Modeling VOC concentration increases near oil and gas well drilling, completion, and production operations

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SPOD1035

DJ Basin air monitoring approach

- 3 sites, 4 well pads, 3 O&G operators
- CDPHE CAMML
 - Hourly speciated VOCs, CH₄, NO_x, PM_{2.5}
- Weekly integrated VOC canisters
 - 51 speciated VOCs + CH₄
 - 2 near-pad locations plus background reference site
- Continuous PID monitors with event-triggered canister samples
 - 2 near-pad locations
- Mobile measurements
 - CH₄ and VOCs

O&G air emissions

Hydraulic fracturing

Fracking engines Material being pushed down-hole Truck traffic Drilling
Diesel/NG/Grid-powered
Drilling mud/shale shakers
Pipe pulling
Truck traffic

Flowback

- On-site storage of flowback/produced water
- Closed-loop/tankless systems
- Emptying sand cans

TRACER pre-production model



TRACER pre-production model emissions



EMISSION DATA SOURCES

EPA O&G Emission Tool

Hecobian et al. (2019)

Gaps & Limitations

- Missing some operations (e.g., coil tubing/mill-out)
- Evolving operational practices (e.g., flowback fluids handling)
- Sometimes lack full VOC speciation

Hecobian et al. (2019) Air toxics and other VOC emissions from UOGD, Env. Sci. Technol. Lett., doi: 10.1021/acs.estlett.9b00591.

Constraining UOGD VOC emission rates



Use multiple linear regression to constrain Broomfield VOC emission rates using AERMOD and ambient VOC concentrations

$$\begin{pmatrix} C_1 \\ \vdots \\ C_n \end{pmatrix} = C_{bg} + \begin{pmatrix} M_{1,1} & \cdots & M_{1,m} \\ \vdots & \ddots & \vdots \\ M_{n,1} & \cdots & M_{n,m} \end{pmatrix} \cdot \begin{pmatrix} e_1 \\ \vdots \\ e_m \end{pmatrix}$$



Ku et al. (2024) Air quality impacts from the development of unconventional oil and gas well pads: Air toxics and other volatile organic compounds. *Atmos. Environ.,* 120187. https://doi.org/10.1016/j.atmosenv.2023.120187.

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1...

20

25

30

35



Constraining UOGD VOC emission rates

- Updated estimates for drilling mud volatilization
 - including synthetic Neoflo

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- Higher than EPA tool and Hecobian et al.
- First emission estimates for coil tubing/millout operations
- >95% reduction in average VOC and benzene emissions from flowback using closed-loop, tankless systems vs. Hecobian et al. green completions
 - EPA Tool → zero VOC emissions for green completions



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Development of model Graphical User Interface (GUI)

- A GUI has been created to enhance accessibility in policymaking and research related to environmental health:
 - Created using Python 3 (PyQt5).
 - Also packaged as a standalone .exe file for Windows.
 - Inputs file are Excel sheets for easy access, except for AERMOD outputs.
 - Evaluated model performance with DJ air monitoring results.



Operation timelines

Detail operation logs from operators.

Start Time	End Time	Operation	Start Time	End Time	Operation
2022/09/06 18:00	2022/09/12 06:00	Move/Skid - Nipple Up	2023/03/15 00:00	2023/06/09 23:59	Fracking
2022/09/12 06:00	2022/09/13 14:30	BOP Test	2023/06/10 00:00 2023/07/10 00:00 2023/09/15 00:00	2023/07/09 23:59	MillOut
2022/09/13 14:30	2022/09/13 15:30	Drill VS		2023/09/15 23:59	Flowback
2022/09/13 15:30	2022/09/13 20:30	Drill Curve		2023/03/31 23:59	Production
2022/09/13 20:30	2022/09/15 13:15	Drill Hz	2023/03/13 00.00		
2022/09/15 13:15	2022/09/16 01:00	Trip out & Circulate			
2022/09/16 06:00	2022/09/16 22:00	Case & Cement			

Simulate operation timelines (MAES):

- Monte Carlo approach;
- Duration distributions are from real-world pad development timelines.







Emission factors

- The GUI comes with three sets of emission factors, offering options for various practices.
- Users can adjust the emission factors directly.

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 V		< 0.082
Fracking	Diesel Engine 🗸		< 0.082
MillOut	Diesel Engine	Uncontrolled Vent	< 0.082
Flowback	Green with Tanks \sim		6.330
Production	Normal Production \sim		0.330



Median Mean

EPA Emission Tool

Hecobian et al. (2019)

Atmospheric dispersion

Gaussian plume model:

- Users can modify atmospheric settings and receptor positions (distance/height).
- Three preset locations are included for convenience.



AERMOD model:

• The GUI can read AERMOD outputs directly.

Cmodel (µg/m³)

Model evaluation through air monitoring

Observation and UOGD timelines:



Model configuration:

- Detailed operation timelines;
- Inverse-modeled emission rates (Zhang-2025) and EPA Emission Tool;
- AERMOD simulations for monitoring locations.

Evaluation: Weekly VOC Concentrations

- Updated emission factors better represent drilling and coil-tubing emissions
 - Including C₈ C₁₀ n-alkanes from drilling muds
 - Higher than EPA tool during drilling and coil-tubing
- VOC concentrations during early production show large variability
 - Underestimated by both Zhang-2025 and EPA Tool at site 1; but overestimated by EPA Tool at 3 (not shown).
 - Changing practices need further investigation



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Evaluation: benzene hourly exceedance (9 ppbv)

- The low early production emission rate of Zhang-2025 leads to the underestimation of benzene exceedance events.
- EPA Emission Tool significantly overestimates the number of exceedance events during early production.

	Site 1 Drilling	Site 2 Drilling	Site 3 Fracking	Site 3 Fracking & Coil-Tubing	Site 3 Coil- Tubing & Production	Site 3 Early Production
CAMML	1	0	0	0	8	4
observations						
Model with	0	0	0	1	5	0
Zhang-2025						
emission rates						
Model with EPA	0	0	0	0	5	19
emission rates						

Study highlights - modeling

- New TRACER UOGD pre-production model. Enables stakeholders to
 - Predict air quality impacts and their timing during specific operational phases
 - Evaluate air quality benefits of best management practices such as
 - drill rig electrification
 - drilling mud choice
 - closed-loop/tankless fluids handling
 - altering schedule to different season



- Recent DJ Basin UOGD preproduction activities studied to improve model emission rate inputs for current UOGD practices
- Reasonable performance for DJ Basin UOGD pre-production activities but needs to be tested in other basins