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Reconciling Top-Down and Bottom-Up Methane Emissions Estimates in the Delaware Basin

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Abstract: Methane is a greenhouse gas and identified as a key driver of near-term climate change. Bottom-up approaches estimate annual methane loss from US natural gas production and transport at 6 Tg, but recent studies suggest this may be an underestimate. To investigate this possibility, an equipment-based emissions inventory, using EPA emission factors, was developed to calculate methane emissions from oil and gas operations in the Delaware Basin, USA. Emission factors and activity data were then updated using contemporary and region-specific measurement data. The original inventory estimated emissions at 315 Gg CH_4 y^{-1} (gas production-normalized rate of 0.6% loss), while the updated inventory estimated emissions of 1,500 Gg CH_4 y^{-1} (2.8% loss).   The largest changes resulted from large fugitive emissions from oil production (+430 Gg CH_4 y^{-1}), updating maintenance activity emissions (+214 Gg CH_4 y^{-1}), considering flaring inefficiency (+174 Gg CH_4 y^{-1}), and the inclusion of associated gas venting (+136 Gg CH_4 y^{-1}). This study suggests that a systematic underestimate probably exists in current bottom-up inventories and identifies sources currently missing or may be incorrect.   We also strongly recommend that emission factors should be validated through direct comparison against measurement campaigns that include long-tail distributions typical of oil and gas activities.

Keywords: Methane; Inventory; Bottom-up; Reconciliation; Oil and Gas

1. Introduction

Methane (CH_4) is a greenhouse gas with a 100-year warming potential 25 times higher than carbon dioxide [1,2] and is the largest constituent part of natural gas.   Currently, bottom-up methods estimate that 6 Tg of methane is lost from producing, processing, transmitting, storing, and distributing natural gas in the US each year [3]. Recent studies have shown differences between top-down and bottom-up methane emission estimates [4–8], and studies suggest bottom up approaches may miss some sources [6] or that emission factors derived decades ago may now be unrepresentative of current emissions processes [7,9,10].

As part of the Paris Agreement [11], countries including the US report greenhouse gas emissions to the Intergovernmental Panel on Climate Change (IPCC) and the United Nations. Typically, greenhouse gas emissions including methane are derived using bottom-up methods which multiply process-specific emission factors by process activity levels [12–14]. Total methane emissions across all sectors of the economy in the US are typically calculated using US Environmental Protection Agency (EPA) approved emission factors [13] and are used to generate the annual Inventory of U.S. Greenhouse Gas Emissions and Sinks (GHGI).   Complementary to the GHGI is the Greenhouse Gas Reporting Program (GHGRP) which collects emissions data from the facilities emitting more than 25,000 metric tons carbon dioxide equivalent (CO_2e) annually [15]. The GHGI provides high level (national and state emissions) data over the past 25 years while the GHGRP compares individual facility emissions across sectors since 2010.

Oil and gas emission factors used in the GHGI were generated from studies funded by the EPA [16–18], some of which were conducted decades ago and are still in use today [7,19,20]. Recent studies suggest that these currently used emission factors may not accurately represent contemporary

emissions or management/engineering practices, particularly in the oil and gas industry [7–9,21–24]. The EPA has updated some emission factors using field studies, such as those reported by [25] for gathering compressor stations.   Therefore, it is suggested that emissions calculated from bottom-up inventories may significantly underestimate total area emissions [7,20,26].   Using IPCC emission factors, a recent study reported bottom-up CH_4 emission estimates of 1.2 Tg CH_4 y^{-1} from the Permian Basin in Texas [20] while a top-down study estimated emissions from the same region at 3.7 Tg CH_4 y^{-1} [27]. Overall, greenhouse gas emission estimates that are essential for climate modelling have the highest integrity when verified by direct, top-down atmospheric flux measurements [9,28–31].

