



Modeling air emissions from complex facilities at detailed temporal and spatial resolution: The Methane Emission Estimation Tool (MEET)



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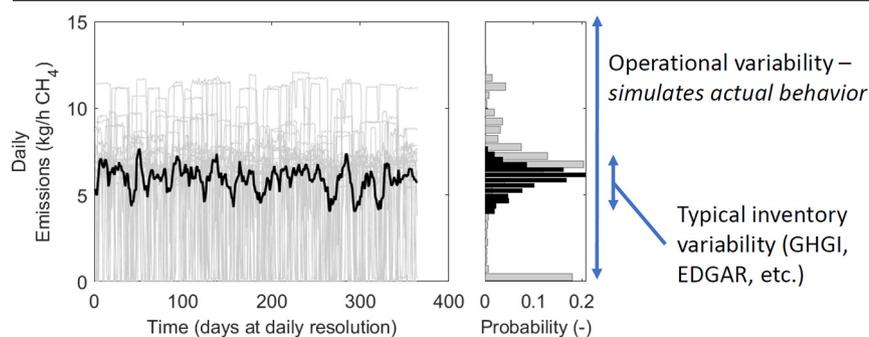
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HIGHLIGHTS

- Anthropogenic methane emissions are a key driver of climate change.
- Traditional inventory methods do not account for spatial and temporal variability.
- MEET model uses novel methods to capture mechanistic drivers of emissions.
- Most emissions studies fail to collect information needed to model variability
- Modeling temporal & spatial variability highlights uncertainty in measurements.

GRAPHICAL ABSTRACT



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ABSTRACT

Recent attention to methane emissions from oil and gas infrastructure has increased interest in comparing measurements with inventory emission estimates. While measurement methods typically estimate emissions over a few periods that are seconds to hours in length, current inventory methods typically produce long-term average emission estimates. This temporal mis-alignment complicates comparisons and leads to underestimates in the uncertainty of measurement methods. This study describes a new temporally and spatially resolved inventory emission model (MEET), and demonstrates the model by application to compressor station emissions – the key facility type in midstream natural gas operations. The study looks at three common facility measurement methods: tracer flux methods for measuring station emissions, the use of ethane-methane ratios for source attribution of basin-scale estimates, and the behavior of continuous monitoring for leak detection at stations. Simulation results indicate that measurement methods likely underestimate uncertainties in emission estimates by failing to account for the variability in normal facility emissions and variations in ethane/methane ratios. A tracer-based measurement campaign could estimate emissions outside the 95% confidence interval of annual emissions 30% of the time, while ethane/methane ratios could be mis-estimated by as much as 50%. Use of MEET also highlights the need to improve data reporting from measurement campaigns to better capture the temporal and spatial variation in observed emissions.

1. Introduction

Methane is a powerful greenhouse gas and atmospheric methane concentrations have increased steadily since 1980 (N. US Department of Commerce, n.d.). Evidence indicates that a substantial portion of the increase is due to anthropogenic sources, including fossil fuel development

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(Turner et al., 2019; Zhang et al., 2021; Milkov et al., 2020). This increase coincides with increases in natural gas production globally, driving interest in methane emissions from the natural gas supply chain as well as emissions of hazardous air pollutants and CO₂. Multiple recent studies have also indicated that large emitters from oil and gas (O&G) operations are likely under-represented in current inventories of O&G methane emissions and that these emitters likely originate from abnormal process conditions at O&G production and midstream operations (Duren et al., 2019; Cusworth et al., 2021; Lauvaux et al., 2021; Lyon et al., 2021). In response, several organizations independent of regulators or the O&G industry have started large-scale aircraft – and in some cases satellite – campaigns to identify large emitters and publish them in open data portals, including the Environmental Defense Fund's *Permian Map* project (Fund, n.d.), the Jet Propulsion Laboratory's *Methane Source Finder* (Jet Propulsion Laboratory, n.d.), and CarbonMapper's open data portal (CarbonMapper, n.d.).

Data from these large-scale measurement efforts indicate that a substantial fraction of the detected large emitters behave stochastically: While a similar number of large emitters may be seen on multiple days of measurement, the location and size of the emitters varies substantially. Emissions with highly variable temporal and spatial behavior are poorly captured in current inventory methods, such as those utilized by national inventories (e.g. U.S. Environmental Protection Agency (EPA) Greenhouse Gas Inventory (GHGI) and many modeling studies, including recent work modeling national-scale emissions for transmission and storage (T&S) (Zimmerle et al., 2015), gathering and processing (G&P) (Marchese et al., 2015; Zimmerle et al., 2020), and distribution systems (Lamb et al., 2015). Since these emitters are poorly captured in inventory methods, it is difficult to compare results of aircraft/satellite surveys ('top down') with inventories ('bottom up') that represent emissions as averages over extended periods and large regions – typically annual averages at basin-to-continental scales. These challenges are reflected in several comparisons of top-down measurements to bottom-up inventories (Vaughn et al., 2018; Zavala-Araiza et al., 2015a; Zavala-Araiza et al., 2015b).

The work presented here introduces a new approach to bottom-up inventory methods that increases both spatial and temporal resolution, building upon modeling done for basin scale studies in the Fayetteville Shale region (Vaughn et al., 2018) and the Barnett production basin (Allen et al., 2017) in the USA. This approach supports more accurate comparisons between measurement surveys and inventories by better incorporating normal variability in emissions as well as recent data on large emitters and abnormal process conditions. As an illustration of this method, the work focuses on one sector of the natural gas supply chain – midstream – and compares to several commonly utilized facility-scale methods to the improved inventory method. The same tool and method could be made utilized for other natural gas sectors or for other anthropogenic source categories that exhibit high variability.

The midstream sector of the USA natural gas supply chain transports and upgrades an estimated 33×10^{12} standard cubic feet (scf), or 934×10^9 m³, of natural gas from US production basins to distribution companies and industrial consumers using over 400,000 miles (640,000 km) of natural gas pipelines (EIA, n.d.) and associated compressor stations and processing facilities.

Compressor stations in all sectors of the natural gas industry receive gas from one or more pipelines originating at well pads or other compressor stations, compress the gas, and inject it into downstream pipelines. Stations often host equipment to support connected pipelines, such as pig launchers and receivers, and metering equipment. In gathering and storage applications, stations often include equipment that upgrades gas quality, including dehydrators and acid gas removal units (AGRU). Compressor equipment found in these sectors is also found at gas processing plants to inject processed gas into transmission pipelines.

