PNNL-33345

User's Guide

for the

Geospatial Risk Analysis Tool

V 1.0.1

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1 General Information

1.1 System Overview

Performing back trajectory and forward trajectory using the Hybrid Single-Particle Lagrangian Integrated Trajectory Model (HYSPLIT) is a reliable approach for assessing particle transport after release among mid-field atmospheric models (Draxler et al. 2020; Stein et al. 2015). HYSPLIT has an externally facing online interface that allows non-expert users to run the model trajectories without requiring extensive training or programming. However, the existing HYSPLIT interface is limited if simulations have a large amount of meteorological data and timesteps that are not coincident. The existing HYSPLIT Graphical User Interface (GUI) does not easily permit computations of trajectories of a dataset of meteorological data in high temporal frequency. To improve the performance of trajectories computation from a large dataset and enhance risk analysis of the accidental release of material at risk, a Geospatial Risk Analysis Tool (GRAT-GUI) is created to allow large data sets to be processed instantaneously and provide ease of visualization (Hou et al., 2023). In order to perform safety analysis properly, the DOE standard recommends that at least five-years of meteorological data be used (DOE, 2014), therefore the ability to handle big data is highly necessary (Zhou et al., 2022).

The Geospatial Risk Analysis Tool (GRAT) is developed by the Pacific Northwest National Laboratory (PNNL) in collaboration with Oak Ridge National Laboratory (ORNL). This software package is designed to enable batch processing of the Hybrid Single-Particle Lagrangian Integrated Trajectory (HYSPLIT), an open source software developed by the National Oceanic and Atmospheric Administration (NOAA) Air Resources Laboratory and the Australian Bureau of Meteorology Research Center in 1998 for computation of air parcel trajectories, transport, and dispersion. Specifically, the function of trajectory prediction is used in this tool. PSDF is an improved statistical function based on the well-known Potential Source Contribution Function (PSCF) in establishing the air pollutant source and receptor relationship (Pekney et al., 2006; Ren et al., 2019). Performing this analysis requires a range of meteorological and pollutant concentration measurements to be statistically meaningful.

GRAT is used to batch process meteorological data into ARL format to permit more rapid trajectory calculations. While the HYSPLIT GUI limits users to convert meteorological data up to six time stamp points per operation, GRAT allows users to convert a significantly large amount of data within one operation. For example, 10 years of meteorological data can be converted within 5 minutes using a standalone personal computer. When coupled trajectory results with the Potential source distribution function (PSDF), GRAT can be used to determine the areas influenced by the emission of hazardous chemicals.

1.2 Software Requirements

The GRAT will run using any of the following operating systems:

- Windows 10 64bits Software:
- Python 3. x with the following packages:
  - numpy
  - openpyxl
  - scipy
  - matplotlib
  - basemap
  - basemap-data-hires
  - daal4py

1.3 Hardware Requirements

Systems running the SFC software require:

- At least Pentium 233-megahertz (MHz) processing
- At least 64 megabytes (MB) of RAM (128 MB recommended)
- At least 1.5 gigabytes (GB) of available space on the hard disk.

2 System Installation

2.1 System Pre-Installation

To assure proper performance of GRAT, HYSPLIT and Python need to be installed in the computer that will be used for using GRAT. Users can download HYSPLIT from https://www.ready.noaa.gov/HYSPLIT.php and extract it to C:\HYSPLIT. They can also download Python from https://www.python.org/downloads/, and follow installation instructions. Then they can use PIP to install the following Python packages: numpy, openpyxl, scipy, matplotlib, basemap, basemap-data-hires, daal4py.

2.2 Geospatial Risk Analysis Tool Installation

A compressed file will be provided for the GRAT program installation.

Step 1: Navigate to the installation file location.

Step 2. Unzip the compressed file to a local folder. Two files are required for installation:

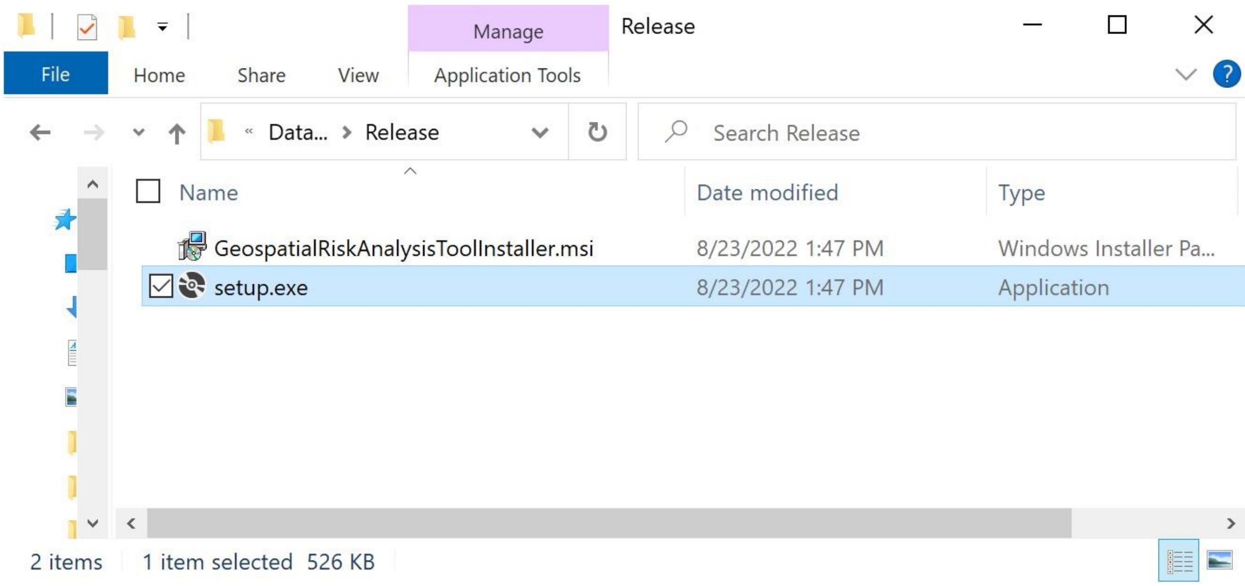


Figure 1. The setup.exe file for GRAT installation.

Step 3: Double-click the "setup.exe" file to begin the installation process. The Setup Wizard will begin the installation process, as depicted in the following figures.

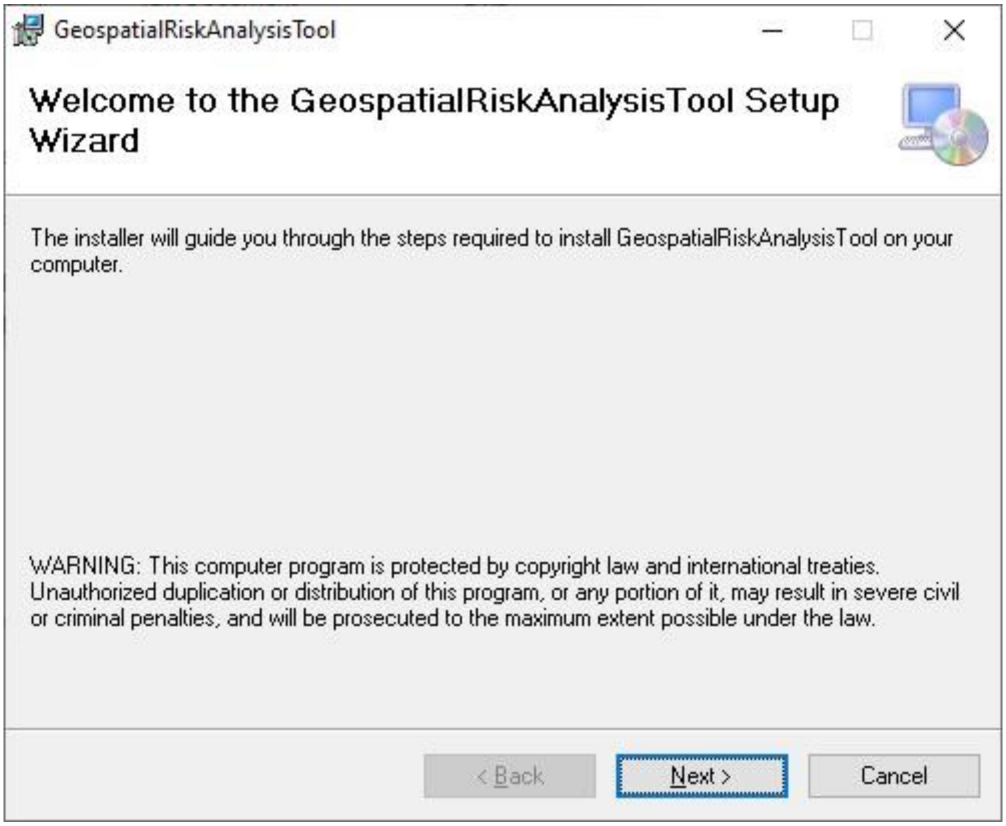


Figure 2. The GRAT installation wizard welcome page.

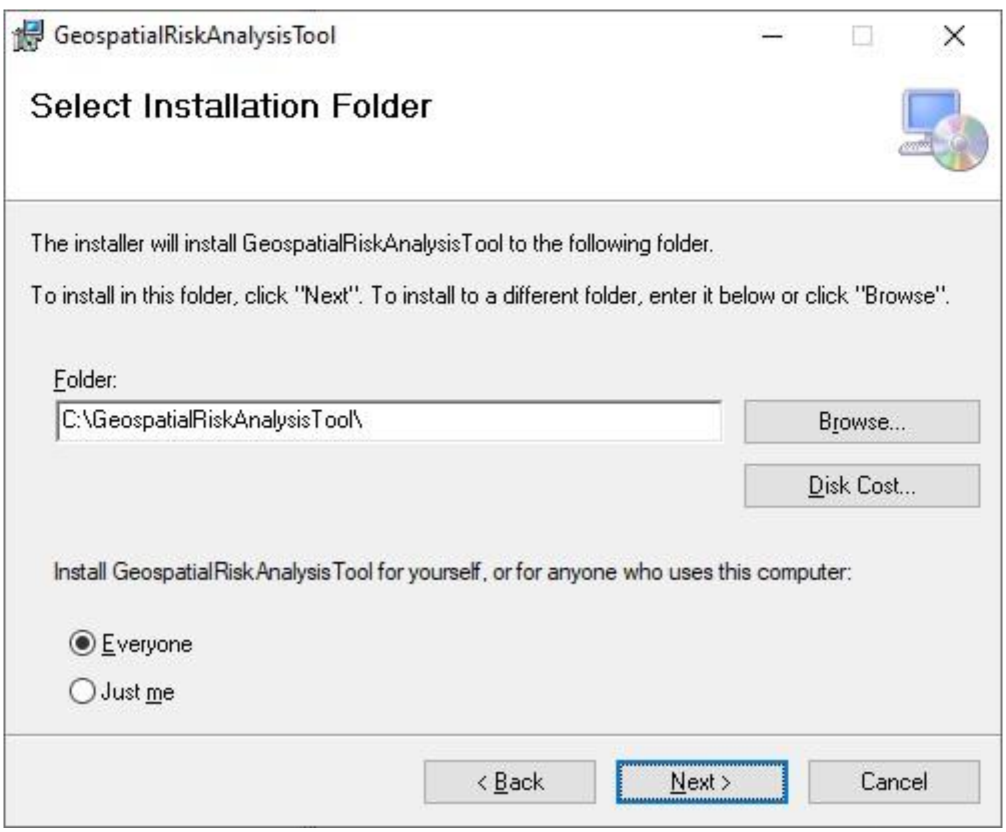


Figure 3. The GRAT installer folder page.