Technological advances in instrumentation have been key to raising concerns over the veracity of bottom-up models' emission estimates.   Methane specific analysers, capable of measuring mixing ratios to ppb-level, are now routinely deployed as part of mobile surveys to detect and quantify point source emissions [8,32,33].   These analysers are fixed at one spot and used to observe mixing ratios in the boundary layer to infer landscape emission [26,34–36], or can be mounted on a satellite and used to observe area emissions by measuring the mixing ratios in a column of air in the atmosphere [20,37].

One continuous top-down regional quantification method is the tall tower approach, where towers are used to quantify methane concentrations in well mixed air in the boundary between 10 am and 5 pm local time [26,34,38,39]. Concentration data, an atmospheric transport model, and a prior emission estimate are combined through an atmospheric inversion to estimate methane emissions.   For example, the approach described in Barkley et al. (2023) uses four tower sites in the Delaware basin, Texas, to continuously quantify methane emissions from oil and gas operations in the region between March 2020 and April 2022 at between 146 and 210 Mg CH_4 h^{-1}, corresponding to a gas-normalized rate of 2.5% to 3.5% [26].

Satellite based continuous top-down monitoring includes using the TROPOspheric Monitoring Instrument (TROPOMI) launched in 2017 that produces daily global coverage at 5.5 × 7 km^2 pixel resolution of methane concentrations at regional scales, based on measurements made at ~13.30 local overpass time [40–43]. Varon et al., (2023) reported weekly methane emissions, between May 2018 to October 2020, at 25 × 25 km^2 resolution from the Permian Basin calculated using inverse analysis of satellite observations from TROPOMI [27]. The Permian basin comprises the Delaware basin and Midland basin, which were not disaggregated by this study [27]. Mean methane emissions, almost solely attributed to oil and gas operations in the basin, were estimated at 3.7 ± 0.9 Tg CH_4 y^{-1}, corresponding to a gas-normalized rate of 4.6 % ± 1.3 %. Varon et al., (2023) conclude that emissions inferred using methane concentration measurements made by the TROPOMI satellite are six times higher than the current GHGI bottom-up estimate.   Note here that the non-O&G emissions were calculated using emission-factor, which have also not been updated for extended periods, but are largely based on biogeochemical process that are likely more stable than oil and gas related emissions.

Given the apparent discrepancy between bottom-up and top-down approaches (a factor of between 3 and 6), this study aims to investigate any uncertainty in bottom-up emission inventories from oil and gas production. Specifically, the study investigates how changes to emission factors could improve emission estimates by considering regional variation using: 1. Tier 1 IPCC emission factors; 2. Tier 2/3 EPA emission factors for the Permian basin; and 3. a mechanistic air emissions simulator (MAES) that can temporally resolve emissions. In each case we will review current emission factors, identify discrepancies between bottom-up estimates and top-down observations, and identify the largest sources of uncertainty. The overall aim of this study is to identify which emission sources are least well parameterized and where future measurement campaigns could be used to improve emission factors and potentially reduce discrepancies between top-down and bottom-up estimates.

2. Materials and Methods

2.1 Tier 1 Emissions Inventory–Production based Inventory

Tier 1 methodologies are the simplest form of generating an emission inventory and require relatively little information about sources. For oil and gas production and midstream sectors, emissions can be calculated solely using gas and oil production rates as the activity factor. This study calculates Tier 1 methane emission estimates from oil and gas production in the Delaware basin using published oil and gas production values [44] and emission factors presented by the IPCC [12]. A range of emission factors and associated uncertainties are categorized as fugitive, vented, or flared emissions from gas production, oil production, servicing, gas transport, condensate transport, oil transport, and gas processing (Table S1) for three classifications of countries: developed, developing, and "economies in transition" [1,2,45].

