C11,"",A11,"",D11,"");)

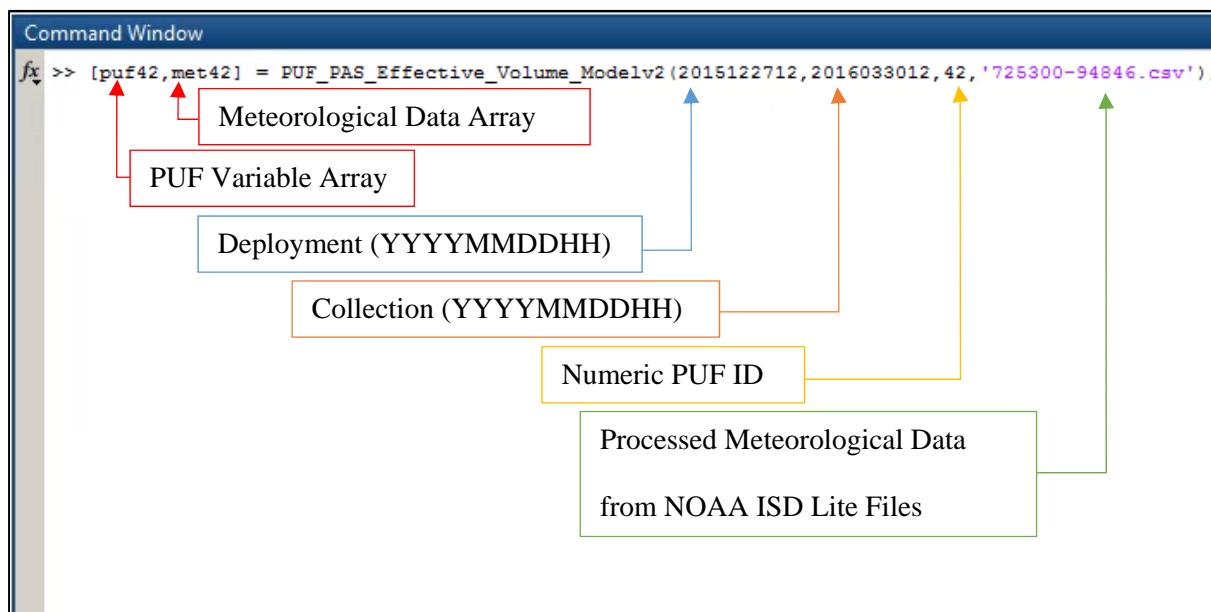
| | A | B | C | D | E | F |
|----|----------------|---|------------|--------------------|---|---|
| 1 | PUFID --> | Numerically Assigned PUF ID for identification in output data | | | | |
| 2 | Deployment --> | Deployment Date formatted as YYYYMMDDHH | | | | |
| 3 | Collection --> | Collection Date formatted as YYYYMMDDHH | | | | |
| 4 | Met_ID --> | AWS Site ID formatted as a string 'XXXXXX-XXXXX' | | | | |
| 5 | | | | | | |
| 6 | PUF_ID | Deployment | Collection | MET_ID | | Run Command |
| 7 | 5 | 2014111712 | 2014122812 | '725300-94846.csv' | | PUF_PAS_Effective_Volume_Modelv2(2014111712,2014122812,5,'725300-94846.csv'); |
| 8 | 9 | 2015012812 | 2015031412 | '725300-94846.csv' | | PUF_PAS_Effective_Volume_Modelv2(2015012812,2015031412,9,'725300-94846.csv'); |
| 9 | 10 | 2015011112 | 2015031612 | '725300-94846.csv' | | PUF_PAS_Effective_Volume_Modelv2(2015011112,2015031612,10,'725300-94846.csv'); |
| 10 | 11 | 2015020712 | 2015032612 | '725300-94846.csv' | | PUF_PAS_Effective_Volume_Modelv2(2015020712,2015032612,11,'725300-94846.csv'); |
| 11 | 14 | 2015020812 | 2015040912 | '725300-94846.csv' | | =CONCATENATE("PUF_PAS_Effective_Volume_Modelv2(",B11,"",C11,"",A11,"",D11,"");) |
| 12 | 15 | 2015031012 | 2015041712 | '725300-94846.csv' | | PUF_PAS_Effective_Volume_Modelv2(2015031012,2015041712,15,'725300-94846.csv'); |
| 13 | 16 | 2015031012 | 2015041712 | '725300-94846.csv' | | PUF_PAS_Effective_Volume_Modelv2(2015031012,2015041712,16,'725300-94846.csv'); |
| 14 | 19 | 2015030612 | 2015042112 | '725300-94846.csv' | | PUF_PAS_Effective_Volume_Modelv2(2015030612,2015042112,19,'725300-94846.csv'); |
| 15 | 20 | 2015031012 | 2015042112 | '725300-94846.csv' | | PUF_PAS_Effective_Volume_Modelv2(2015031012,2015042112,20,'725300-94846.csv'); |