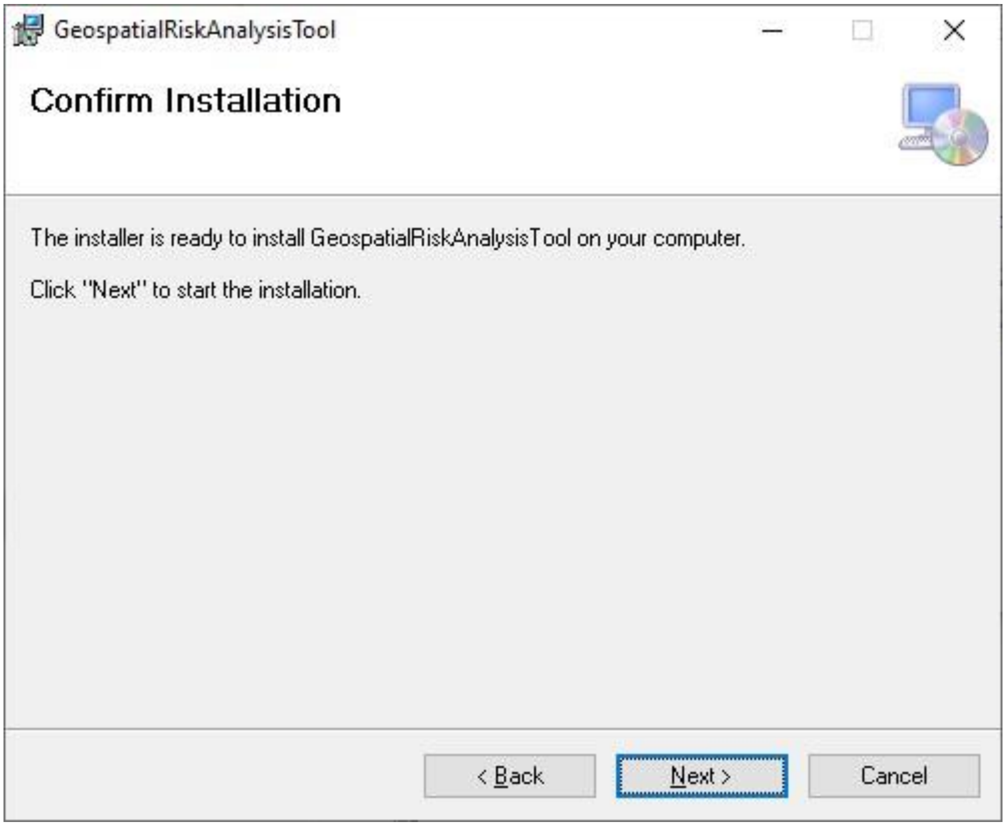


Figure 4. The GRAT installation page.

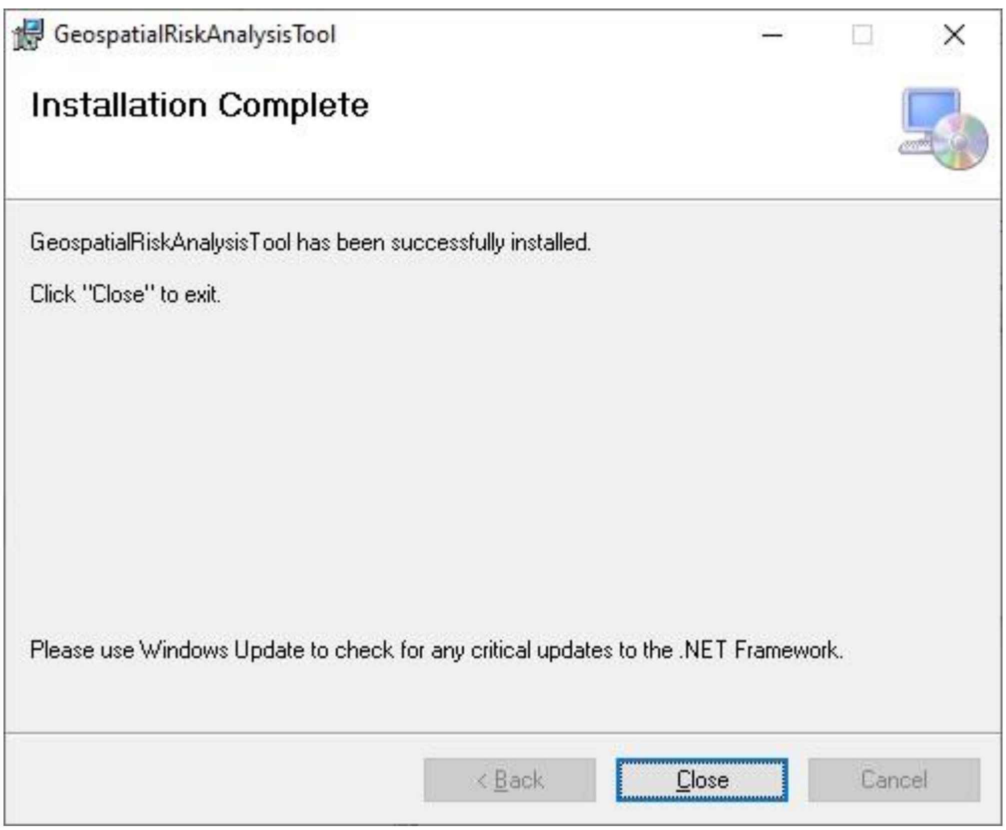


Figure 5. The GRAT installation complete information.

3 Getting Started

3.1 Launching the Application

There are two ways to start the GRAT application:

- Click the Windows Start icon. Select “All Programs” and navigate to and select “GeospatialRiskAnalysisTool”.
- Go to the installation file specified when installing the program (Section 2.2).

The startup screen will open:

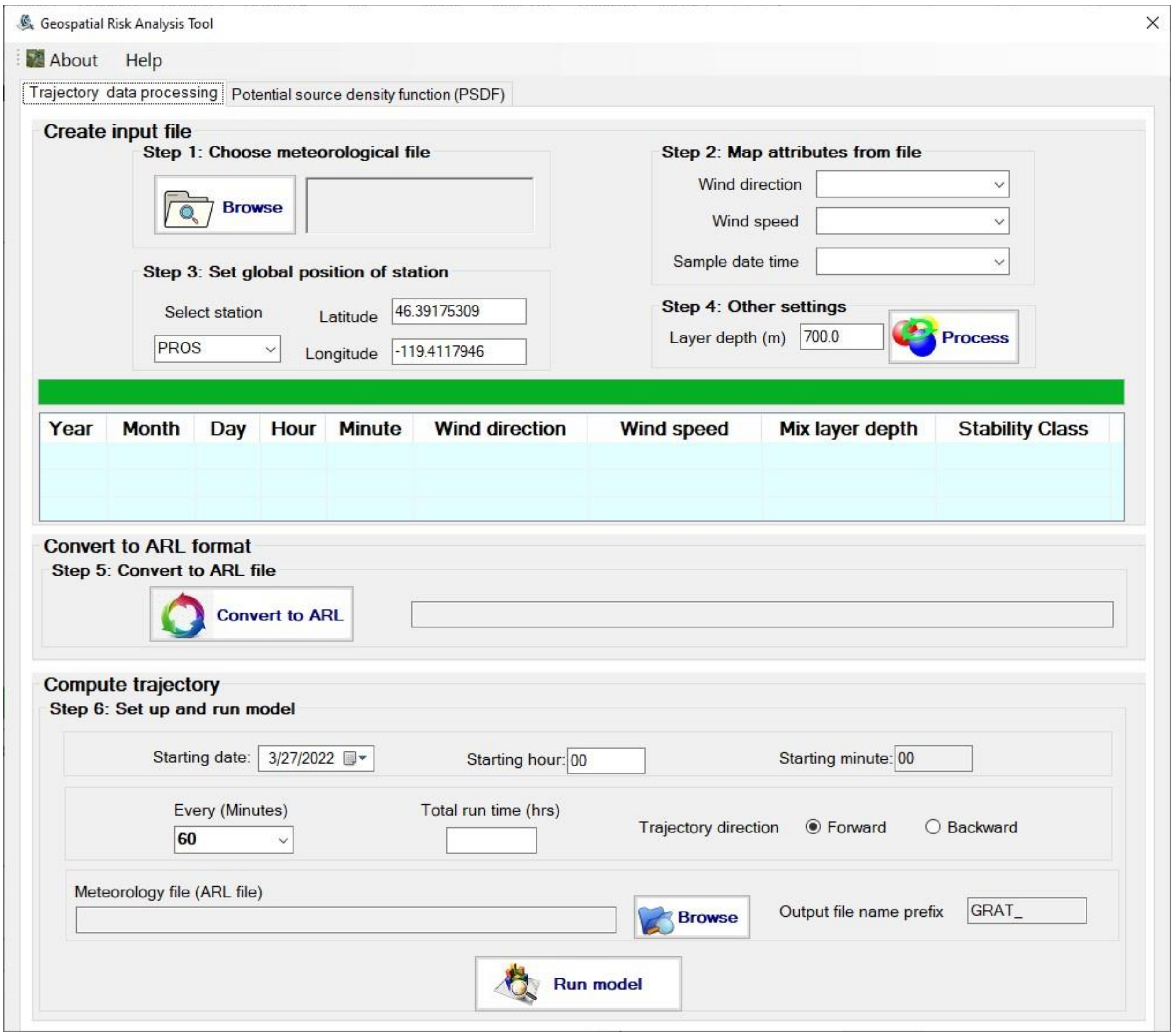
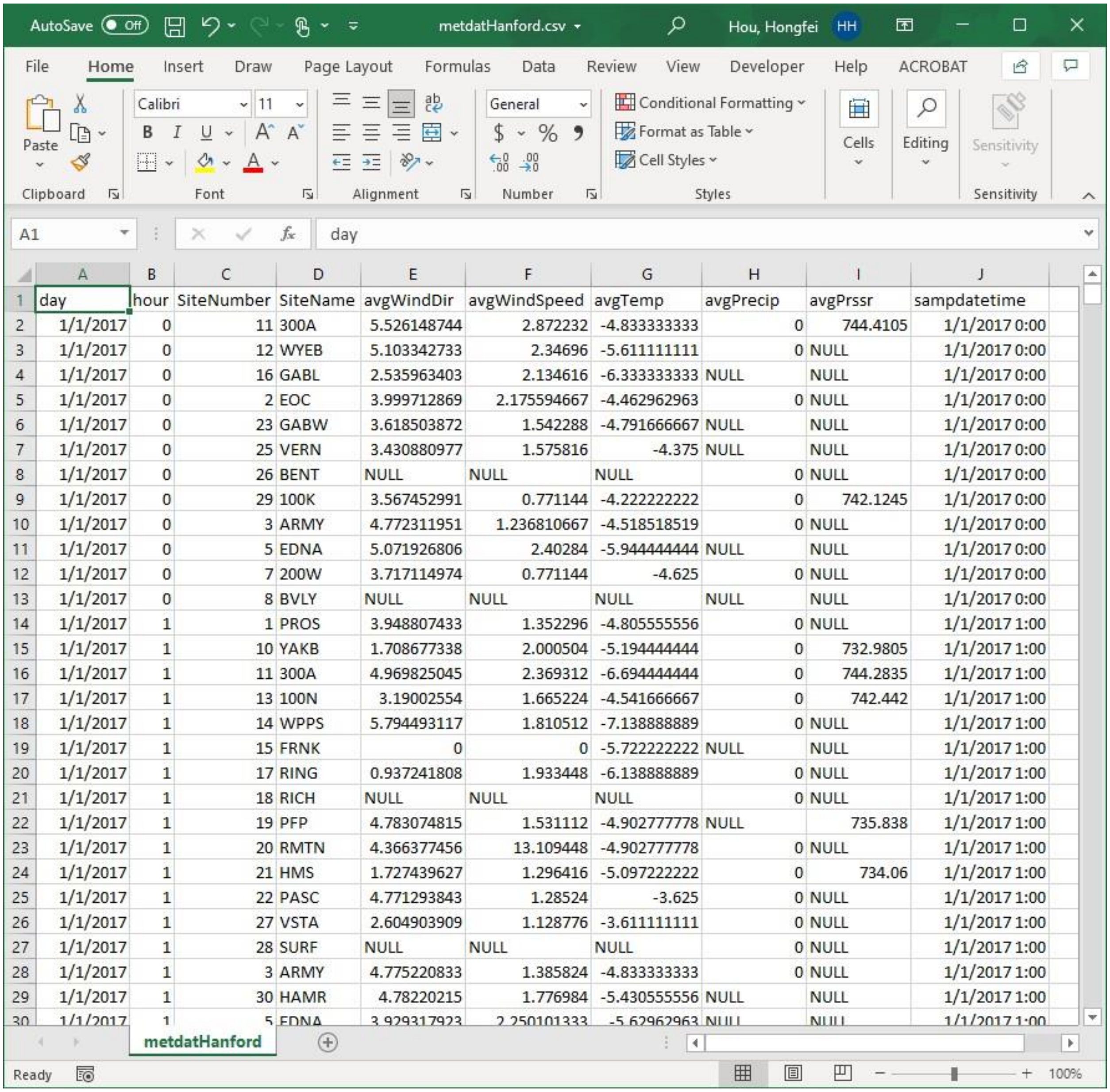


