Technical Notes for Pre-Production Module for the TRACER Model

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1. General Information

Unconventional oil and gas development (UOGD) in the US has surged in recent years, leading to significant emissions of volatile organic compounds (VOCs). Current emission models often fail to accurately represent recent UOGD practices and emission factors. In this study, we introduce the TRAcking Community Exposures and Releases (TRACER) model for pre-production VOC emissions, based on the Mechanistic Air Emissions Simulator (MAES, formerly known as MEET). The TRACER model can simulate emissions of over 50 VOC species, including light and heavy alkanes, alkenes, and aromatics, from complex pre-production activities such as drilling, hydraulic fracturing, mill-out, coil-tubing, and flowback, with detailed temporal resolution. The model incorporates adjustable emission factors from various sources, making it versatile for applications like emission inventory compilation, health impact assessment, and air quality evaluation. Additionally, the TRACER pre-production model features a Graphical User Interface (GUI) to facilitate broader use in policymaking and environmental health research.

The GUI of the Pre-Production Module is built using Python 3 and has been compiled into a standalone executable compatible with Windows platforms. The module's input data is organized and stored in Microsoft Excel spreadsheets (".xlsx" format). More details are provided in the following sections.

2. Installation and Quick Start

2.1. Installation

The GUI can be downloaded as from https://github.com/dp7-PU/HEI_TRACER_Preproduction. To use the module, download all files in the repository and run the exe application in the folder.

2.2. Quick Start

Run "HEI_GUI.exe" to start the program. Ensure that the "config," "input," and "output" folders are in the same directory as "HEI_GUI.exe." After 5 - 10 seconds, a graphical interface, as shown in Fig. 1, will appear.