Here, we calculate a Tier 1 emission estimate from the Delaware Basin as a range with a 'best-guess' estimate, which is the average of the maximum and minimum emission factors (Table S1). Activity data to calculate the emissions was the 2020 production of natural gas and oil in the Delaware basin, at 3.7×10^9 Mcf per year and 8.4×10^8 bbls per year, respectively [44]. Methane content of natural gas in the Delaware basin has been taken as 80% [26,27]; this is an external estimate which may or may not reflect changes in production practices over the last decade. For the critical review of the bottom-up estimate using production values, we will critically assess the provenance of Tier 1 emissions factors and then compare the best-guess emission estimate against values presented in a range of peer-reviewed articles for each of the categories.

2.2 Tier 2/3 Emissions Inventory–Equipment Counts based Inventory

A Tier 2/3-based bottom-up emission estimate for the Delaware basin can be calculated using emission factors and activity published by the EPA for petroleum systems [46] and natural gas systems [47]. For each source type, an emission factor is presented typically in kg CH_4 per source type. For some activities, a regional emission factor is presented, e.g., associated gas flaring, miscellaneous production flaring, associated gas venting, and for this study, we have used the values for the Permian basin (code 430) [46,47]. Similarly, partial activity data are also presented by basin and are calculated using region specific values of equipment numbers per well head. Collated emission factors and activity data are presented in Table S1 for petroleum systems and Table S2 for natural gas systems for the 45,686 oil (30,610) and gas (15,076) well heads in the Delaware basin [44], where an oil well is defined as having a gas to oil ratio of less than 4,000 cf bbl^{-1} [48]. As with the Tier 1 inventory, the Tier 2/3 emission estimate used the 2020 production of natural gas and oil in the Delaware basin at 3.7×10^9 Mcf per year and 8.4×10^8 bbls per year, respectively.

2.3 Mechanist Air Emissions Simulator (MAES)–Temporally Resolved Inventory Model

The MAES is an emissions simulation tool that has been developed at Colorado State University and has the capability to employ both traditional methods and mechanistic models for estimating emissions originating from Oil and Gas production and midstream sites. The tool utilizes the Monte Carlo method to incorporate variability in emissions and provides spatial and temporal resolution, with a 1-second interval.

Traditional methods rely on the multiplication of emission factors by activity factors to estimate emissions. In contrast, mechanistic models take into account chemical and physical processes occurring at the equipment level to simulate emissions. In this context, fluid flows, such as gas throughput, and the equipment's state play a pivotal role in influencing the emissions.

To simulate emissions for the Delaware basin utilizing MAES, this study used two facility configurations, based on analyses from previous studies, which classified facilities into simple and complex sites [49]. Sites classified as simple include only well heads, separators, and other minor miscellaneous equipment on-site. Conversely, complex sites are facilities with equipment from simple sites plus any of the following: oil tanks, water tanks, and compressors. The Delaware basin

extends over the southeast part of New Mexico and the northwestern part of Texas. Out of the approximately 20,833 well sites estimated in the New Mexico section of the basin (calculated as 25,000 well heads divided by an average of 1.2 wells per site), 66.6% were classified as simple, and the rest as 'complex. This classification was done through human assessment using satellite imagery. In another study that aimed to quantify methane emissions with TROPOMI data [20], this prior assumption (67% simple and 33% complex) was employed in their analysis. This assumed that the same distribution applied uniformly across the entire Permian basin, without conducting additional analysis. Consequently, we extended this classification percentage (67% simple and 33% complex) to encompass the entire Delaware basin.