Figure 6. The GRAT setup page.

3.2 Data Preparation

The expected input files for GRAT should be in .csv format. Each file should contain at least three columns, including wind direction, wind speed, and the timestamp values obtained from meteorological measurements. Here is an example:



day	hour	SiteNumber	SiteName	avgWindDir	avgWindSpeed	avgTemp	avgPrecip	avgPrssr	sampdatetime
1/1/2017	0	11	300A	5.526148744	2.872232	-4.833333333	0	744.4105	1/1/2017 0:00
1/1/2017	0	12	WYEB	5.103342733	2.34696	-5.611111111	0	NULL	1/1/2017 0:00
1/1/2017	0	16	GABL	2.535963403	2.134616	-6.333333333	NULL	NULL	1/1/2017 0:00
1/1/2017	0	2	EOC	3.999712869	2.175594667	-4.462962963	0	NULL	1/1/2017 0:00
1/1/2017	0	23	GABW	3.618503872	1.542288	-4.791666667	NULL	NULL	1/1/2017 0:00
1/1/2017	0	25	VERN	3.430880977	1.575816	-4.375	NULL	NULL	1/1/2017 0:00
1/1/2017	0	26	BENT	NULL	NULL	NULL	0	NULL	1/1/2017 0:00
1/1/2017	0	29	100K	3.567452991	0.771144	-4.222222222	0	742.1245	1/1/2017 0:00
1/1/2017	0	3	ARMY	4.772311951	1.236810667	-4.518518519	0	NULL	1/1/2017 0:00
1/1/2017	0	5	EDNA	5.071926806	2.40284	-5.944444444	NULL	NULL	1/1/2017 0:00
1/1/2017	0	7	200W	3.717114974	0.771144	-4.625	0	NULL	1/1/2017 0:00
1/1/2017	0	8	BVLY	NULL	NULL	NULL	NULL	NULL	1/1/2017 0:00
1/1/2017	1	1	PROS	3.948807433	1.352296	-4.805555556	0	NULL	1/1/2017 1:00
1/1/2017	1	10	YAKB	1.708677338	2.000504	-5.194444444	0	732.9805	1/1/2017 1:00
1/1/2017	1	11	300A	4.969825045	2.369312	-6.694444444	0	744.2835	1/1/2017 1:00
1/1/2017	1	13	100N	3.19002554	1.665224	-4.541666667	0	742.442	1/1/2017 1:00
1/1/2017	1	14	WPPS	5.794493117	1.810512	-7.138888889	0	NULL	1/1/2017 1:00
1/1/2017	1	15	FRNK	0	0	-5.722222222	NULL	NULL	1/1/2017 1:00
1/1/2017	1	17	RING	0.937241808	1.933448	-6.138888889	0	NULL	1/1/2017 1:00
1/1/2017	1	18	RICH	NULL	NULL	NULL	0	NULL	1/1/2017 1:00
1/1/2017	1	19	PFP	4.783074815	1.531112	-4.902777778	NULL	735.838	1/1/2017 1:00
1/1/2017	1	20	RMTN	4.366377456	13.109448	-4.902777778	0	NULL	1/1/2017 1:00
1/1/2017	1	21	HMS	1.727439627	1.296416	-5.097222222	0	734.06	1/1/2017 1:00
1/1/2017	1	22	PASC	4.771293843	1.28524	-3.625	0	NULL	1/1/2017 1:00
1/1/2017	1	27	VSTA	2.604903909	1.128776	-3.611111111	0	NULL	1/1/2017 1:00
1/1/2017	1	28	SURF	NULL	NULL	NULL	0	NULL	1/1/2017 1:00
1/1/2017	1	3	ARMY	4.775220833	1.385824	-4.833333333	0	NULL	1/1/2017 1:00
1/1/2017	1	30	HAMR	4.78220215	1.776984	-5.430555556	NULL	NULL	1/1/2017 1:00
1/1/2017	1	5	EDNA	3.929317923	2.250101333	-5.62962963	NULL	NULL	1/1/2017 1:00

Figure 7. An example of measured meteorological data as input to use in GRAT.

3.3 Choose the Meteorological Data

Select the "Trajectory data processing" tab, and click the "Browse" button in "Step 1", then select the desired data file and click the "Open" button in the pop-up window:

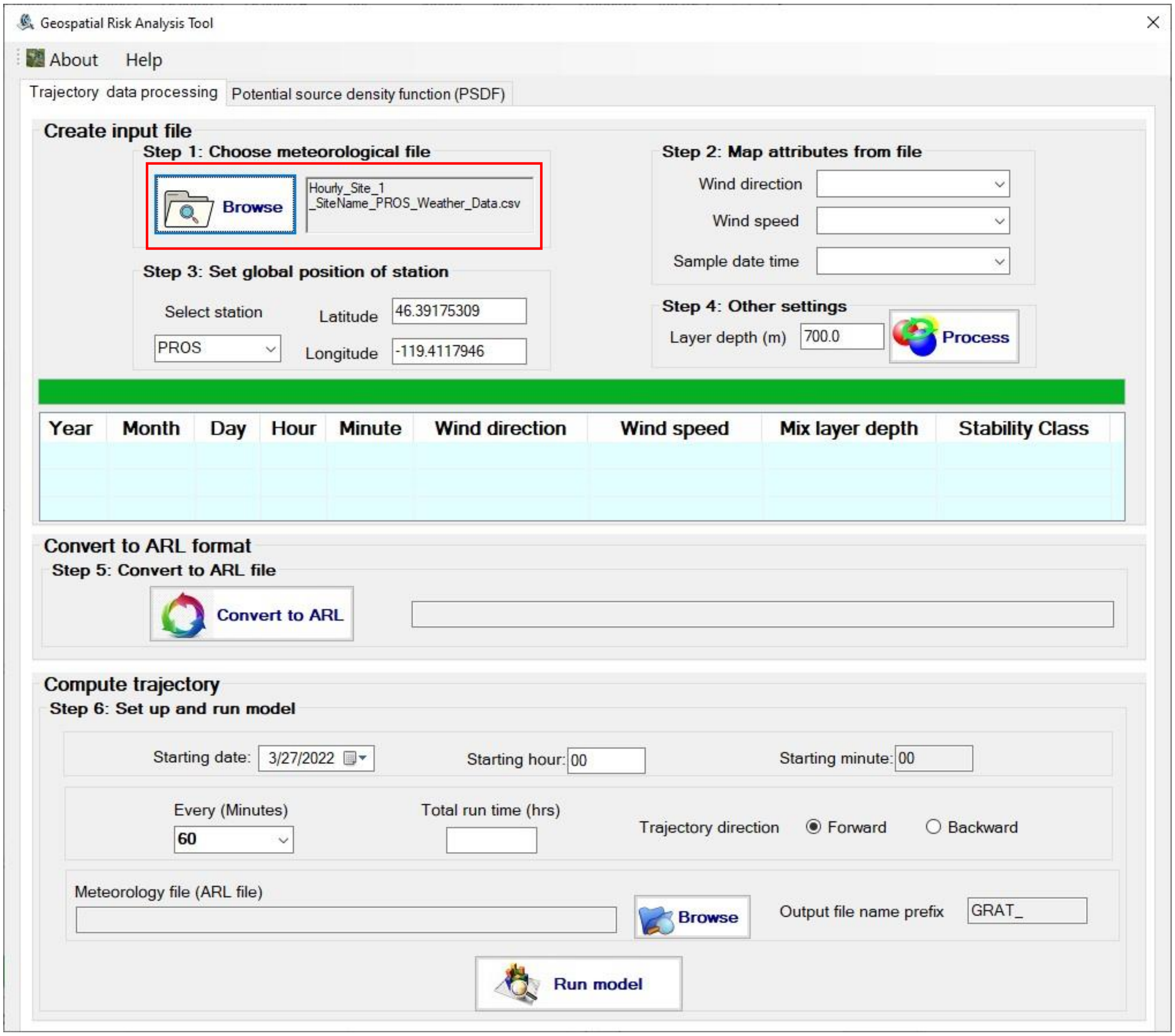


Figure 8. The “Trajectory data processing” tab.