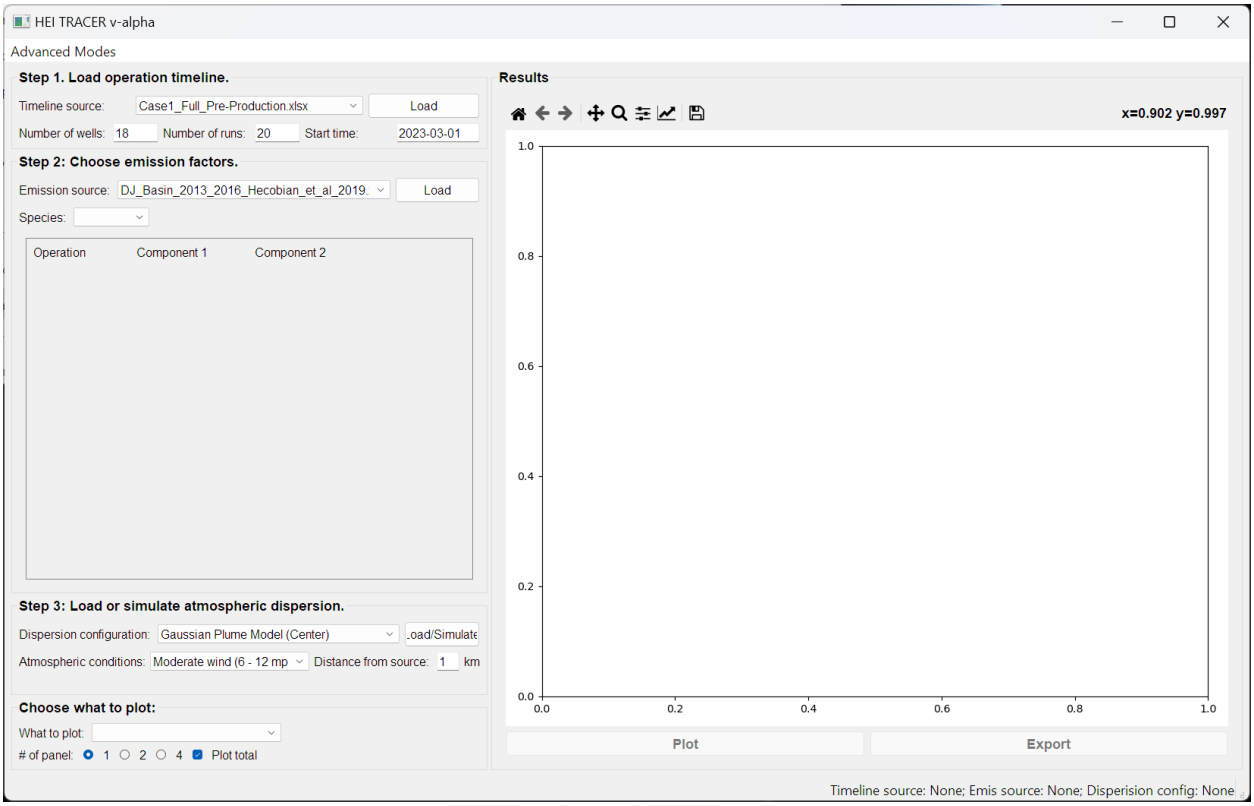

Figure 1. Typical user interface of the Pre-Production Module for the TRACER Model.

The program requires inputs for the operation timeline, emission factors, and atmospheric dispersion parameters, which are processed in three steps.

Step 1. Load operation timeline.

- Use the "Timeline source" pull-down menu to select a pre-defined operation timeline and click "Load".
- Number of wells, number of runs, and start time will be automatically updated.
- After this step, the operation timeline and operation durations will be ready for plotting.

Step 2. Choose emission factors.

- Use the "Emission source" pull-down menu to select pre-defined emission factors and click "Load".
- After loading, emitting components of each operation will appear, as shown on the right. Use the pull-down menus to change the corresponding emitting components. For example, rig preparation can be changed from powered by electricity or a diesel engine.

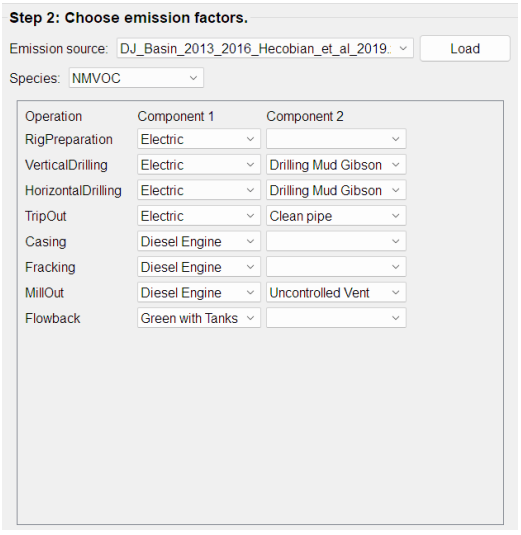

Figure 2. An example of emission sources.

- Use the “Species” pull-down menu to select the pollutant of interest.
- After this step, the emission timeline, emission factors, and total emissions will be available for visualization.

Step 3. Load or simulate atmospheric dispersion.

- Use the “Dispersion configuration” pull-down menu to select an atmospheric dispersion model. There are several options for the Gaussian plume model for simulating concentrations at the center of the plume and locations off center.
- For the ***Gaussian plume model***:
    - Use the “Atmospheric conditions” pull-down menu to select a set of conditions that represents the typical conditions of interest. Note that daytime and nighttime dispersion characteristics are different even for the same wind and cloud category.
    - Enter the downwind distance of interest.
- For the ***AERMOD model***:
    - Use the “AERMOD file” pull-down menu to select AERMOD simulation output file.
    - Enter site ID to obtaOptin simulated results for a specific location of interest. Site ID can be found in the output file (the highlighted column below).

```
* AERMOD (23132 ):  HEI - WRF MET data                                                    04/01/24
* AERMET ( 23132):                                                                        16:28:22
* MODELING OPTIONS USED:   RegDFAULT  CONC  ELEV  RURAL  ADJ_U*  MMIF_Data  BULKRN
*         POST/PLOT FILE OF CONCURRENT  1-HR VALUES FOR SOURCE GROUP: ALL
*         FOR A TOTAL OF     4 RECEPTORS.
*         FORMAT: (3(1X,F13.5),3(1X,F8.2),2X,A6,2X,A8,2X,I8.8,2X,A8)
*        X             Y      AVERAGE CONC    ZELEV    ZHILL    ZFLAG    AVE     GRP      DATE     NET ID
* ____________ ____________  ____________  ______  ______  ______  ______  ________ ________  ________
  530852.48000 4395601.48000       0.00000  1743.40  1743.40     0.00    1-HR  ALL      22010101  LTNE
  530900.96000 4395376.59000       0.00000  1739.50  1739.50     0.00    1-HR  ALL      22010101  LTE
  530016.87000 4394877.09000       0.00000  1726.10  1726.10     0.00    1-HR  ALL      22010101  LTSW
  533783.22000 4395917.35000       0.00000  1702.90  1702.90     0.00    1-HR  ALL      22010101  LTBG
  530852.48000 4395601.48000       0.00000  1743.40  1743.40     0.00    1-HR  ALL      22010102  LTNE
```