The gathering compression stations, compressors at gas processing plants, and the inter-connecting pipelines between these stations represents the sizable G&P sector of the U.S. onshore natural gas industry. The T&S system, which transports processed gas to consumers, consists primarily of transmission stations interconnected by pipelines, and storage stations

that buffer gas supplies for use in peak demand periods. These two sectors make up an estimated half (U. EPA Inventory of U.S. greenhouse gas emissions and sinks, 1990) of U.S. methane emissions from the onshore natural gas system. Therefore, emissions from these facilities are of strong interest for both air quality and greenhouse gas reasons.

Emissions from these sectors have traditionally been estimated using 'inventory' or 'bottom-up (BU)' methods, including the EPA GHGI (U. EPA Inventory of U.S. greenhouse gas emissions and sinks, 1990). Inventories estimate emissions by multiplying a measure of activity ('activity factor') – such as component or equipment counts, or operating hours – by an estimated emission rate ('emission factor') for the activity. For example, connector leak emissions at a facility would be estimated by multiplying the average emission rate for all connectors on a gathering compressor station with the number of connectors on that station. Generally, both activity and emission factors represent long-term averages of both quantities, and are suitable for calculating total emissions over extended time periods (months to years), for a large area, such as a nation or state, although some recent work has looked at gridded inventories with finer spatial resolution. (Maasackers et al., 2016; Vaughn et al., 2018; Allen et al., 2017)

Recently, however, there has been increasing interest in BU estimates that are more representative of shorter time periods and higher spatial resolutions. Examples include comparing top-down (TD) aircraft estimates of basin emissions to BU inventories of those basins (Peischl et al., 2016; Peischl et al., 2015; Karion et al., 2015; Karion et al., 2013); comparing TD estimates to inventories based on BU measurements (Schwietzke et al., May 2017); or comparing downwind facility-level measurements with BU inventories of those facilities (Vaughn et al., 2017; Bell et al., 2017; Omara et al., 2016; Robertson et al., 2017; Yacovitch et al., 2015; Roscioli et al., 2015). In each case, measurement using downwind or mass balance methods occur during short time periods (typically minutes) and are often constrained to afternoon working hours during the week, while the comparison inventory methods are long-term averages that include no temporal variability or spatial heterogeneity. These differences have stimulated concerns about the representativeness of inventory methods and spurred an interest in understanding the emission variation in bottom-up models (Vaughn et al., 2018).

This study describes BU inventory modeling using Methane Emissions Estimation Tool (MEET), an inventory emissions model expressly designed to model time scales ranging from seconds to years, resolved to the spatial resolution of individual facilities or major equipment units. MEET models track any gas species which are available in emissions data, typically CO₂, methane, and other light alkanes, although other species are readily accommodated. A companion paper (Cardoso-Saldaña et al., 2021) describes the calculation of gas and fluid compositions that serve as inputs to MEET. Of particular interest is the comparison between short-duration measurements – here represented by full-facility measurement method – and inventory methods, including both variability in emissions and gas species ratios, which are often utilized by TD methods for source attribution (for example, references (Peischl et al., 2015; Karion et al., 2015; Schwietzke et al., May 2017)). Additionally, the study also illustrates how continuous monitoring can be analyzed using temporally-resolved emissions.

To demonstrate these capabilities, we utilize natural gas compressor stations. Compressor stations represent one of the most concentrated and temporally variable sources of greenhouse gas (GHG) emissions in the natural gas supply chain. The large compressors (0.5–50 MW) on these facilities cycle on/off with demand, and other equipment on the stations increases/decreases loading and associated emissions as compressor loads change. In addition, many compressor drivers (typically large engines or turbines) often burn some of the gas passing through the station for power. Driver exhaust gases often represent one of the largest sources of emissions on a station (Zimmerle et al., 2015; Vaughn et al., 2017; Zimmerle et al., 2020; Zimmerle et al., 2019a). Compressor equipment also releases short duration, high-rate, emissions as equipment is depressurized when idled (blown down) or started (gas starters). This variability has a substantial impact on emissions which may be measured by

short-duration methods, leading to an interest in improving the modeling of compressor station emissions.

2. Methods

MEET implements a robust framework for emissions modeling built around a *discrete event simulator (DES)*, a common multi-agent simulation methodology where individual ‘agents’ model the behavior of specific processes and interact with each other via a central event queue. Agent models (hereafter ‘models’) currently implemented in MEET include models for well pads and compressor stations, each of which combine models for major equipment, components, leaks, and operational changes on these facilities. The model framework is extensible to other sectors, equipment and facility types, as well as processes which interact with these facilities, such as leak detection and repair (LDAR) surveys, liquid transport, or equipment modifications. Events in MEET are resolved to the second, but can be queried at time resolutions from seconds to years. MEET resolves spatial dimensions to the major equipment level if those data are available.

An overview of the MEET simulation process is shown in Fig. 1. The analyst defines activity data and either selects or populates emissions data. MEET runs multiple Monte Carlo (MC) iterations and saves results to event logs. After simulation, the analyst extracts time-series of emissions from the desired MC iterations at the desired time resolution. Using multiple calls to the time series extraction tools, the analyst can drill down to finer time resolution in periods and facilities of interest. For both simulation and extraction, individual MC iterations and time-period queries are independent and can be executed in parallel on multi-core and cluster servers.

As with all inventory models, emissions and activity data completely define the behavior of the emissions model. However, the introduction of spatial resolution and time varying behavior introduces several unique aspects into MEET’s models, which are discussed below.

Emitter population: The compressor station model, like all facility models in MEET, is organized into a three-level hierarchy matching that used in several recent studies (Zimmerle et al., 2020; Vaughn et al., 2017; Zimmerle et al., 2015) [SI Section S-1]:

1. **Station or Facility:** A physical group of equipment, typically surrounded by a fence or some other outer marker.

2. **Major equipment unit:** A major, integrated, equipment unit at the station. Six types of major equipment at compressor stations are modeled for this study: Compressors, dehydrators, acid gas removal units (AGRUs), station separators, tanks, and flares. The limit of each unit of major equipment is defined by the flanges which connect it to the gas transport piping on the station. All equipment not assigned to another major equipment unit is grouped into a single unit of major equipment termed ‘yard piping,’ as in Zimmerle et al. (2019b).

3. **Components:** Each major equipment unit includes many components. Nine types of components (threaded and flanged connectors, open-ended lines (OELs), valves, meters, pressure reducing valves (PRVs), regulators, gauges, and gas-driven pneumatic controllers) cover the general-purpose component categories found on all major equipment categories. Compressors include several additional types of compressor-specific components (blowdown and isolation valves, rod packing or shaft seals, pocket vents, gas starter valves, and combined vents). Additional specialized categories, such as station vents, are also modeled [SI Section S-1.1].