3.4 Select Map Attributes from the File

Click the combo box on the immediate right of the “Wind direction” label and choose the column which contains the measured wind direction data. Make similar selections for wind direction and time stamp.

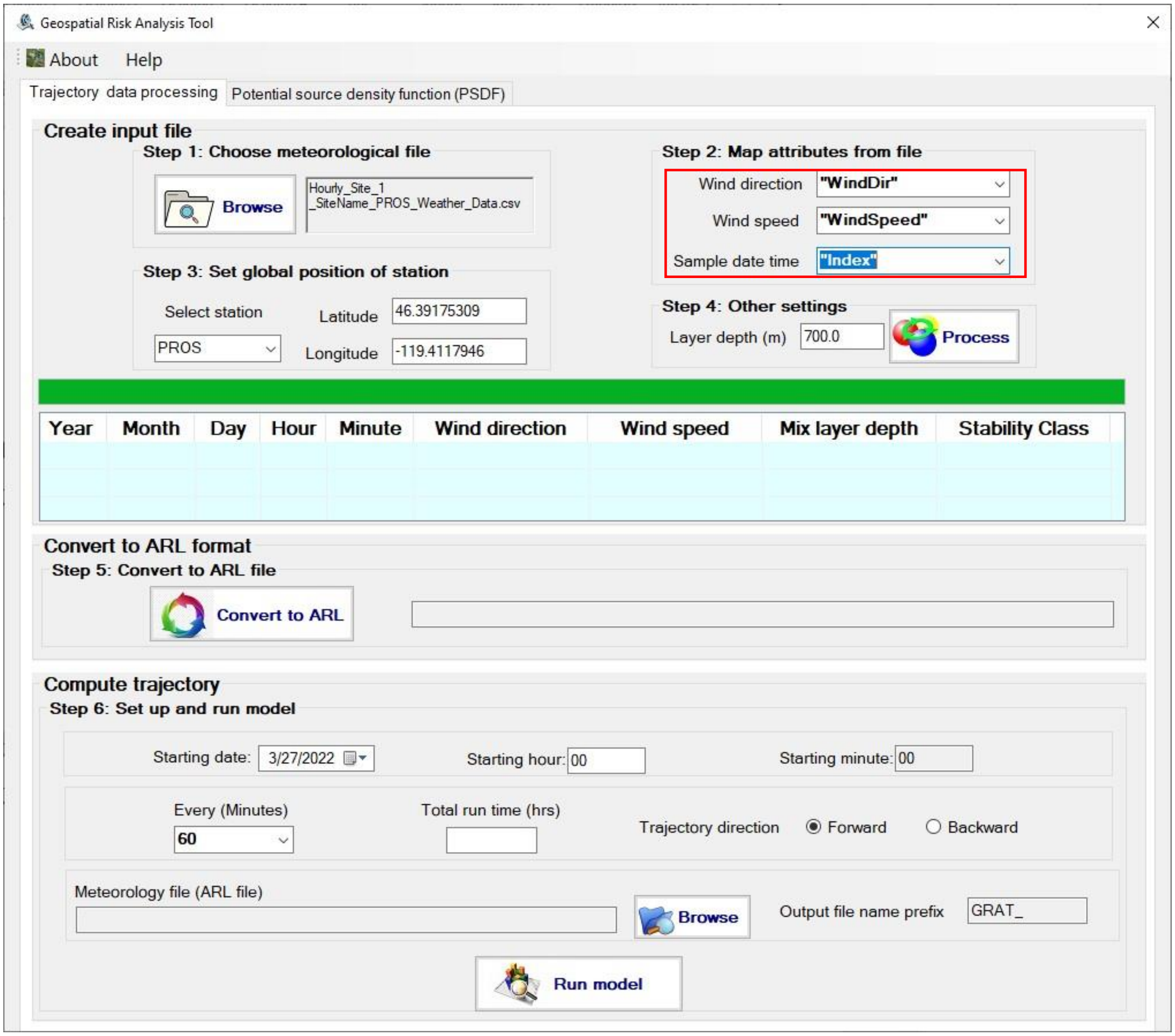


Figure 9. The meteorological data selection tab.

3.5 Input the Measurement Station Information

Click the combo box right below the “Select station” label and select the station where data was measured. If there is no matching item in the combo list, input the station and fill in the corresponding latitude and longitude.

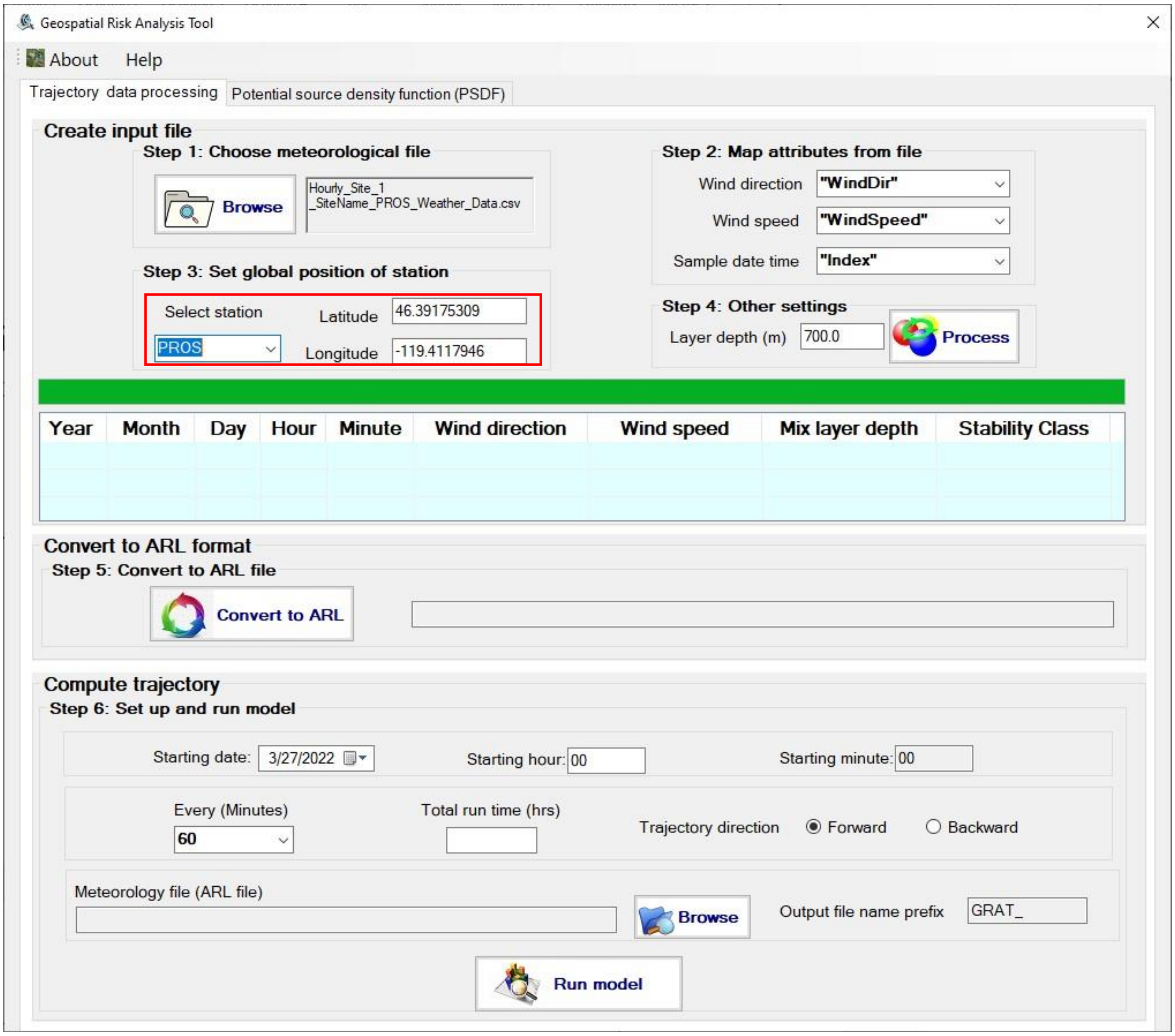


Figure 10. Input the measurement station information.

3.6 Set the Boundary Layer Height

The users can input the estimated boundary layer height within which the wind direction and wind speed are assumed to be constant. Based on the HYSPLIT user's guide (Draxler et al 2022), the default value is 150 meters; and it is related to the typical vertical resolution of the meteorological data. A resolution near the surface of 15 hPa is typical of pressure-level data files. This suggests that it is difficult to infer a mixed layer depth of less than 150 m (10 m per hPa) for most meteorological input data.