Figure 3. An example of AERMOD model outputs.

- Once relevant model parameters have been specified, click the “Load/Simulate” button.
- After this step, the concentration timeline will be available for plotting.

Step 4. Plotting and exporting the results

- Use the “What to plot” menu to select the data for plotting.
- Click the “Plot” button in a specific canvas to plot the corresponding results.
- When plotting a timeline, averaging time can be specified.
- Use the buttons above the canvas to customize the figure.
- Click the “Export" button to export data as a csv file to the “ExportData" folder in the output directory.
- Use the “# of panel” to change the number of panels presented in the interface. Up to four panels can be plotted for intercomparison.

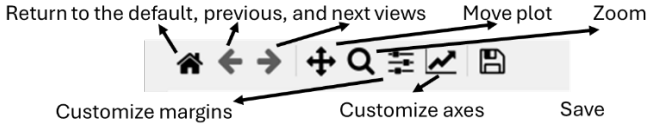

Figure 4. Plot customization toolbar.

3. Detailed configurations and data sources

3.1. Operation Timeline

3.1.1. Using a Real Operation Timeline

When operation logs are available from the operator, the start and end times of relevant operations should be recorded in an Excel spreadsheet in the ".xlsx" format. Table1 defines the operations, and Fig. 5 illustrates the sequence of the operations. The number of wells on the pad should also be specified in the second row of the corresponding column ("Number of Wells"). An example can be found in the "Case1_Full_Pre-Production.xlsx" file. The completed operation timeline should be saved in the "input/RealLogFiles" folder. The GUI lists all available timelines the "Timeline source" pull-down menu.

Table 1. Definition of UOGD operations and corresponding codes for the Pre-Production Module for the TRACER Model.

Phase	Operation code	Description	Potential emission sources
Drilling - Rig preparation (Ri	Move/Skid -Nipple Up	Move the drilling rig to the target well and set up the drilling rig.	Drilling rig engines.
	BOP Test	Blowout prevent test.	Drilling rig engines.
Drilling - Vertical drilling	Drilling VS	Vertical drilling to reach target depth.	Drilling rig engines;, and drilling mud degassing.
Drilling - Horizontal drilling	Drilling Curve	Curve drilling to enter into the "pay" zone. Here, we categorize them into horizontal drilling.	Drilling rig engines, and drilling mud degassing.
	Drilling Hz	Horizontal drilling within the "pay" zone.	Drilling rig engines, and drilling mud degassing.
Drilling - Tripping Out	Trip out & Circulate	Tripping out the pipes, and circulation is needed to prevent issues like kicks.	Drilling rig engines, and residual mud on the pipes.
Drilling - Casing	Case & Cement	Casing and cementing.	Cementing engines.
Hydraulic fracturing	Fracking	Hydraulic fracturing.	Fracturing Engines.
Coil-tubing and mill-out	MillOut	Milling out previously installed plugs with coil-tubing.	Engines, and direct emissions from the well.
Flowback	Flowback	Flowback processes.	Emissions from produced water; Emissions from flairing processes.
Production	Production		

