HEI Energy Collett Research Report 232

Measuring and Modeling Air Pollution and Noise Exposure Near Unconventional Oil and Gas Development in Colorado

Jeffrey L. Collett Jr. et al.

Appendix D. Technical Notes for Preproduction Module for the TRACER Model

Correspondence may be addressed to Dr. Jeffrey L. Collett Jr., Colorado State University, Atmospheric Science Department, Fort Collins, CO 80523-1371; email: collett@atmos.colostate.edu

Although this report was produced with partial funding by the United States Environmental Protection Agency under Contract No. 68HERC19D0010 to the Health Effects Institute, it has not been subjected to the Agency's peer and administrative review and may not reflect the views of the Agency; thus, no official endorsement by the Agency should be inferred. This report also has not been reviewed by private party institutions, including those that support HEI Energy, and may not reflect the views or policies of these parties; thus, no endorsement by them should be inferred.

Appendix D. Technical Notes for Preproduction Module for the TRACER Model

Table of Contents

D.1. General Information

Unconventional oil and gas development (UOGD) in the United States 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 preproduction VOC emissions, which is 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 preproduction 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 preproduction model features a graphical user interface (GUI) to facilitate broader use in policymaking and environmental health research.

The GUI of the preproduction module was 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.

D.2. Installation and Quick Start

D.2.1. Installation

The GUI can be downloaded as a ZIP file archived on a GitHub repository (see main report for link). To use the module, simply extract all the files into a single folder, and it will be ready to run.

D.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 a few seconds, a graphical interface, as shown in Figure D1, will appear.