- d. If this is done the output file will have the same format as previously described preceding down the columns in the order the PUF were run

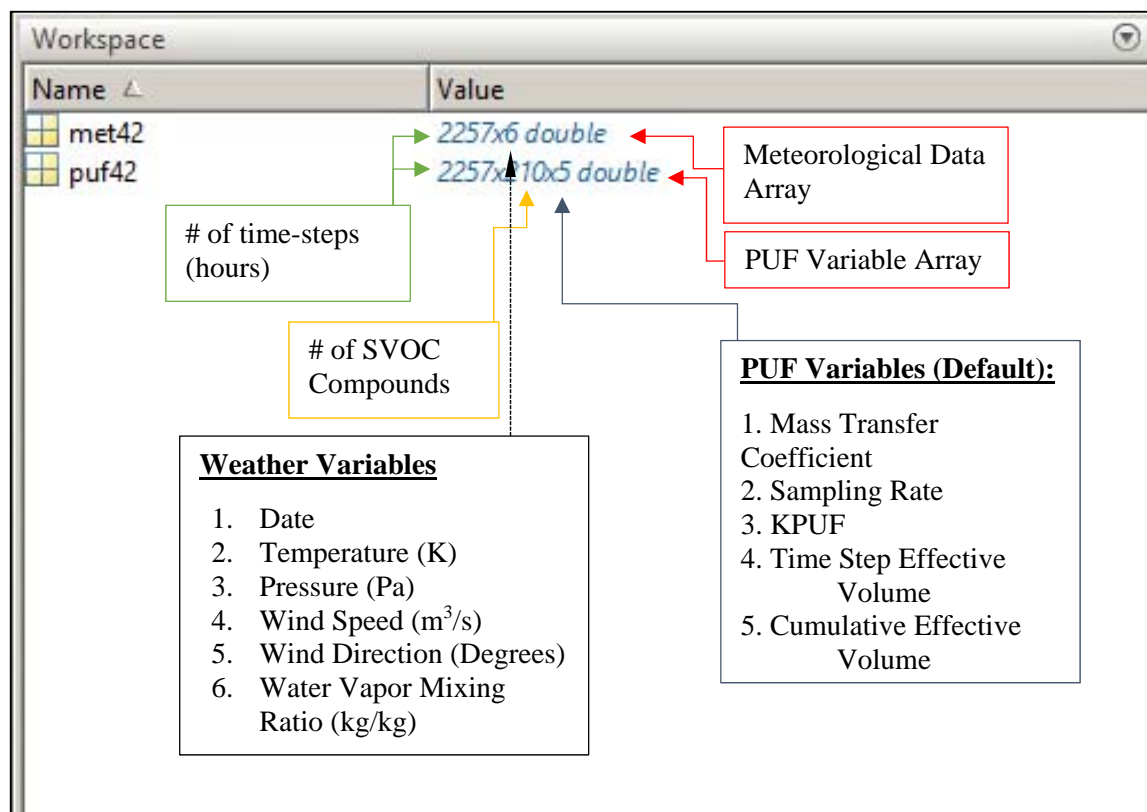
| | A | B | C | D | E | F | G | H | I | J | K | L |
|----|----|------------|------------|------|---|----------|----------|----------|----------|----------|----------|----------|
| 1 | 42 | 2015122712 | 2016033012 | 2257 | 1 | 83.9329 | 146.3399 | 153.1927 | 184.3405 | 250.7427 | 242.1082 | 228.2342 |
| 2 | 42 | 2015122712 | 2016033012 | 2257 | 2 | 4.042036 | 4.042036 | 4.042036 | 3.822283 | 3.822283 | 3.822283 | 3.822283 |
| 3 | 5 | 2014111712 | 2014122812 | 985 | 1 | 84.81323 | 112.1122 | 114.3797 | 119.5428 | 135.1852 | 133.3942 | 130.4054 |
| 4 | 5 | 2014111712 | 2014122812 | 985 | 2 | 3.977707 | 3.977707 | 3.977707 | 3.761451 | 3.761451 | 3.761451 | 3.761451 |
| 5 | 9 | 2015012812 | 2015031412 | 1081 | 1 | 102.028 | 127.9264 | 129.9152 | 132.4777 | 145.3332 | 143.9184 | 141.5383 |
| 6 | 9 | 2015012812 | 2015031412 | 1081 | 2 | 3.756365 | 3.756365 | 3.756365 | 3.552143 | 3.552143 | 3.552143 | 3.552143 |
| 7 | 10 | 2015011112 | 2015031612 | 1537 | 1 | 112.3437 | 155.7359 | 159.3482 | 168.7878 | 194.0246 | 191.1479 | 186.3505 |
| 8 | 10 | 2015011112 | 2015031612 | 1537 | 2 | 3.71422 | 3.71422 | 3.71422 | 3.512289 | 3.512289 | 3.512289 | 3.512289 |
| 9 | 11 | 2015020712 | 2015032612 | 1129 | 1 | 86.67014 | 117.8895 | 120.5463 | 127.4841 | 145.9213 | 143.7802 | 140.2118 |