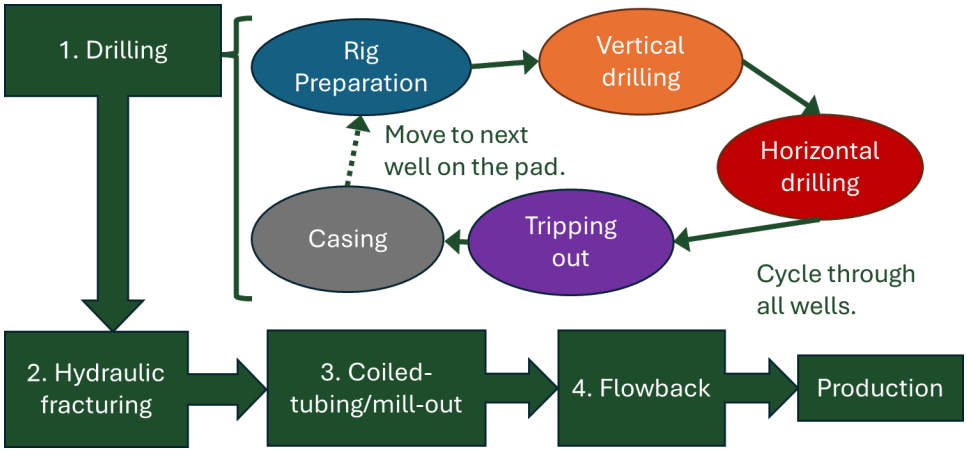

Figure 5. Operation sequences of pre-production activities.

3.1.2. Simulating an Operation Timeline

When detailed operation start and end times may not be available. In this case, the user can use the "Simulate Timeline" function in the advanced modes. This function is based on the Mechanistic Air Emissions Simulator (MAES, formerly known as the Methane Emissions Estimation Tool (MEET, (Allen et al., 2022)). The MAES model randomly simulates durations of different operations using a Monte Carlo approach based on the real operation durations of provided by operators in the DJ basin. Figure6 shows the statistical summary of the durations. Multiple operation timelines will be simulated to form an ensemble.

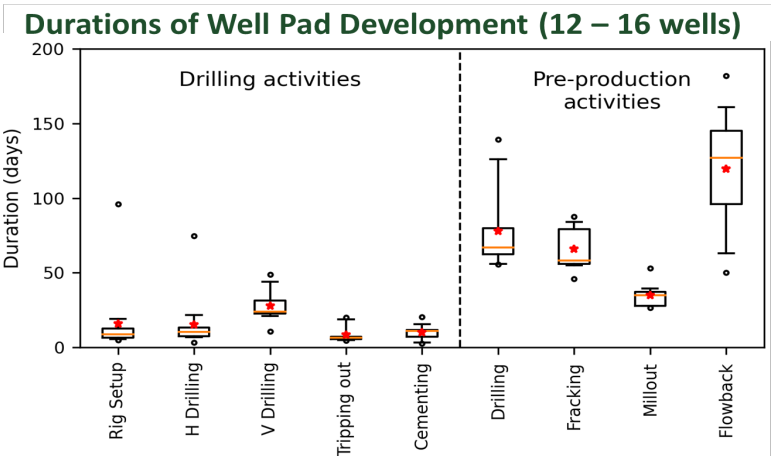

Figure 6. Statistical summary of operation durations obtained from different operators in the DJ Basin, Colorado. The boxes and whiskers show 5th, 25th, 50th, and 95th percentiles, and the red stars show the mean values.

To simulate a new ensemble of operation timelines, follow the steps below (Fig. 7):

Step 1: Configure the Operation Timeline Mode:

- Navigate to the **"Load or create operation timeline"** panel.
- Select the option **"Generate new"** to create a new timeline for your simulation.

Step 2: Choose the Duration File

- Locate the **pull-down menu** within the interface.
- From the menu, select the **duration file** that contains the duration samples relevant to your simulation. **Currently, there is only one duration file generated based on operation logs obtained from operators in the DJ Basin.**

Step 3: Set Simulation Parameters

- Input the **number of wells** to include in the simulation.
- Specify the **number of runs** to define the number of simulated timelines in the ensemble.
- Define the **Start time** for the operation timeline simulation.