Activity data are defined by enumerating individual stations and the major equipment units on the station, while components are instantiated using population distributions for each component type [SI Section S-1].

Emission labels: In addition to chemical species, BU emissions simulation also provides insight into the origin and cause of emissions, and allows analysts to compare relative, interacting, emission rates between source types and causes. To support these analyses, MEET labels emissions with their source and cause. *Source* is identified by using user-supplied activity identifiers, which follows the hierarchy above. Currently, MEET supports the three labels for the *cause* of an emission:

1. **Fugitive:** Unintended emissions of uncombusted gas from components; commonly called ‘leaks,’ but also including excess venting and abnormal process conditions that release gas to atmosphere.

2. **Vented:** Emissions of uncombusted gas as part of regular site operations. Examples include venting from gas-powered pneumatic controllers and blowdowns of pressurized equipment.

3. **Combusted:** Emissions from onsite combustion. These emissions include combustion products (this study tracks only CO₂) and unburned fuel entrained in the combustion exhaust, commonly called ‘combustion slip,’ from engines, flares, heaters, dehydrator still vents and other sources.

For labeling to be effective, activity and emissions data must support the classification of emissions into the appropriate categories. Emissions from a single location may change labels depending upon the operating state of equipment, the emissions behavior (size, duration, etc.), or via interaction with external agents (e.g. leak repair). Several special cases need to be considered.

First, in most venting categories, there is an intended emission rate and duration. Two possibilities exist: (a) Emissions below the intended rate *and* within the intended duration are classified as *vented* emissions; and (b) Emissions above the intended rate or longer than the intended duration are *fugitive* emissions. Unfortunately, few published data sources include sufficient information to separate vented emissions measurements between (a) and (b). For example, low- and intermittent-bleed gas pneumatic controllers are specified with an intended emission rate and, for intermittent bleed controllers, an expected duration for each actuation. (Luck et al., 2019a) However, most data on pneumatic controller emissions provide only total emissions (Allen et al., 2015; Lamb et al., 2015; Zimmerle et al., 2015) which are not segmented into vented and fugitive components. Luck et al. (2019b) provide a prototype of how emissions could be segmented, but the data are limited in scope. Ideally, future field studies would collect and publish these data.

Second, properly operating combustion devices typically emit a fraction of the fuel gas uncombusted. For example, flares are specified to have a ‘combustion efficiency’ – typically 98% – which indicates that 2% of the combustible hydrocarbons sent to the flare are released uncombusted. Similarly, dehydrator still vents, engine exhaust, AGRU reboilers, etc. have similar specifications for properly functioning emissions. When malfunctioning, efficiency may drop substantially, and these emissions should be classified as fugitive emissions. As with pneumatic controllers, these data are not generally available.

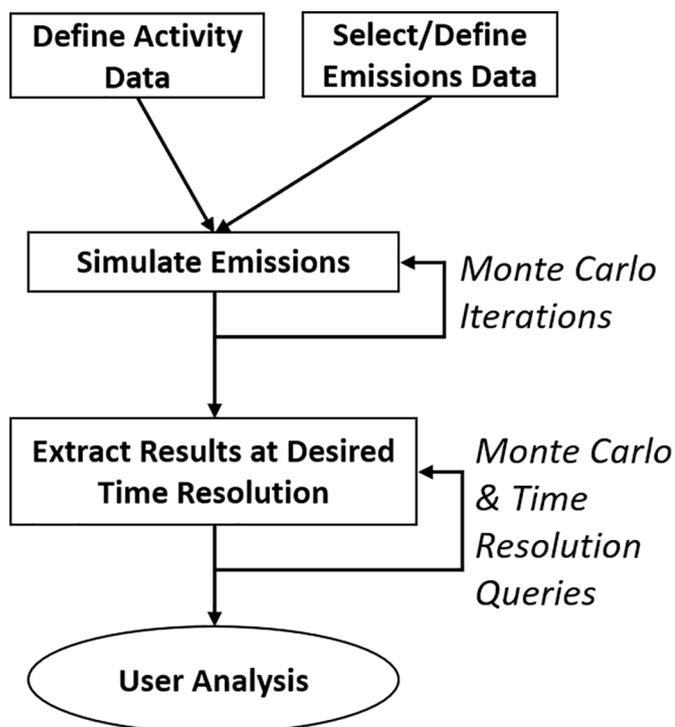


Fig. 1. Overview of MEET process.

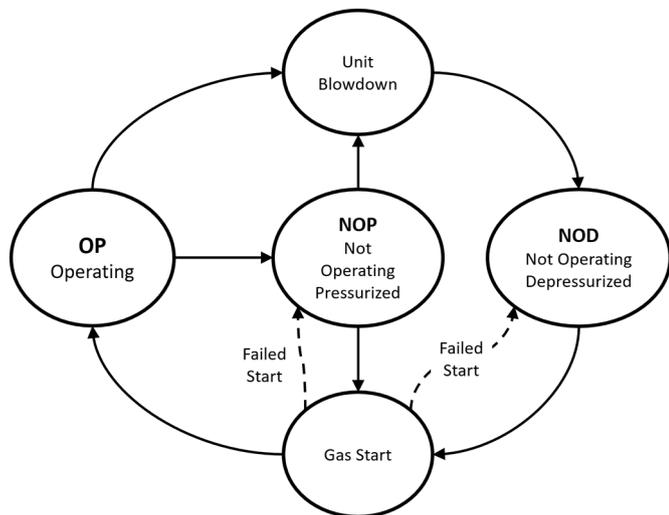


Fig. 2. Compressor unit operating states. The diagram illustrates the principal operating modes of the compressor and its associated driver. Valid state transitions are shown with arrows. Current model does not implement failed starts.

Due to these data limitations, available input data forces emissions to be coarsely labeled in the current model. SI Table S-2 summarizes labeling for each category of modeled emissions, SI Section S-6 describes episodic venting (gas starters and blowdowns), and SI Section S-7 describes non-episodic vented sources.

Time domain behavior: Since emissions models in MEET are DES agents, changes in one model may impact the behavior of other models. For example, a leak detection agent could identify a fugitive emission, trigger a leak repair agent, which in turn mitigates the fugitive emission.