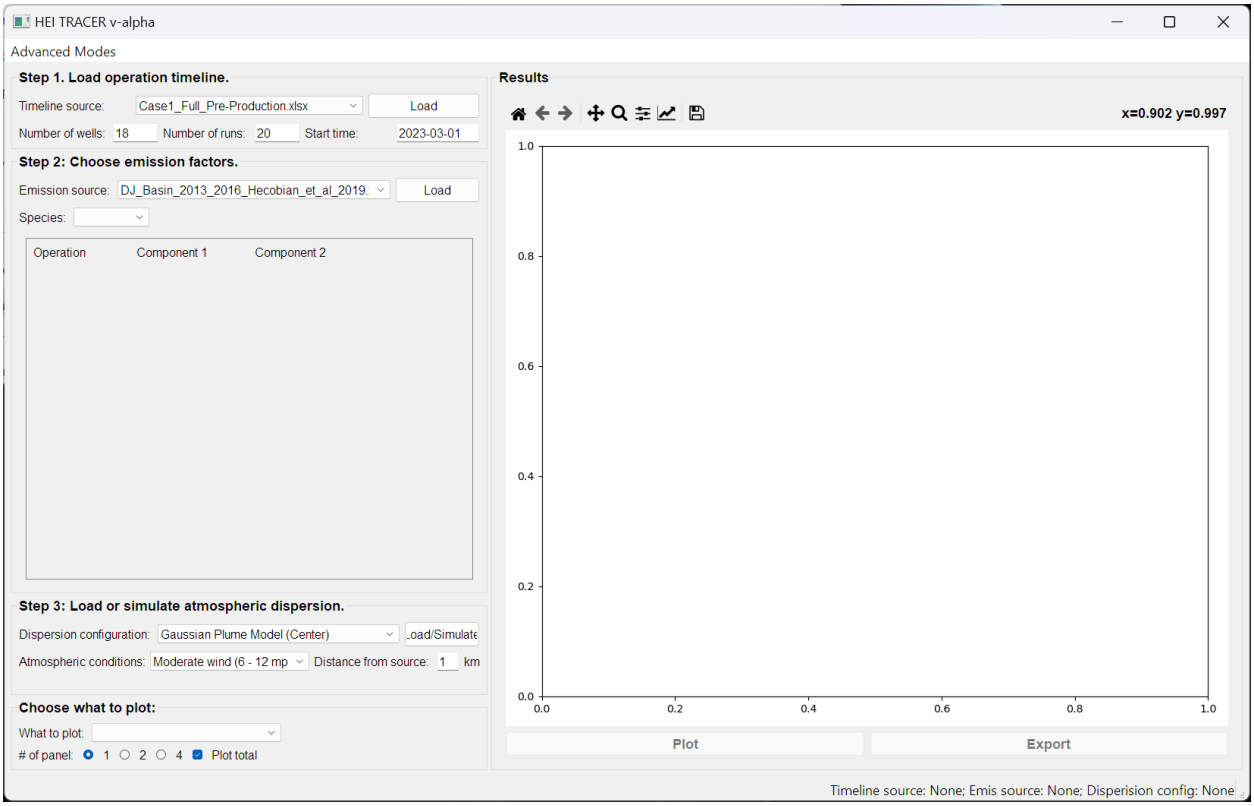


Figure D1. Typical user interface of the preproduction module for the TRACER Model.

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 predefined 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 predefined 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

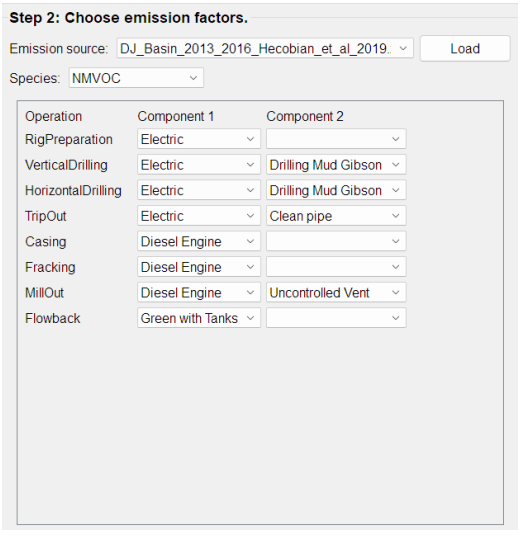


Figure D2. An example of emission sources.

emitting components. For example, rig preparation can be changed from being powered by electricity or a diesel engine.

- 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 the AERMOD simulation output file.
    - Enter site ID to obtain Optin-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 D3. 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, the 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.

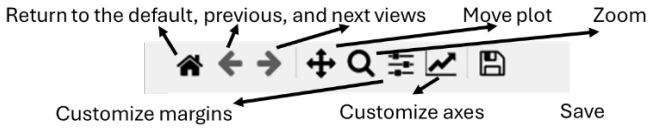


Figure D4. Plot customization toolbar.

D.3. Detailed Configurations and Data Sources

D.3.1. Operation Timeline

D.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. Table D1 defines the operations, and Figure D5 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 in the "Timeline source" pull-down menu.

Table D1. Descriptions of UOGD Operations and Corresponding Codes for the Preproduction 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; 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; drilling mud degassing
	Drilling Hz	Horizontal drilling within the "pay" zone	Drilling rig engines; 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; 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 flaring processes.
Production	Production		

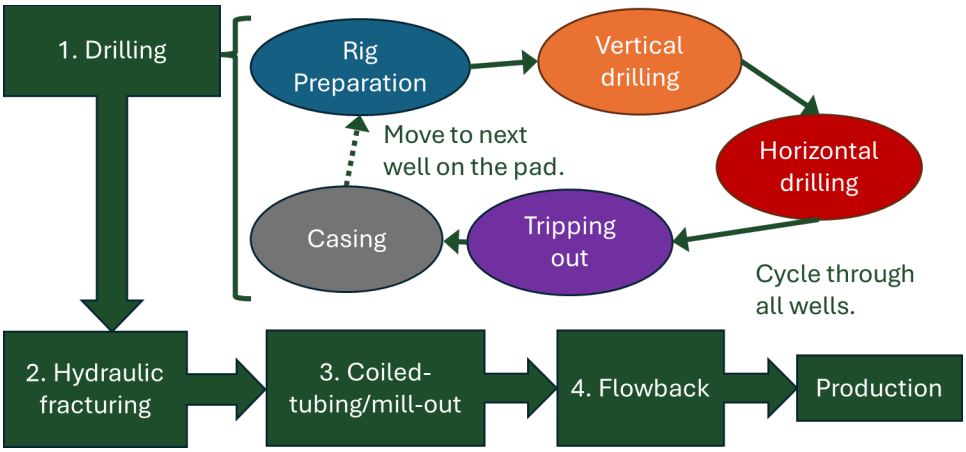


Figure D5. Operation sequences of preproduction activities.