Step 4: Start the Simulation

- Click on the **"Generate MAES"** button to initiate the simulation process. Depending on the number of runs, it may take a few minutes to finish the simulations.

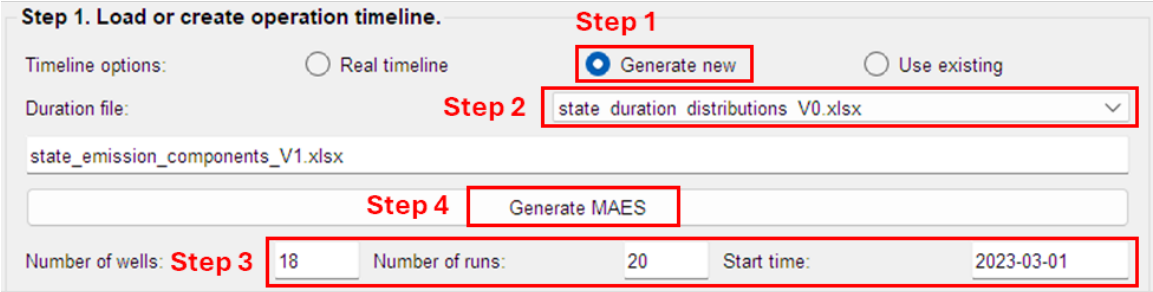

Figure 7. Steps for simulating a new ensemble of operation timelines using MAES.

To load a previously generated timeline ensemble, follow the steps below (Fig. 8):

Step 1: Configure the Operation Timeline Mode:

- Navigate to the **"Load or create operation timeline"** panel.
- Select the option **"Use existing"** to create a new timeline for your simulation.

Step 2: Load a Previously Generated Timeline.

- Use the pull-down menu to select a previously generated timeline ensemble.
- Click the "Load" button to load the ensemble. Depending on the number of runs, it may take a few minutes to load.

Figure 8. Steps for loading an existing ensemble of operation timelines.

Figure 9 shows an example of a timeline ensemble. The transparent lines show individual simulations while the solid line illustrates the ensemble mean.

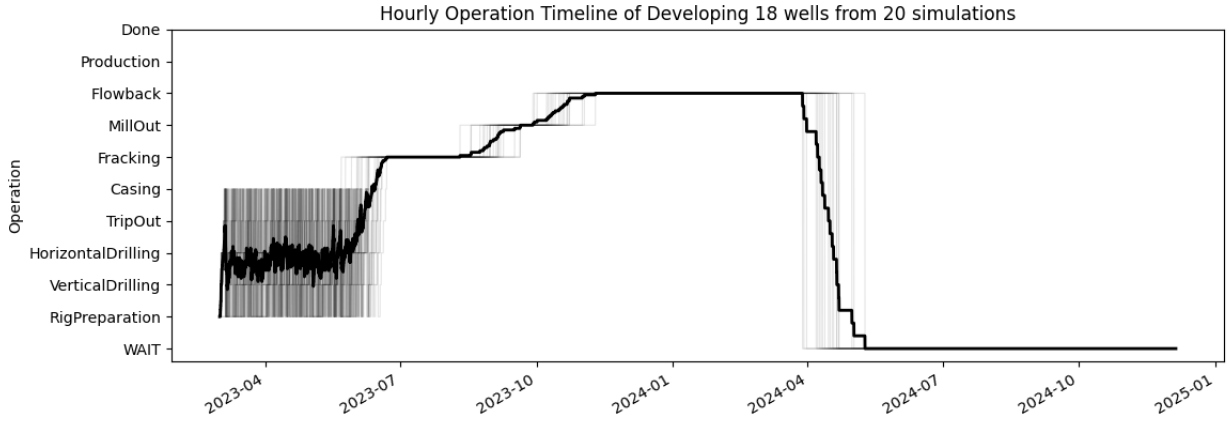

Figure 9. An example of MAES simulated operation timelines. The transparent lines show individual simulations while the solid line illustrates the ensemble mean.