For compressor stations, the operating mode of the on-site compressors represents the single largest driver of temporal variations in emissions, due to the large exhaust emissions of the compressor drivers (Vaughn et al., 2017; Zimmerle et al., 2020), and the high-rate, short-duration, gas releases when compressors are started or blown down. For emissions purposes, each compressor is at all times in, or transitioning into, one of three principle operating modes: Operating (OP); not operating pressurized (NOP); and not operating depressurized (NOD). State transitions are shown in Fig. 2. To depressurize the unit, the compressor passes (briefly) through the unit blowdown state, when the blowdown valve is opened and pressurized gas in the compressor is vented, typically to atmosphere. When entering OP mode from either NOP or NOD, the compressor must pass through a short-duration ‘start’ state to start the compressor driver; if a gas starter is present, gas will be vented during this state. In some cases, the start fails (dotted lines), resulting in a return to the previous state. (Failed starts were not implemented for this study due to the lack of data for the frequency at which they occur).

Major compressor valves (isolation, blowdown, starter) change state with the compressor operating mode [SI Section S-1.3, S-6]. Emissions through the valve seal when the valve is closed are fugitive emissions. When open, there are no emissions or emissions are intentionally vented emissions. For example, during unit blowdowns, the blowdown valve is opened and emissions are vented (i.e. intended). When the compressor is pressurized (OP and NOP modes), the blowdown valve is closed, and any leaks through the valve seal are fugitive (i.e. unintended) emissions. When the compressor is depressurized (NOD mode), the blowdown valve is typically left open, and causes no emissions; any emissions observed at the blowdown vent are due to leaks in isolation valve seals [SI Table S-1, Fig. S-3]. A similar analysis was performed on other emitter categories, as shown in Table 1 [More detail in SI Table S-2].

Intermittent gas pneumatics also cycle between two operating states – a near-zero emission waiting period and a short, high-emitting, actuation. Actuation rates vary between near-zero to frequent actuations (Luck

et al., 2019b). Typically, actuation emission rates peak at 75 slpm (150 scfh) whole gas, and may interact with other processes, such leak detection.

Inter-dependencies between emitters: Gas throughput for a station is determined by the number of compressors operating and the current throughput of each unit. The operation of other equipment on the station, such as dehydrators, flares and tanks, varies with the station throughput. Variations can include both gas throughput for individual units, or the number of units on-line at any one time. The frequency of dump valve actuations on station separators is also dependent upon throughput and the quantity of liquid in the incoming gas. Unfortunately, little data exists to link the operation of non-compressor equipment to the current throughput of the station. For example, vent emissions from dehydrators depend upon throughput, but also re-circulation rate and other settings that vary somewhat independently of throughput.

Due to lack of public data, MEET’s current example inputs do not coordinate compressor operations with other equipment. However, when analysts select input data, they can coordinate the throughput-related loadings between equipment types. Assuming the availability of the required data, future extensions of the model could coordinate throughput for all facility equipment.

Leak models: A primary focus of BU models is an accurate treatment of fugitive (leaks and other unexpected) emissions behavior. MEET uses one leak model for all facility types; it requires three sets of information:

1. Distributions of component/source counts for each component/source category, for each major equipment type. Component count distributions are typically derived from field studies that counted components, or from internal company data.
2. The fraction of each component category that is leaking.
3. Distribution of emission rates for *leaking components*, commonly called a ‘leaker factor’ or ‘leaker distribution.’ Note that leaker data is *not* the same as *average* or *population* emission factors. (Zimmerle et al., 2019b)

Since many distributions are highly skewed, empirical distributions from field studies are preferred for both activity and emission data.

Most field studies of leaks are ‘snapshots’ in time that identified and measured individual leaks. In contrast, MEET needs not only the leak size, but also a measure of the frequency at which new leaks appear. To estimate these parameters, MEET makes a number of assumptions to emulate a time-varying leak count with variable leak size. Key steps are discussed below; SI Section S-5.1 provides mathematical detail on the formulation of the model.

First, the model assigns component counts for each component type on each unit of major equipment (e.g. a compressor). Counts are pre-set for some source types [SI Section S-1.1] or drawn from an empirical distribution of counts for others [SI Section S-4].

Second, at the start of the simulation, MEET assumes that the fraction of components leaking in each component category equals the fraction observed in field data. MC methods are used to populate these initial leaks.

Table 1

Emission labels for emitter categories on compressors that change with compressor mode.

Emitter category	OP	NOP	NOD	START	BLOW- DOWN
Components leaks	F	F		F	F
Gas pneumatics ^a	V	V		V	V
Blowdown valve	F	F		F	V
Isolation valve		F	F		F
Starter valve	F	F	F	V	F
Rod packing ^b	V	F	F		
Wet/dry seals	V				
Combined unit vents	F	F		F	
Compressor driver exhaust	C				

Key: F: fugitive, V: vented, C: exhaust, and blank indicates the emitter is inactive, but not mitigated.

^a Emissions from intermittent pneumatic controllers may be either fugitive or vented emissions.

^b Rod packing emissions are drawn from different distributions for each compressor operating mode.

Leak count may vary substantially between MC iterations, but will converge over a sufficiently large number of MC iterations to the fraction of components seen leaking in the field study. This method assures that the facilities modeled in MEET reflect the conditions seen in the field study at the start of the simulation.

Finally, later in the simulation, additional leaks will start. Leaks may also be repaired, either through routine facility maintenance or via specific LDAR processes. To generate additional leaks, an assumption must be made on the frequency at which leaks appear on the simulated equipment. Most emissions models are populated with data from field campaigns that screened for leaks at many field locations (operator records from LDAR programs may also be used). In most cases, the facilities screened for leaks in these studies have been subject to prior LDAR activities. The frequency of LDAR surveys, and the fraction of detected leaks repaired, impact how these data reflect the *generation rate* of new leaks. Unfortunately, these qualifying data are seldom published. Therefore, the model makes several assumptions to produce a realistic leak generation rate.

First, the model assumes that (a) facilities in the field study were subject to periodic LDAR surveys; (b) all leaks were detected; and (c) all detected leaks were fixed shortly after detection, prior to the next survey. Therefore, leaks detected during any survey – including the study's field campaign – reflect the number of new leaks since the last survey. Since field campaigns typically measure facilities at arbitrary times, on average they visit facilities half way between LDAR surveys. Leaks detected therefore represent, on average, half the leaks generated at the facility per LDAR survey.

Unfortunately, leak survey frequency for studied facilities is not typically published with field studies. Therefore, MEET assumes that LDAR surveys occur annually, a common frequency, and therefore the field data represent new leaks which appeared in six months. Different survey frequencies can be accommodated, if known, by adjusting the leak generation rate parameters.