D.3.1.2. Simulating an Operation Timeline

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 provided by operators in the DJ basin. Figure D6 shows the statistical summary of the durations. Multiple operation timelines will be simulated to form an ensemble.

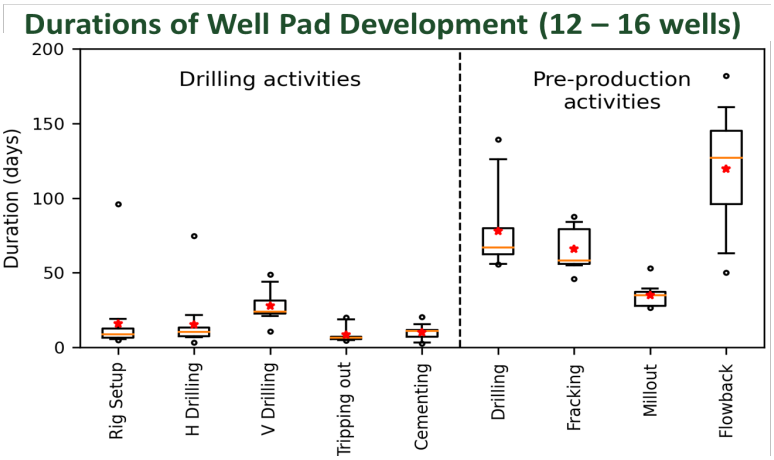


Figure D6. Statistical summary of operation durations obtained from different operators in the DJ Basin, Colorado. The boxes and whiskers show 5th, 25th, 50th, and 95th percentiles, and the red stars show the mean values.

To simulate a new ensemble of operation timelines, follow the steps below (Figure D7):

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.

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.

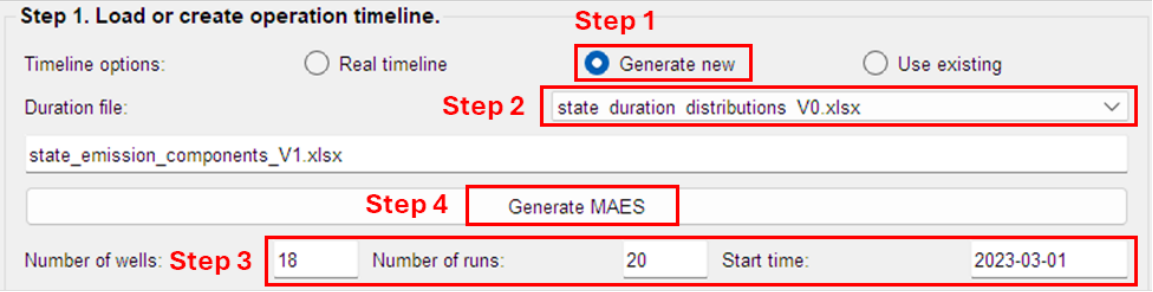


Figure D7. Steps for simulating a new ensemble of operation timelines using MAES.

To load a previously generated timeline ensemble, follow the steps below (Figure D8):

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 D8. Steps for loading an existing ensemble of operation timelines.

Figure D9 shows an example of a timeline ensemble. The transparent lines show individual simulations, whereas the solid line illustrates the ensemble mean.