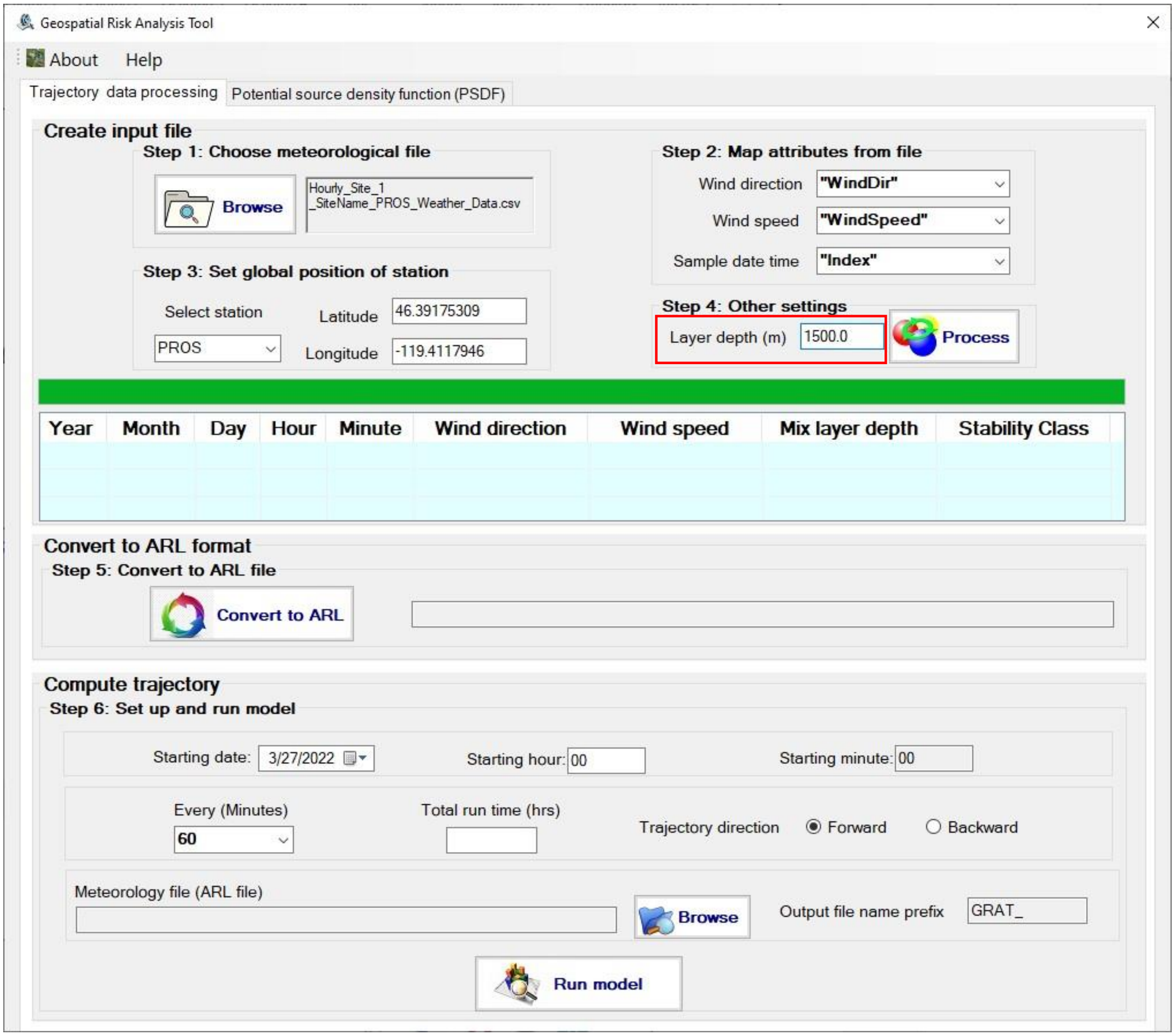


Figure 11. User's input of the boundary layer height in the meteorological data tab.

After clicking the "Process" button, the GRAT software will prepare an associated input file from the select meteorological data file for conversion. The stability class for each measurement will be automatically assigned to 4. Please refer to the following page for more information: https://www.ready.noaa.gov/READYpgclass.php:

A corresponding row will be created for each row from the selected data file:

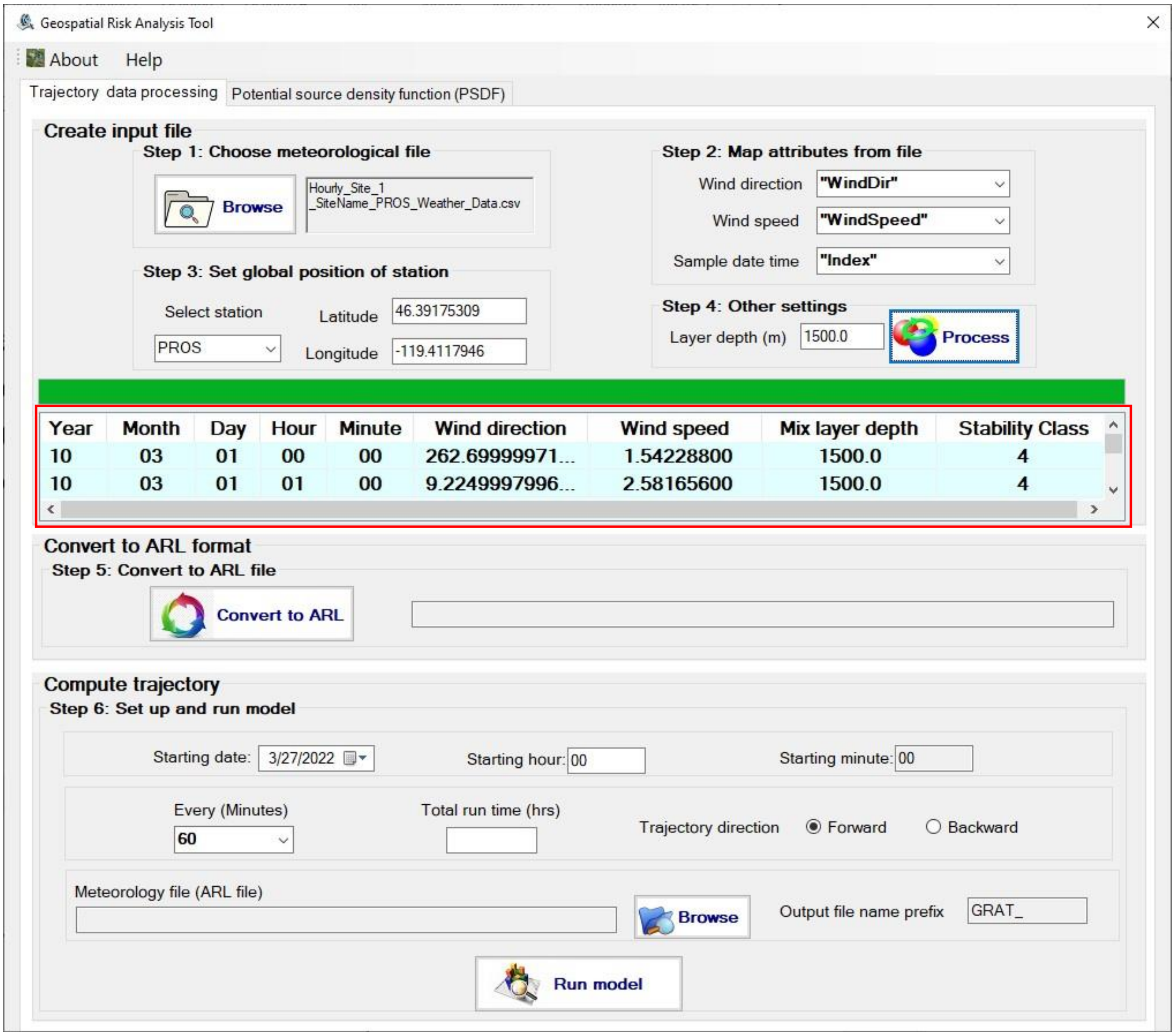


Figure 12. The processed meteorological data depicted in the user interface.

3.7 Convert to ARL file

Next, the users can click the "Convert to ARL" button to convert the dataset produced in section 3.6 to the ARL format. GRAT uses the executable `stn2arl.exe` from the HYSPLIT program to accomplish this. This process is time-consuming, and it takes approximately 4 minutes to convert a 10-year of hourly meteorological data file. The following pop-up window will show after the conversion is done.

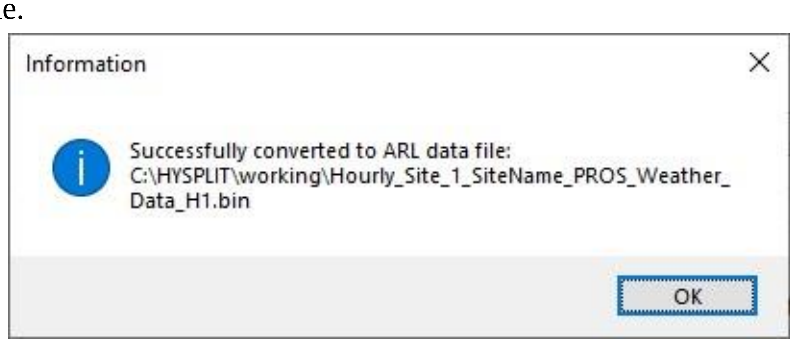


Figure 13. The pop-up window showing completion of data conversion to the ARL format.

3.8 Set up and Run the Model

The following shows the steps to set up and run the model:

1. Select the start date and start time, for example, 8/29/2017 at 23:00.
2. Set the value for "Every (Minutes)" as the measurement interval of the data file, such as 60 minutes, and so on.
3. Input the expected hours of data to run. For example, 312 hours for data for the duration of December.
4. Choose the "backward" trajectory or "forward" trajectory depending on applications.
5. Click the "Browser" button to choose the ARL file, for example: "C:\HYSPLIT\working\Hourly_Site_1_SiteName_PROS_Weather_Data_H1.bin".
6. Fill in the output file name prefix. For example, "tj.PNNL.PROS.".
7. Click the "Run model" button.