Second, if leaks are generated but not repaired, the number of leaks will increase throughout the simulation. This may be the desired behavior, for example, to test the efficacy of several LDAR programs. However, in the default case, where leak repair actions are not independently simulated, MEET simulates repair actions such that leaks are repaired at the same rate as they are generated. Since repair actions are generated independently from leak generation, the number of leaks will vary, but will converge to the desired leak frequency over a sufficiently large MC simulation.

The availability of leak data varies substantially between compressor stations in different industry sectors, and current sources require specific pre-processing to be included in a MEET model [SI Sections S-5.2 to S-5.5].

Gas composition: For this study, MEET simulates CO₂, CH₄, and light alkane emissions. During the DES simulation, the event log notes the type of gas emitted (e.g. whole gas, combustion exhaust, etc.) and gas compositions are applied when data is extracted to a time series.

For compressor stations, gas composition data varies between incoming gas, gas after dehydration, and flash gas from liquid storage tanks. However, these data are not generally available for compressor stations. Therefore, the current MEET model utilizes a single gas composition for all *whole gas* emissions from the facility (vented or fugitive), while combusted emissions are computed using models which are specific to the type of equipment [SI Section S-3].

Sources not modeled: Several sources are not included in current MEET models for compressor stations, due to the lack of public data to design these models. Combustion emissions from heaters (e.g. AGRU steam heaters, dehydrator reboilers) are not modeled. MEET also assumes all AGRU vents are routed to flares. Full or partial station blowdowns are not modeled; these events are infrequent. While only marginally interesting for method comparisons, they must be included to estimate annual emissions. Unlike the MEET production facility model, tank flash emissions are not modeled since little information exists on the composition of liquids sent to the tanks. Finally, emissions from dehydrators and flares are drawn randomly from Greenhouse Gas Reporting Program (GHGRP) reports, and, as a result, there may be mismatch between the size of these emitters and other equipment on the compressor station in some MC iterations.

For ease of use, MEET defaults any data not specified by the analyst. For example, if the number of compressors are specified, but the size and type of compressor driver is not specified, these values are drawn randomly from published data, and will vary substantially between MC iterations. Alternatively, if these values are specified, then major compressor emissions, such as compressor driver exhaust, will show only minor variation between iterations.

3. Results and discussion

To demonstrate the model, a set of eight compressor stations was constructed. Seven of the stations are modeled after facilities measured in a recent basin study (Vaughn et al., 2017), including the size and number of compressors and the type of compressor driver. After configuring the facility equipment, the run time of the compressors was manipulated to create a variety of operating characteristics across a range of compressor loading (fractional load when running) and utilization (fraction of the time the compressor is running). The eighth station (station ID 1), utilizes compressor types, loads, and utilization taken from T&S data (Zimmerle et al., 2015). Key characteristics of the stations are summarized in Table 2, and SI Table S-6.

The stations were simulated for a year, using a relatively small number of Monte Carlo iterations (20), since the primary purpose is to illustrate the functionality of the model. Across all iterations, 3131 emitters were active at some time. Large emitters were included by modifying default emissions distributions [SI S-9.3]; the 25 emitters larger than 10 kg/h are summarized in SI Table S-9. These emitters appeared in 14 Monte Carlo iterations, and on 6 of the eight stations, in at least one iteration, and 6 sources emitted over 100 kg/h.

Daily total emissions were extracted for all emitters, and a set of 26 randomly-selected half-day periods were extracted at one-minute resolution to simulate measurement methods. Fig. 3 provides an example of daily and minute resolution time series.

To demonstrate the model, we consider three test cases which model aspects of methods in active use: error bounds when estimating emissions using a downwind tracer flux method, variability in ethane/methane ratio, and the probability that a continuous monitor can identify a fugitive emission given a substantial background of vented and combusted emissions.

Table 2
Key operating characteristics of test stations.

Station ID	Sector	Size	Compressor COUNT	Total station power (10 ³ HP)	Total station power (MW)	Compressor loading when operating	Utilization	Operating fraction
1	T	–	2	9.78	7.29	90%	Very low	35%
2	G	Typical	8	12.5	9.29	80%	Typical	79%
3	G	Typical	5	8.88	6.62	98%	Typical	85%
4	G	Small	2	3.55	2.65	104%	High	90%
5	G	Small	2	3.55	2.65	50%	High	90%
6	G	Large	24	40.9	30.5	90%	Typical	79%
7	G	Small	2	6.23	4.65	0%	Zero	0%
8	G	Typical	7	12.5	9.29	90%	Low	58%
All	G&T	–	52	97.8	72.9	86%	Typical	73%

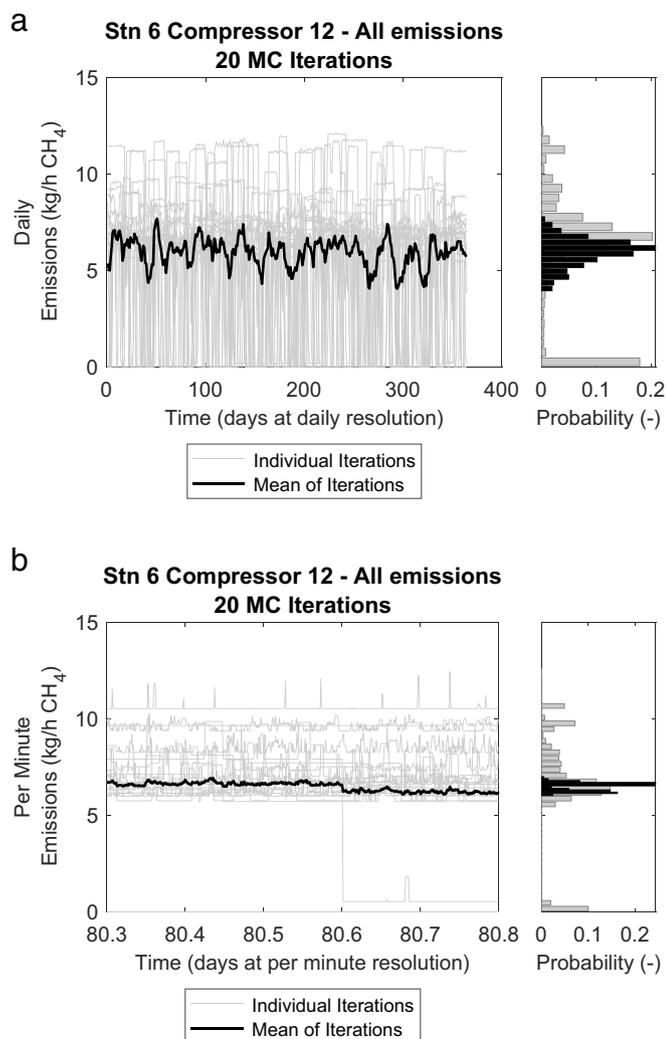


Fig. 3. Simulation examples for compressor 12 on station 6. Left panel displays the time series. Light gray lines indicate the 20 individual Monte Carlo iterations and the dark line indicates the mean over all iterations. Right panel displays the same data as a histogram of values.