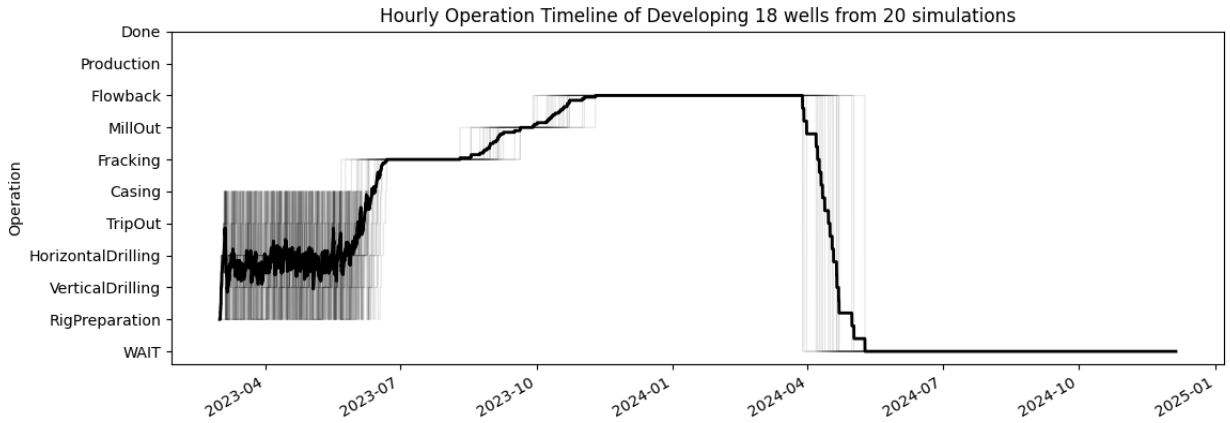


Figure D9. An example of MAES simulated operation timelines. The transparent lines show individual simulations, while the solid line illustrates the ensemble mean.

D.3.2. Emission Rates

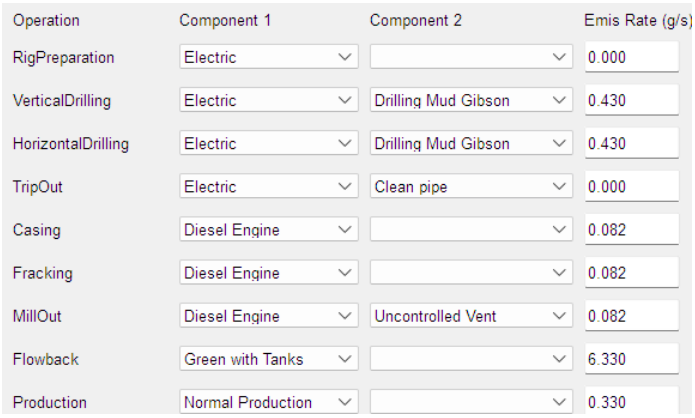
Three sets of emission rates are provided with the GUI:

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. 2025);
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 preproduction 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 and colleagues (2019) only have 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 Figure D10.



Operation	Component 1	Component 2	Emis Rate (g/s)
RigPreparation	Electric		0.000
VerticalDrilling	Electric	Drilling Mud Gibson	0.430
HorizontalDrilling	Electric	Drilling Mud Gibson	0.430
TripOut	Electric	Clean pipe	0.000
Casing	Diesel Engine		0.082
Fracking	Diesel Engine		0.082
MillOut	Diesel Engine	Uncontrolled Vent	0.082
Flowback	Green with Tanks		6.330
Production	Normal Production		0.330

Figure D10. An example of the emission rate panel, the advanced mode "Customize Emission Rates."

D.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.

D.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 follows:

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

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 follows:

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

Parameters are listed in Table D2 (Hanna, 1982). The Gaussian plume model used here considers plume reflection from the ground.

Table D2. 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 Table D3. 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 Figure D11.

Table D3. Conditions of the Predefined 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

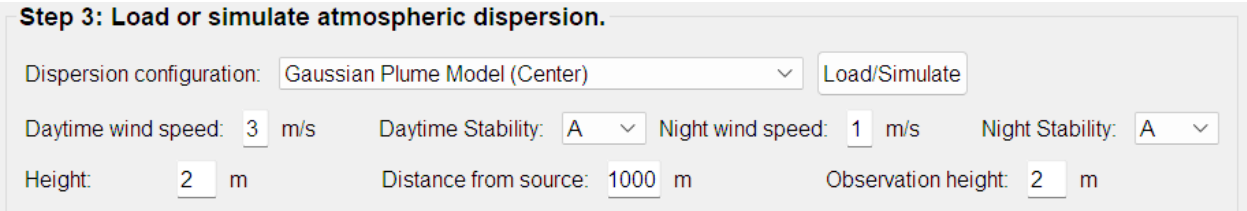


Figure D11. An example of the panel for modifying the meteorological conditions.

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.

D.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.

D.4. References

Allen, D. T., Cardoso-Saldaña, F. J., Kimura, Y., Chen, Q., Xiang, Z., Zimmerle, D., 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.

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.

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

Zhang, W., Pan, D., Ku, I.-T., Pierce, J., & Collett, J. J. (2025). Using ambient concentration measurements to quantify volatile organic compound emissions from unconventional oil and gas operations.Environmental Science & Technology, 16 December 2025.