3.2. Emission Rates

Three sets of emission rates are provided with the GUI:

1. **"DJ_Basin_2019_2023_Zhang_et_al_2025.xlsx"** contains the emission rates inverted from the observations that were made in Broomfield between 2019 and 2023 (Zhang et al., in preparation);
2. **"DJ_Piceance_Basin_2013_2016_Hecobian_et_al_2019.xlsx"** contains the emission rates derived from tracer ratio experiments conducted between 2013 and 2016 in the DJ and Piceance basins by Hecobian et al. (2019);
3. The file **"EPA_Oil_and_Gas_Tool_2020.xlsx"** contains emission rates derived from the 2020 EPA Nonpoint Oil and Gas Emissions Estimation Tool (EPA, 2020). Emission rates for pre-production activities are directly converted from emission factors, while the production emission rate is calculated by dividing the total annual production emissions in Colorado by the number of active wells.

Each file has several tabs consisting of mean and median emission rates for each potential source. Note that Hecobian et al. (2019) only has median emission rates, and the EPA Emission Tool only has mean emission rates. Detailed emission rates can be found in the specific files.

The user can create their own emission file following the format of the provided spreadsheets. Once the emission file is added to the "input/EmissionFiles/" folder, it will be included in the "Emission Source" pull-down menu.

The user can directly adjust emission rates by enabling the advanced mode "Customize Emission Rates". Once enabled, the emission rate for each UOGD phase can be adjusted directly in the GUI as illustrated in Fig. 10.

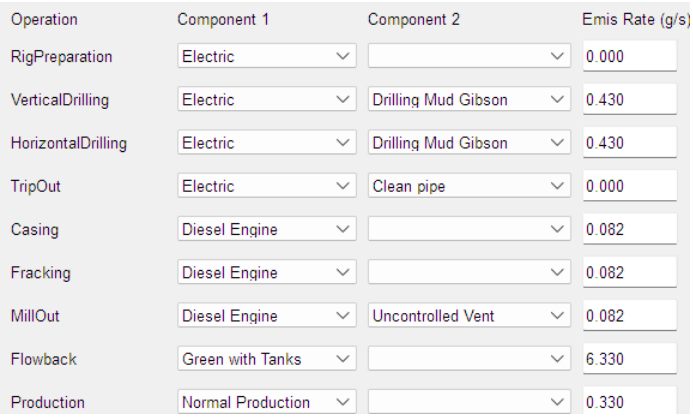

Figure 10. An example of the emission rate panel when the advanced mode "Customize Emission Rates".

3.3. Dispersion Models

The GUI can couple the simulated emission timeline with a Gaussian plume model or previously generated AERMOD simulations as described earlier.

3.3.1. Gaussian plume model

Using the Gaussian plume model, the concentration at a location (x, y, z) of a pollutant emitted from a source located at (0, 0, H) is calculated as:

$$c(x,y,z) = \frac{Q}{2\pi\sigma_y\sigma_z U}\exp\left[-\frac{y^2}{2\sigma_y^2} - \frac{(z-h)^2}{2\sigma_z^2} - \frac{(z+h)^2}{2\sigma_z^2}\right] \quad (D1)$$

where Q and U are emission rate (g/s) and wind speed (m/s). σ_y and σ_z are crosswind and vertical dispersion parameters, respectively. σ_y and σ_z are calculated as:

$$\sigma_y(x) = \exp[I_y + J_y \ln x + K_y(\ln x)^2]\,; \sigma_z = \exp[I_z + J_z \ln x + K_z(\ln x)^2].$$

Parameters are listed in Table2 (Hanna, 1982). The Gaussian plume model used here considers plume reflection from the ground.

Table 2. Parameters for calculating the crosswind and vertical dispersion parameters in the Gaussian plume model.

	Stability Class					
Coefficient	**A**	**B**	**C**	**D**	**E**	**F**
I_y	-1.104	-1.634	-2.054	-2.555	-2.754	-3.143
J_y	0.9878	1.035	1.0231	1.0423	1.0106	1.0148
K_y	-0.0076	-0.0096	-0.0076	-0.0087	-0.0064	-0.007
I_z	4.679	-1.999	-2.341	-3.186	-3.783	-4.49
J_z	-1.7172	0.8752	0.9477	1.1737	1.301	1.4024
K_z	0.277	0.0136	-0.002	-0.0316	-0.045	-0.054

Six cases are provided for simple simulations, and the corresponding conditions are listed in Table3. The user can also modify the meteorological conditions using the advanced mode "Customize Gaussian Plume Model Conditions". An example of the panel for modifying the meteorological conditions is shown in Fig. 11.