Tracer Flux Simulation: Single- and dual-tracer flux methods are well-established methods for estimating facility-scale emissions (Vaughn et al., 2017; Zimmerle et al., 2015; Bell et al., 2017; Yacovitch et al., 2015; Yacovitch et al., 2017), following methods developed in the 1990s (Lamb et al., 1995) and extended recently with the use of more advanced trace gas analyzers (Roscioli et al., 2015). Briefly, the method utilizes one or more tracer gasses – acetylene and nitrous oxide are common – released at a known rate near a suspected emission source. A mobile instrument transects the emission plume downwind of the release, covering sufficient distance to measure both background and plume concentrations of both tracer and target species. Emission rates are calculated from the ratio of the target species to the known tracer emission rate [SI Section S-9.4].

In this study, tracer measurements were simulated using the one-minute resolution data. Each transect (or ‘plume’) was calculated as the mean of 3 min of data with a measurement error standard deviation of 15%. The plume duration is a conservative assumption (which improves the tracer estimates) by averaging over a longer time than a typical transect. Measurement error is typical of estimated error from prior studies. (Yacovitch et al., 2015; Roscioli et al., 2015; Mitchell et al., 2015). A single tracer measurement was the mean of multiple (2 to 8) plumes, which were spaced 5 to 15 min apart. The resulting simulations were ‘best case’ tracer method estimates, with no confounding sources, and neglecting any issues due to spatial misalignment of emission sources relative to tracer release location,

poor road access, or challenging wind conditions. Results are summarized in Fig. 4 and SI Table S-10.

The tracer simulation demonstrates that the method correctly estimates emissions for all station types and sizes over a large number of days and simulated measurement events. Errors in mean estimated emissions range from -2% to 0.9% for individual stations, and -0.5% for measured emissions on the group of 8 stations. This illustrates that the method itself produces correct estimates in the mean.

However, no measurement campaign includes a large number of days and measurements; campaigns are economically limited to a few samples of each station (Vaughn et al., 2017; Roscioli et al., 2015; Mitchell et al., 2015), typically occurring on one or two days. Therefore, the accuracy of any measurement campaign is more correctly reflected by the accuracy of individual measurements, which is far lower than large ensembles of measurements. For individual stations 30% of measurements are outside the confidence interval of the annual estimate, with more estimates (24%) underestimating emissions than overestimating (5.3%). For the station group, 28% of measurements are outside the annual confidence interval (21% under the lower CI and 7% over the upper CI). Therefore, due only to natural variability in emissions from these midstream sites, a measurement campaign has a one in three chance of estimating emissions outside the 95% confidence interval of annual emissions.

Given that the simulated measurements do not reflect all of the challenges of actual field measurements, these simulations illustrate that the uncertainty in tracer measurements – arguably one of the most accurate of field measurement techniques – is higher than commonly estimated. In particular, error estimates typically include only the measurement process, and do not account for the unknown variability in the facility’s operating state and emissions behavior.

Gas Ratio Impact: Regional measurements often utilize ethane/methane (C2/C1) ratio to attribute greenhouse gas emissions to a mixture of thermogenic and biogenic sources in a region. For production basins and urban areas, a common assumption is that thermogenic natural gas emissions will have a C2/C1 ratio that corresponds to the gas production in the basin, or delivered gas in a distribution system area. The time-resolved simulations of the MEET model allow an estimate of both long-term mean and variability in C2/C1 ratio.

All compressors on the stations simulated here are equipped with lean-burn natural gas engines as drivers. Lean-burn engines are common in gathering and transmission, accounting for 66% of all compressor drivers in a recent gathering study [14, Tables S3–19]. When operating, a fraction of the natural gas fuel is emitted, uncombusted, in the engine’s exhaust, an emission source commonly called ‘combustion slip.’ Further, C2 + hydrocarbons are preferentially oxidized in the engine (and potentially in the exhaust catalyst), leading to excess methane emissions relative to the fuel gas composition.

The C2/C1 ratio based upon daily simulations is shown in Fig. 5. Station 7, which has no operating compressors, exhibited a C2/C1 ratio matching that of the natural gas transported through the station. In contrast, Stations 3 and 6, with 5 and 24 compressors, respectively, and high compressor utilization and loads, exhibited C2/C1 ratios approximately half that of the gas passing through the station. It is common for gathering stations to operate at relatively high utilization (>80%) and high loads. When operating in this common mode, the stations may produce emissions which have one half the C2/C1 ratio of the field’s produced gas. For basin-level estimates, underestimating C2/C1 ratio for any source type is likely to lead to under-attributing emissions to that source, and/or increasing attribution to a source with higher relative ethane emissions. A recent basin-level study that modeled emissions variability indicated that gathering station emissions were similar in size to production facility emissions (Vaughn et al., 2018). In this case, underestimating C2/C1 ratio of gathering by ≈50% could underestimate that ratio by 25% for all oil and gas operations, and potentially skew source attribution away from gathering toward production or other gas infrastructure.

A similar analysis conducted on facilities with high liquid production could see an opposite effect; gas dissolved in the liquids and emitted from

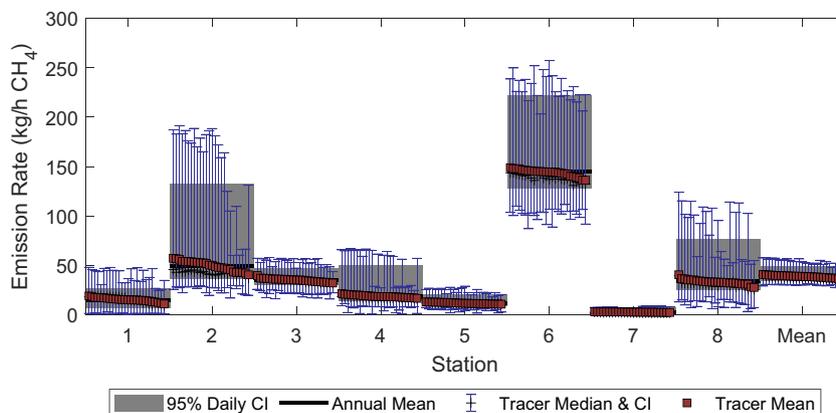


Fig. 4. Results of tracer simulation. Data are grouped by station, with tracer estimates in declining order by median estimate. Results from all stations combined are shown as a per-station estimate labeled ‘Mean’. Gray blocks represent the confidence interval (CI) for station emissions based upon 365 days of simulated emissions. Tracer estimates for each day are shown as median and mean points and bars with 95% confidence intervals. Confidence interval bars extending outside the gray region represent the probability that a field measurement campaign measuring each of these facilities on one day would estimate emissions outside the confidence interval of annual emissions for these facilities.

tank vents could be relatively richer in ethane than the produced gas composition.