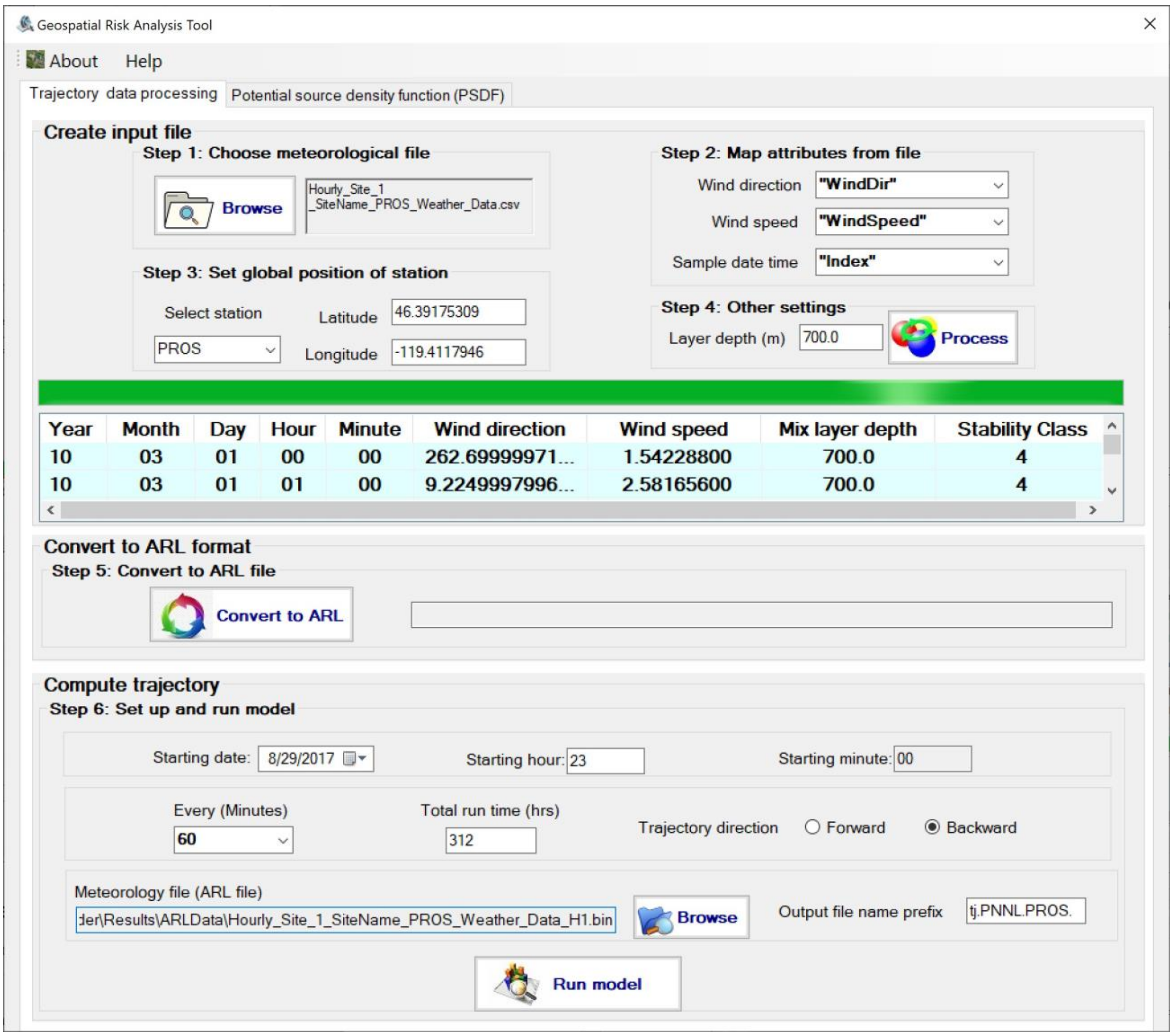


Figure 14. The panel to set up and run the model.

GRAT uses the executable `hyts_std.exe` from HYSPLIT to accomplish this. This process can be time consuming; and it takes about 12 minutes for the data for the whole of December using the Hanford meteorological measurement from one monitoring station.

Figure 15. The pop-up window showing that the trajectory modeling is completed.

The converted trajectory files are stored under C:\HYSPLIT\working directory:

3.9 Run the Potential Source Density Function (PSDF)

The users can use the following steps to run PSDF in the software.

1. Choose the PTR-MS[1] data file, then choose the chemical from the list:

[1] The computed particle transport trajectories, combined with the online Proton Transfer Reaction-Mass Spectrometry (PTR-MS) data (https://doi.org/10.5281/zenodo.7369298), can be used to identify and quantify the sources and influenced area of the hazardous chemicals' emission using the PSDF.

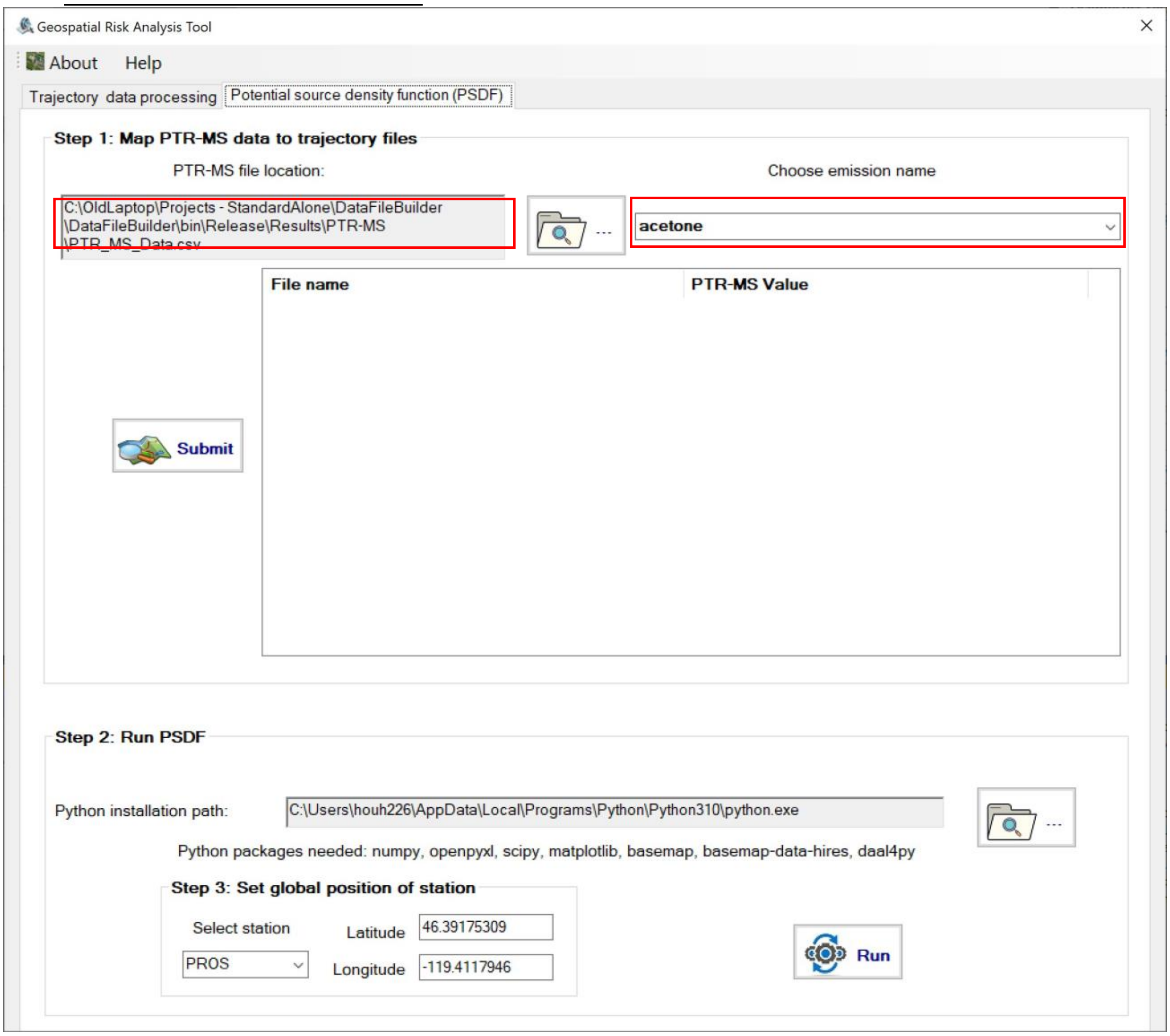


Figure 16. Selection of measurement data of hazardous chemicals.

2. Click "Submit", and it will generate the file containing the trajectory file names and the corresponding PTR-MS value for the selected chemical.

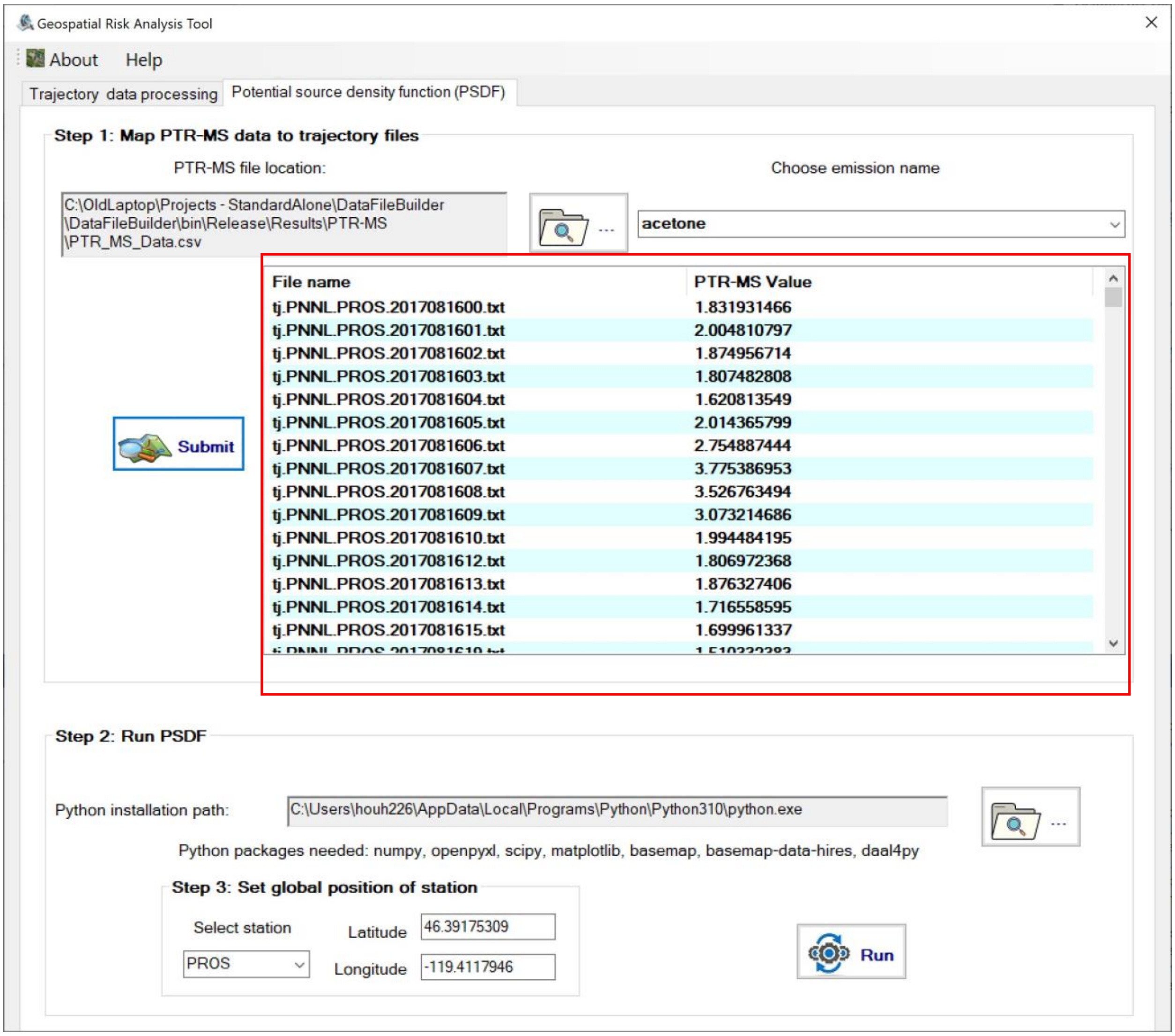


Figure 17. An example showing PSDF calculations using PTR-MS measurements.

3. Choose the full path of the executable “python.exe”, then choose the monitoring station. Click “Run”. This process may take several minutes. A plot will show up once the execution is done.