| 10 | 11 | 2015020712 | 2015032612 | 1129 | 2 | 3.79848 | 3.79848 | 3.79848 | 3.591968 | 3.591968 | 3.591968 | 3.591968 |
| 11 | 14 | 2015020812 | 2015040912 | 1441 | 1 | 79.04936 | 122.1513 | 126.2901 | 141.6948 | 174.3018 | 170.2964 | 163.7176 |
| 12 | 14 | 2015020812 | 2015040912 | 1441 | 2 | 3.877414 | 3.877414 | 3.877414 | 3.666611 | 3.666611 | 3.666611 | 3.666611 |
| 13 | 15 | 2015031012 | 2015041712 | 913 | 1 | 56.45844 | 83.43417 | 86.00739 | 95.20475 | 114.5389 | 112.1347 | 108.1748 |
| 14 | 15 | 2015031012 | 2015041712 | 913 | 2 | 3.940206 | 3.940206 | 3.940206 | 3.725989 | 3.725989 | 3.725989 | 3.725989 |

6. (OPTIONAL) The outputs (as well as meteorological data) can be saved directly in MATLAB to create figures and view trends.

a. Assign Variable for the PUF array and meteorological data



b. After running the **PUF_PAS_Flowrate_Modelv2.m** script, the Meteorological Data Array and PUF Variable Array are available in the workspace.



References

1. Herkert, N. J.; Martinez, A.; Hornbuckle, K. C., A Model Using Local Weather Data to Determine the Effective Sampling Volume for PCB Congeners Collected on Passive Air Samplers. *Environ. Sci. Technol.* **2016**, *50*, (13), 6690-6697.
2. Shoeib, M.; Harner, T., Characterization and comparison of three passive air samplers for persistent organic pollutants. *Environ. Sci. Technol.* **2002**, *36*, (19), 4142-4151.
3. Sprunger, L.; Acree, W. E.; Abraham, M. H., Comment on "Systematic investigation of the sorption properties of polyurethane foams for organic vapors". *Anal. Chem.* **2007**, *79*, (17), 6891-6893.