Additionally, day-to-day variability in C2/C1 ratio increases with variability in compressor utilization due to higher variability in the number of compressors operating at any one time. Transmission stations generally have lower utilization than gathering stations to provide capacity for surge demands on the transmission system. Correspondingly, Station 1, a transmission station with 2 large engines, displayed the highest day-to-day variability emission. In the current simulation, compressor utilization for transmission is entirely random. A more representative simulation, however, would reflect seasonal variations in transmission demand, with corresponding seasonality in both emissions and C2/C1 ratio.

These results indicate the need for caution when applying current methods of source-attribution in basin-scale studies. Since bottom-up inventories that are commonly utilized as Bayesian priors for source-attribution do not model differences in C2/C1 ratios, or temporal variation in those ratios, attribution may be skewed between O&G sectors, or between O&G and other methane emission sources.

Continuous Monitoring: ‘Continuous monitoring’ refers to the use of permanently installed sensors, coupled with appropriate analytics, to sense emissions from a facility on a near-continuous basis. This type of sensing has drawn increasing attention due to the development of lower-cost

sensors with higher sensitivity and improved analytic methods for identifying emissions. Recently, Colorado (a centrally-located U.S. state) passed legislation that will require continuous monitoring at many oil and gas facilities. (Fenberg et al., 2019), and proposed regulatory changes by the EPA (2021) also encourage continuous monitoring.

The prior simulation examples, above, were primarily concerned with total emissions from a compressor station. In contrast, a successful continuous monitor must identify unwanted emissions in an environment where the other sources may produced planned emissions. To analyze this scenario, MEET divides emissions into the categories described in the Methods section (‘Emission labels’) and utilized by the EPA and other inventories (US EPA, n.d.; US EPA Inventory of U.S. greenhouse gas emissions and sinks, 1990).

The goal of a continuous monitor installation is to identify *fugitive* emissions in an environment where *vented* and *combusted* emissions are substantial. Therefore, in this example we simulate the mix of emissions at the compressor stations to develop an understanding of what sensitivity and analytic performance would be required for a continuous monitor to detect fugitive emissions.

The simulation assumes that knowledge of the facility’s background (*vented* and *combusted*) emissions is known exactly – i.e. combustion slip from compressors, timing, size and duration of blowdowns and gas starts,

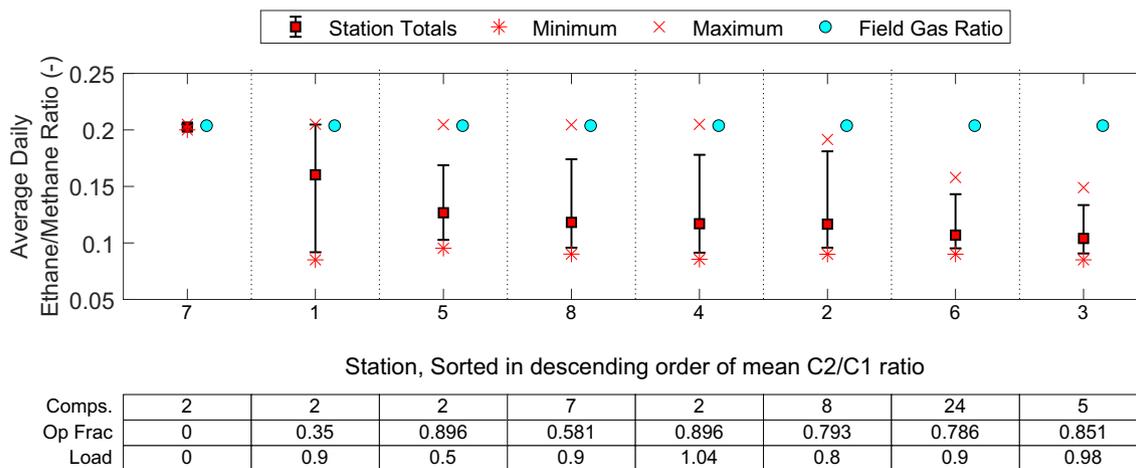


Fig. 5. The ethane-methane ratio of emissions from the simulated compressor stations. In this simulation, all stations handled natural gas with the same C2/C1 ratio (0.204); variation in the C2/C1 ratio is entirely due to changing activity (vented and combusted emissions) and leak emissions at the station.

and gas releases from pneumatic controllers is known precisely and can be ‘tagged’ as vented by the monitoring solution’s analytics. In practice, this type of knowledge is near-impossible to acquire. Therefore, the estimates here provide a rough upper bound on the performance of a continuous monitoring solution [SI Section S-9.5].

To consolidate the complex topic of monitoring performance into a single metric, simulations measure the monitoring solution’s performance using a ‘detection threshold’ defined as “ability to identify fugitive emissions that are X% higher than the *perfectly known* background emissions.” For example, a detection threshold of 20% would indicate that emissions that are $\geq 120\%$ of the known background would trigger a fugitive emissions detection at the station; if fugitives are $<120\%$ of known background, no detection would be triggered. SI Fig. S-5 provides a time series example for Station 6 – a large station with 24 compressors and high utilization – and SI Fig. S-6 for Station 7 – a small station with no compressors running. The simulation utilized methane as the sensed gas species, and both stations have fugitive emissions at all times.

For station 6, a monitor with a 20% detection threshold would detect fugitive emissions on 10% of the one-minute samples in the simulation; the low percentage is primarily due to the high background emissions, primarily from combustion exhaust. In contrast, the same solution on station 7, with no combustion exhaust and lower overall activity levels, would detect fugitives 99% of the time. Extending the analysis, Fig. 6 illustrates results for detection thresholds from 0 to 100% of total emissions.

For stations with higher compressor utilization (i.e. all stations except 1 and 7), the fraction of time a continuous monitor would detect fugitive emissions drops dramatically for detection thresholds larger than 40%, even for stations with a small number of compressors (stations 4 and 5). Given the uncertainty in operating state of equipment and timing of emission events, knowing background emission rates to within 30% is challenging; actual performance would likely require more sophisticated sensing, better analytics, or multiple gas species to achieve detection thresholds below 40%. Stations 1 and 7 have extended periods with no compressors operating. This increases the time when background emissions are lower, increasing the time (i.e. the probability) when fugitive emissions would be detected.