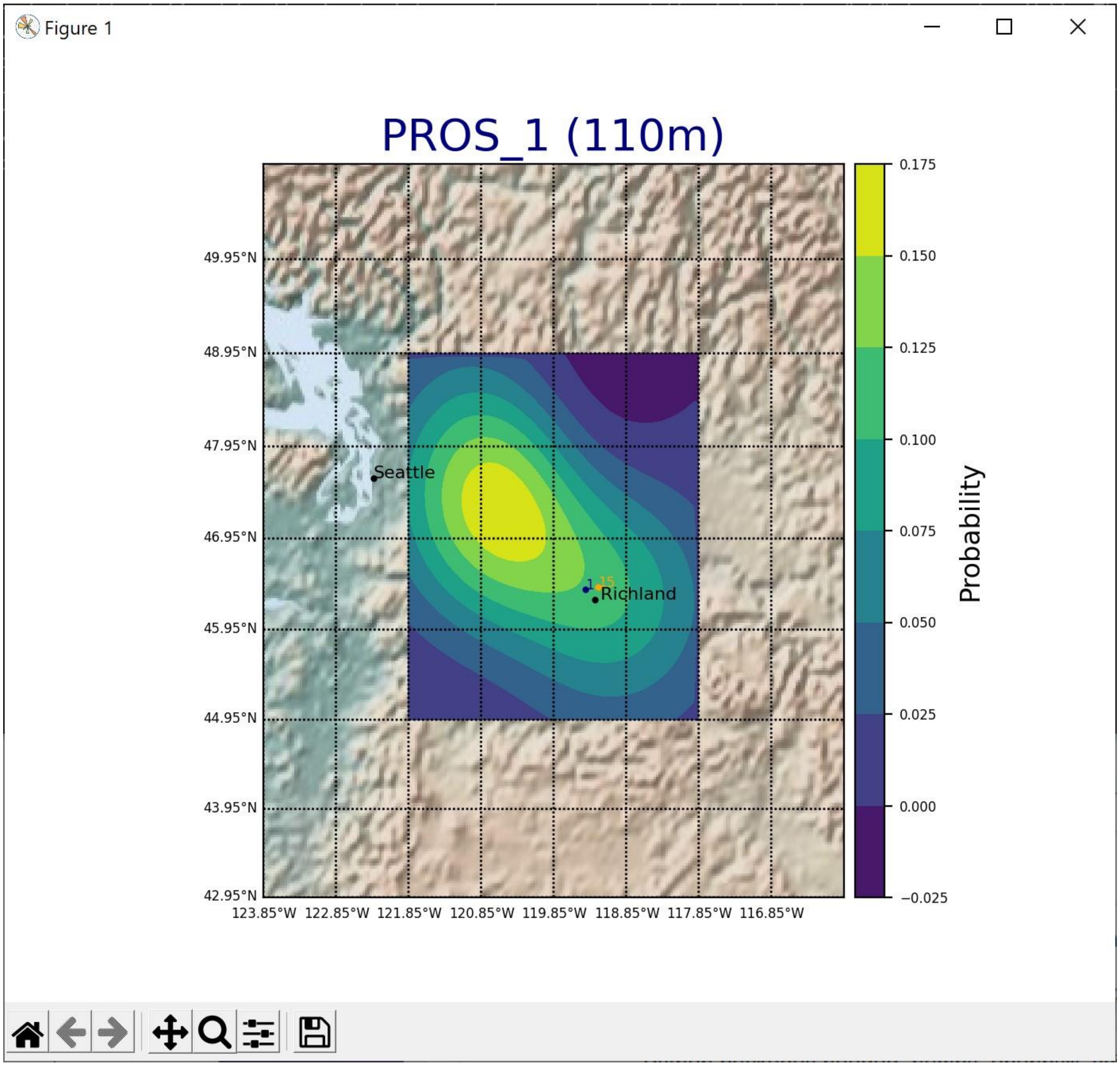
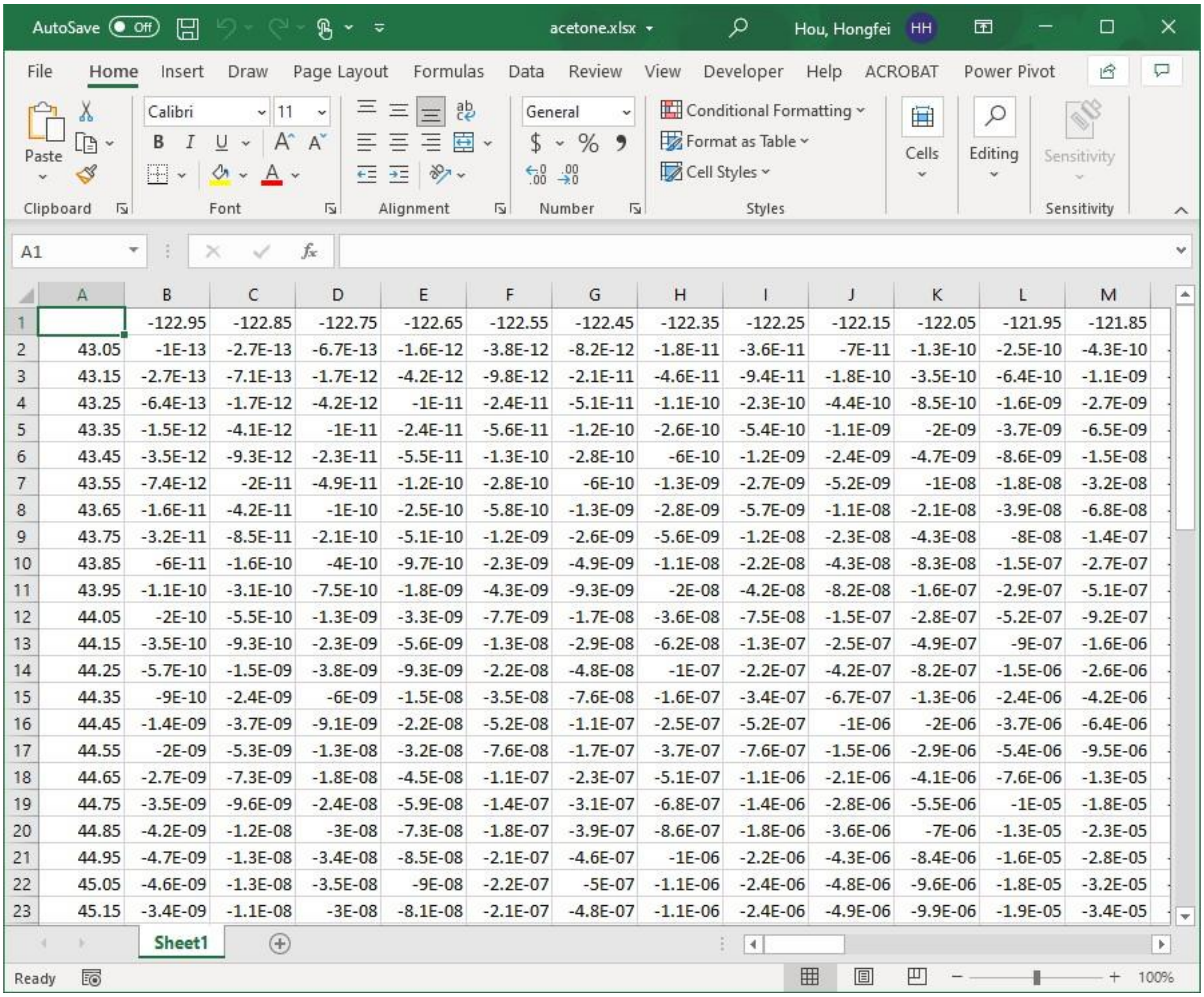


Figure 18. An example PSDF results depicted as a 2D plot superimposed on the map.

4. The "results.xlsx" file will be created under the "Results" subfolder of the installation path, which could be used to calculate the impacted area:



	A	B	C	D	E	F	G	H	I	J	K	L	M
1		-122.95	-122.85	-122.75	-122.65	-122.55	-122.45	-122.35	-122.25	-122.15	-122.05	-121.95	-121.85
2	43.05	-1E-13	-2.7E-13	-6.7E-13	-1.6E-12	-3.8E-12	-8.2E-12	-1.8E-11	-3.6E-11	-7E-11	-1.3E-10	-2.5E-10	-4.3E-10
3	43.15	-2.7E-13	-7.1E-13	-1.7E-12	-4.2E-12	-9.8E-12	-2.1E-11	-4.6E-11	-9.4E-11	-1.8E-10	-3.5E-10	-6.4E-10	-1.1E-09
4	43.25	-6.4E-13	-1.7E-12	-4.2E-12	-1E-11	-2.4E-11	-5.1E-11	-1.1E-10	-2.3E-10	-4.4E-10	-8.5E-10	-1.6E-09	-2.7E-09
5	43.35	-1.5E-12	-4.1E-12	-1E-11	-2.4E-11	-5.6E-11	-1.2E-10	-2.6E-10	-5.4E-10	-1.1E-09	-2E-09	-3.7E-09	-6.5E-09
6	43.45	-3.5E-12	-9.3E-12	-2.3E-11	-5.5E-11	-1.3E-10	-2.8E-10	-6E-10	-1.2E-09	-2.4E-09	-4.7E-09	-8.6E-09	-1.5E-08
7	43.55	-7.4E-12	-2E-11	-4.9E-11	-1.2E-10	-2.8E-10	-6E-10	-1.3E-09	-2.7E-09	-5.2E-09	-1E-08	-1.8E-08	-3.2E-08
8	43.65	-1.6E-11	-4.2E-11	-1E-10	-2.5E-10	-5.8E-10	-1.3E-09	-2.8E-09	-5.7E-09	-1.1E-08	-2.1E-08	-3.9E-08	-6.8E-08
9	43.75	-3.2E-11	-8.5E-11	-2.1E-10	-5.1E-10	-1.2E-09	-2.6E-09	-5.6E-09	-1.2E-08	-2.3E-08	-4.3E-08	-8E-08	-1.4E-07
10	43.85	-6E-11	-1.6E-10	-4E-10	-9.7E-10	-2.3E-09	-4.9E-09	-1.1E-08	-2.2E-08	-4.3E-08	-8.3E-08	-1.5E-07	-2.7E-07
11	43.95	-1.1E-10	-3.1E-10	-7.5E-10	-1.8E-09	-4.3E-09	-9.3E-09	-2E-08	-4.2E-08	-8.2E-08	-1.6E-07	-2.9E-07	-5.1E-07
12	44.05	-2E-10	-5.5E-10	-1.3E-09	-3.3E-09	-7.7E-09	-1.7E-08	-3.6E-08	-7.5E-08	-1.5E-07	-2.8E-07	-5.2E-07	-9.2E-07
13	44.15	-3.5E-10	-9.3E-10	-2.3E-09	-5.6E-09	-1.3E-08	-2.9E-08	-6.2E-08	-1.3E-07	-2.5E-07	-4.9E-07	-9E-07	-1.6E-06
14	44.25	-5.7E-10	-1.5E-09	-3.8E-09	-9.3E-09	-2.2E-08	-4.8E-08	-1E-07	-2.2E-07	-4.2E-07	-8.2E-07	-1.5E-06	-2.6E-06
15	44.35	-9E-10	-2.4E-09	-6E-09	-1.5E-08	-3.5E-08	-7.6E-08	-1.6E-07	-3.4E-07	-6.7E-07	-1.3E-06	-2.4E-06	-4.2E-06
16	44.45	-1.4E-09	-3.7E-09	-9.1E-09	-2.2E-08	-5.2E-08	-1.1E-07	-2.5E-07	-5.2E-07	-1E-06	-2E-06	-3.7E-06	-6.4E-06
17	44.55	-2E-09	-5.3E-09	-1.3E-08	-3.2E-08	-7.6E-08	-1.7E-07	-3.7E-07	-7.6E-07	-1.5E-06	-2.9E-06	-5.4E-06	-9.5E-06
18	44.65	-2.7E-09	-7.3E-09	-1.8E-08	-4.5E-08	-1.1E-07	-2.3E-07	-5.1E-07	-1.1E-06	-2.1E-06	-4.1E-06	-7.6E-06	-1.3E-05
19	44.75	-3.5E-09	-9.6E-09	-2.4E-08	-5.9E-08	-1.4E-07	-3.1E-07	-6.8E-07	-1.4E-06	-2.8E-06	-5.5E-06	-1E-05	-1.8E-05
20	44.85	-4.2E-09	-1.2E-08	-3E-08	-7.3E-08	-1.8E-07	-3.9E-07	-8.6E-07	-1.8E-06	-3.6E-06	-7E-06	-1.3E-05	-2.3E-05
21	44.95	-4.7E-09	-1.3E-08	-3.4E-08	-8.5E-08	-2.1E-07	-4.6E-07	-1E-06	-2.2E-06	-4.3E-06	-8.4E-06	-1.6E-05	-2.8E-05
22	45.05	-4.6E-09	-1.3E-08	-3.5E-08	-9E-08	-2.2E-07	-5E-07	-1.1E-06	-2.4E-06	-4.8E-06	-9.6E-06	-1.8E-05	-3.2E-05
23	45.15	-3.4E-09	-1.1E-08	-3E-08	-8.1E-08	-2.1E-07	-4.8E-07	-1.1E-06	-2.4E-06	-4.9E-06	-9.9E-06	-1.9E-05	-3.4E-05