Table 3. Conditions of the pre-defined conditions for the Gaussian plume model.

Condition	**Daytime wind speed (m/s)**	**Daytime stability class**	**Nighttime wind speed (m/s)**	**Nighttime stability class**
Windy (12 - 18 mph), clear sky	8	C	6	C
Moderate wind (6 - 12 mph), clear sky	5	B	4	D
Calm (0 - 6 mph), clear sky	2	A	1.5	E
Windy (12 - 18 mph), overcast	8	D	6	D
Moderate wind (6 - 12 mph), overcast	5	C	4	E
Calm (0 - 6 mph), overcast	2	B	1.5	F

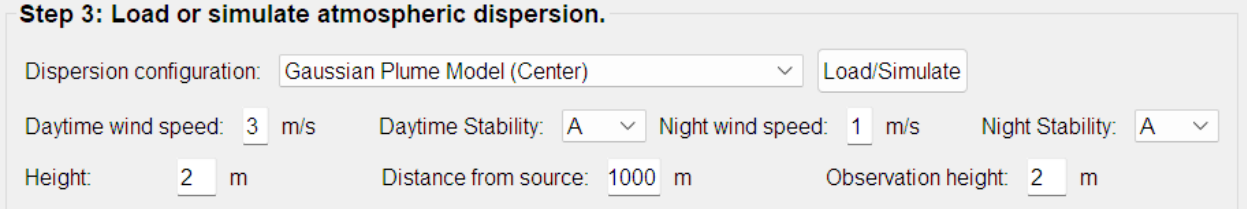

Figure 11. An example of the panel for modifying the meteorological conditions.

The user can choose among three crosswind locations that are 0, 15, and 45 degrees off the prevailing wind direction. The user can also define the distance between the source and receptor.

3.3.2. AERMOD Model

The GUI can directly read AERMOD simulation results stored in the "input/DispersionFiles" folder. The corresponding simulations are listed in the "AERMOD file" pull-down menu. Four sets of AERMOD simulations are provided with the GUI, corresponding to the four well pads at the three sites monitored during the HEI study.

The GUI assumes the emission source in AERMOD has a constant emission rate of 50 g s^{-2} m^{-2} with a radius of 0.6 m. Therefore, a conversion factor of $50 \cdot \pi \cdot 0.6^2$ is required to scale the concentrations to emission rates with units of g/s. If the emission rate used in the AERMOD simulations differs from this default value, the conversion factor must be updated accordingly.

4. References

Allen, T., Cardoso-Saldaña, F. J., Kimura, Y., Chen, Q., Xiang, Z., Zimmerle, , Bell, C., Lute, C., Duggan, J., & Harrison, M. (2022). A Methane Emission Estimation Tool (MEET) for predictions of emissions from upstream oil and gas well sites with fine scale temporal and spatial resolution: Model structure and applications. *Science of The Total Environment*, *829*, 154277.

EPA. (2020). *2020 EPA Nonpoint Oil and Gas Emissions Estimation Tool*.

Hanna, S. (1982). Handbook on Atmospheric Diffusion. *Department of Energy*.

Hecobian, A., Clements, A. L., Shonkwiler, K. B., Zhou, Y., MacDonald, L. P., Hilliard, N., Wells, B. L., Bibeau, B., Ham, J. M., & Pierce, J. R. (2019). Air toxics and other volatile organic compound emissions from unconventional oil and gas development. *Environmental Science & Technology Letters*, *6*(12), 720-726.

Zhang, W., Pan, , Ku, I.-T., Pierce, J., & Collett, J. J. (in preparation). Using Ambient Concentration Measurements to Quantify Volatile Organic Compound Emissions from Unconventional Oil and Gas Operations.