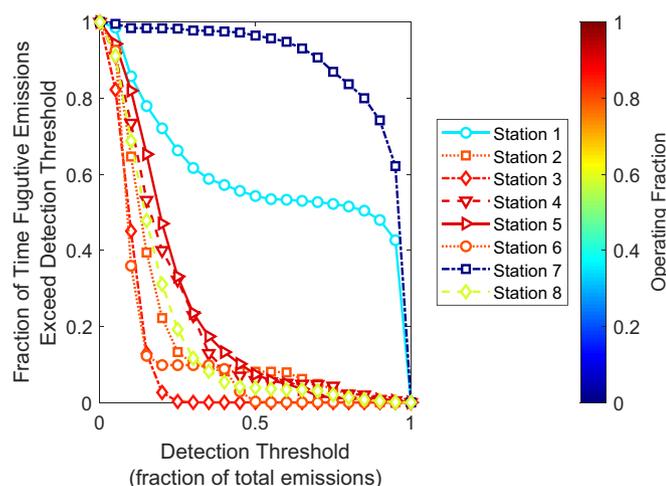


Fig. 6. Fraction of the time that a continuous monitor (CM) would detect fugitive emissions. The horizontal axis shows the detection thresholds for the CM solution, ranging from 0% (a perfect system that can distinguish *any* fugitives within any amount of non-fugitive emissions) to 100% (all emissions must be fugitive emissions for a detection to take place). A detection threshold of 50% indicates fugitive emissions equal non-fugitive emissions. The vertical axis shows that fugitive emissions were occurring. The color scale indicates the time-weighted utilization of compressors on the station, from 0 – no compressors operating – to 1 – all compressor operating.

These results provide a cautionary note regarding the deployment of continuous monitoring solutions. First, applicability of these methods is highly dependent on site type and site operations. Second, the analytics behind continuous monitors will likely need ongoing, near-real-time, information about site operations to estimate combusted and vented emissions in order to distinguish fugitive from these other sources. Finally, even for very large facilities (i.e. station 6), continuous monitoring successfully detects the largest emitters when they occur, as illustrated by the detection pattern in SI Fig. S-7. For this station, all fugitive emitters with rates above 100 kg/h would be detected by a continuous monitor with a 20% detection threshold.

4. Conclusions

The seemingly simple extension of BU inventory methods to accommodate time-varying emissions highlights underestimated uncertainty in measurement methods and emissions monitoring. Results of this study indicate systematic underestimation of uncertainty in common facility-scale measurement methods and basin-scale source attribution methods: Studies typically do not account for variability in emission rates and C2/C1 ratio at midstream facilities, and by extension, other O&G facilities. These increased uncertainties are additive to other method uncertainties which are commonly estimated, such as meteorological uncertainty, instrumentation limits, and modeling limitations. Similarly, interest in continuous monitoring at O&G facilities may obscure limitations on their performance: Most are tested in controlled conditions with little-to-no vented or combusted emissions, then deployed at facilities with high levels of vented and combusted emissions, where these methods may be unable to distinguish fugitive emissions from other planned gas releases.

Use of MEET also highlights significant shortfalls in data available from field studies ... including those performed by the authors. Significant data gaps which could be addressed in future field campaigns include: monitoring of equipment to capture time-varying behavior, such as compressor starts and stops; segmentation of emissions into fugitive and vented components; capturing LDAR survey frequency and the time since the last survey during the field campaign; capturing data to relate equipment operation to overall station throughput; and noting the volume and frequency of unit blowdowns. Each of these data items are of marginal importance to yearly inventory results, but have substantial impact on short-term simulations, as noted in the examples.

Data released in conjunction with component emissions measurements also presents challenges for time series simulation of emissions. Typically, field campaigns note the emission rates of measurements for a component type, and potentially the number of components of that type. However, it is unusual to note the number of components *screened* for leaks – as opposed to total number of components – and the number of detected emissions, including those that could not be measured. These two elements – component count screened and emission count detected – are a necessary ingredient to estimate time series behavior of many emitters [Section S-5]. As an illustration, a study finalized during development of MEET (Zimmerle et al., 2020) provides a prototype of what data should be captured and how it can be presented (see `AvgFactor.xlsx` in study data).

The MEET software will be released as an open source tool in 2021, hosted by the University of Texas (<http://dept.ceer.utexas.edu/ceer/ect/>).

CRediT authorship contribution statement

Daniel Zimmerle: Conceptualization, Methodology, Formal analysis, Writing - Original Draft, Writing - Review & Editing, Visualization, Supervision, Project administration, Funding acquisition; **Gerald Duggan:** Methodology, Software, Data Curation; **Timothy Vaughn:** Data Curation; **Clay Bell:** Methodology, Software, Data Curation, Writing – Review & Editing; **Christopher Lute:** Software, Validation; **Kristine Bennett:** Project administration; **Yosuke Kimura:** Methodology, Data curation; **Felipe J. Cardoso-Saldaña:** Data curation; **David T. Allen:** Conceptualization, Methodology, Supervision, Funding acquisition.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

Daniel Zimmerle reports financial support was provided by Collaboratory to Advance Methane Science. David T Allen reports a relationship with Exxon Mobil Upstream Research Company that includes: funding grants. David T Allen reports a relationship with National Institute for Clean and low Carbon Energy (NICE) that includes: funding grants. Daniel Zimmerle reports a relationship with Chevron Inc. that includes: funding grants. Daniel Zimmerle reports a relationship with BP Plc that includes: funding grants. Daniel Zimmerle reports a relationship with The Environmental Partnership (API) that includes: funding grants. Daniel Zimmerle reports a relationship with Renewable Natural Gas Coalition that includes: funding grants. Daniel Zimmerle reports a relationship with Environmental Defense Fund that includes: funding grants. David T Allen reports a relationship with Eastern Research Group that includes: funding grants. Felipe Cardoza-Saldana reports a relationship with Exxon Mobil Upstream Research Company that includes: employment. Daniel Zimmerle reports a relationship with Colorado Air Quality Enterprise Board, as Colorado State Agency that includes: board membership. Over the past five years, multiple authors have also worked on methane emission measurement projects that have been supported by multiple natural gas producers, developers of leak detection solutions, and the Environmental Defense Fund. Multiple co-authors have been active the funded research projects declared by the Corresponding Author (Zimmerle) and co-Author (Allen).

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.scitotenv.2022.153653>.

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