Figure 19. The sample "results.xlsx" file in the Excel format.

3.10 About

Selecting "About" on the menu bar reveals the software version information and disclaimer as depicted in the screenshot below.

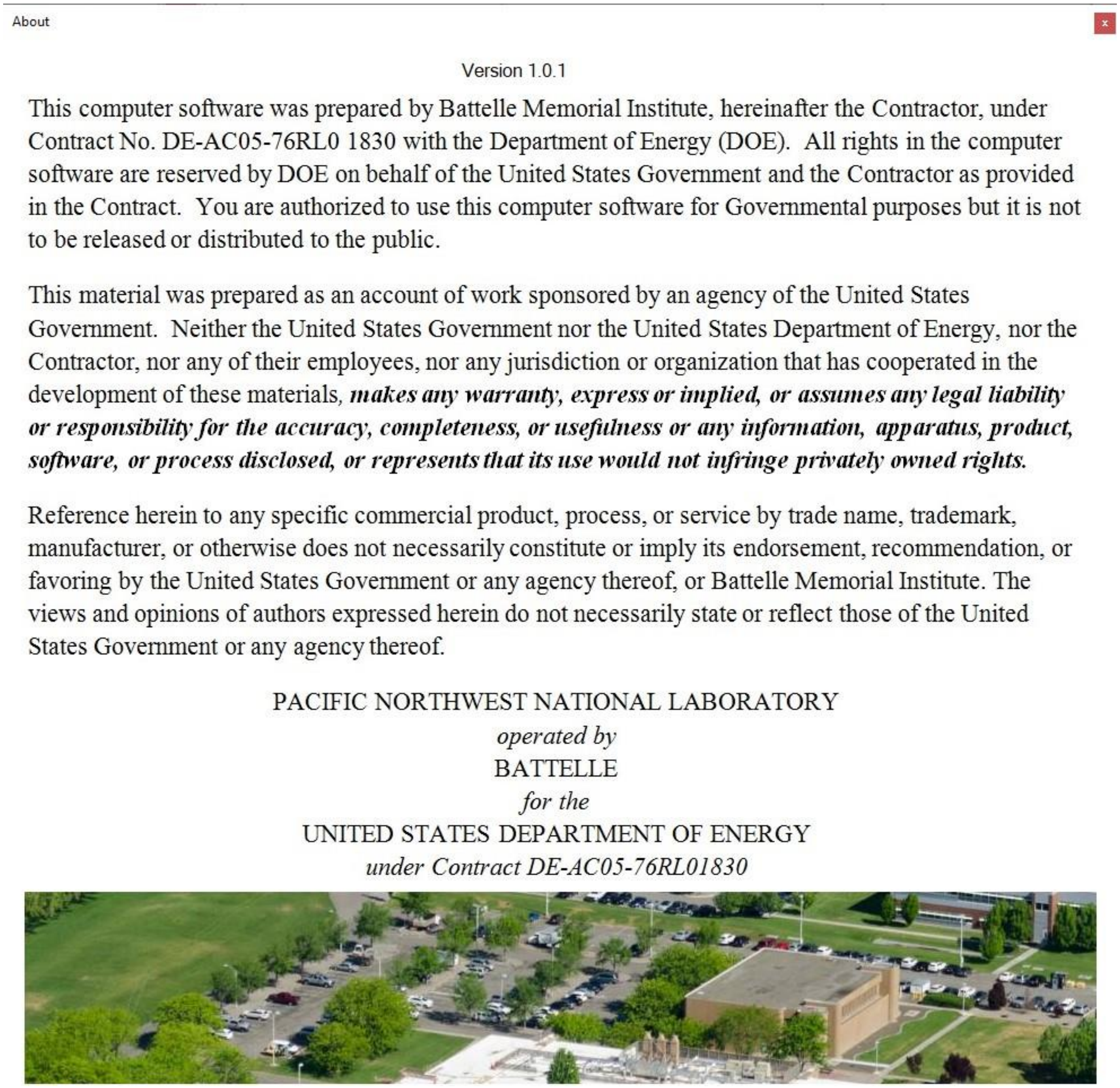


Figure 20. The information and disclaimer page of the software.

3.11 Help

Selecting "Help" in the menu bar will open a copy of the user manual associated with the software version.

4 Uninstall

To uninstall the GRAT program, select the Windows Start button, go to Settings, and select "Apps." In the program list, navigate to and select "GeospatialRiskAnalysisTool," click "Uninstall," and follow the provided instructions.

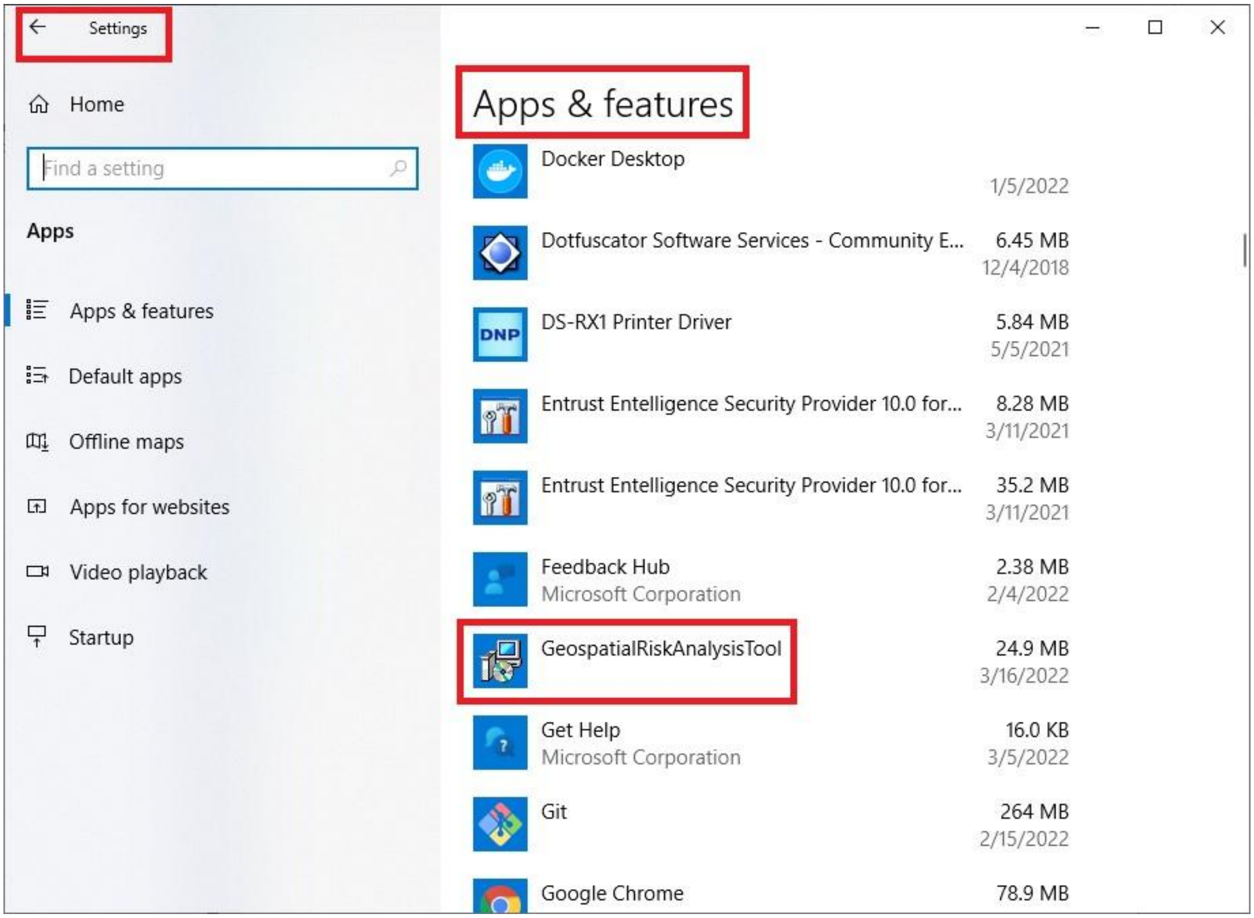


Figure 21. The uninstallation of the GRAT tool.

5 Disclaimer

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