For the MAES analysis, we utilized the two sites' configurations to represent simple (Figure 1A) and complex sites (Figure 1B). These site configurations represent prototypical sites developed in partnership with operators in the DJ basin as part of the Colorado Coordinated Campaign project. These configurations serve as representative models for a group of facilities with similar configurations.   The simple site (Figure 1A) followed descriptions provided in Robertson et al. (2020), where tanks were not observed at the site and liquids were likely transported to other sites for processing.   The complex site typically corresponds with newer sites, with large tank batteries and more stages of separation.   The MAES model assumes such sites are composed of 2 continuous wells; 2x stage 1 separators operating at 118.65 psia, 1x stage 2 separator operating at 39.65 psia, and 1x VRT in the 3rd stage of separation at 16.79 psi; 1x water tank battery; 1x oil tank battery; 1x 1029 kW 4SLB driver for a reciprocating compressor operating as a gas lift; 1x 108 kW 4SRB compressor at the second stage of separation operating as a VRU; 1x 70.8 kW 4SRB compressor at the third stage of separation operating as a VRU; 2 flares: one connected to a water tank and the other to an oil tank.

(A)   (B)

Figure 1. (**A**). Simple site configuration. The MAES model assumes such sites are composed by one continuous well and a high-pressure separator operating at 204.5 psia. (**B**). Complex site configuration. The MAES model assumes such sites are composed of 2 continuous wells; 2x stage 1 separators operating at 118.65 psia, 1x stage 2 separator operating at 39.65 psia, and 1x VRT in the 3rd stage of separation at 16.79 psi; 1x water tank battery; 1x oil tank battery; 1x 1029 kW 4SLB driver for a reciprocating compressor operating as a gas lift; 1x 108 kW 4SRB compressor at the second stage of separation operating as a VRU; 1x 70.8 kW 4SRB compressor at the third stage of separation operating as a VRU; 2 flares: one connected to a water tank and the other to an oil tank.
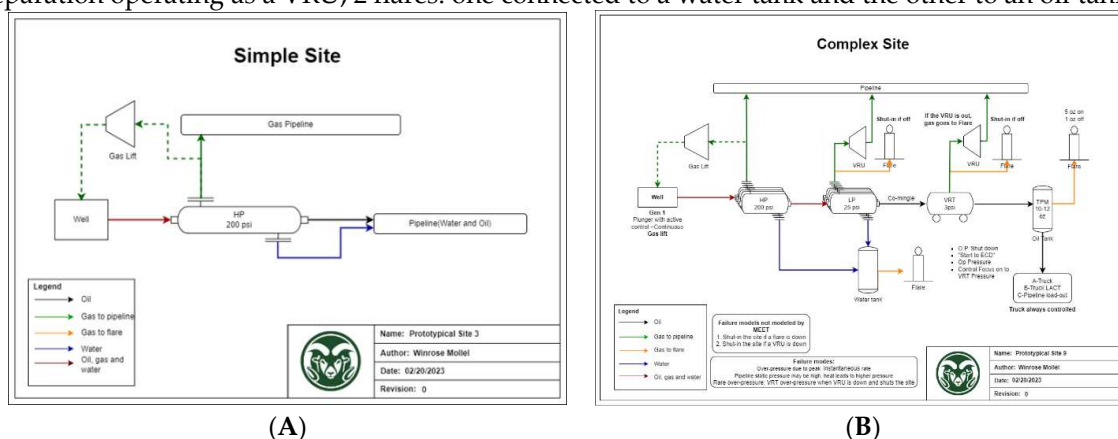
As stated previously, the Delaware basin has a total of 45,686 active wells [44], producing 3.7 x 10^9 Mscf of natural gas per year in 2020. The average of 1.2 wells per site estimated in a previous study [49] indicates 38,072 production sites. Keeping the assumption of 80% methane content for the natural gas produced in the basin, the total methane production in Delaware sums up to 5.5 x 10^{10} kg/year, which averages 1,594 metric tons of methane per site per year. Assuming the same production for both site types, we estimate a well at a simple site produces an average of 7.7 barrels (bbl) of oil per day and a well at the complex produces 6.8 bbl/day.   This assumption is a source of uncertainty as the simple sites are likely older and vertical and probably produce more oil than the newer complex sites. The model also assumes that 1 bbl/day of water is produced for each site. Out

of the total of 38,072 production sites, two-thirds of sites were categorized as simple and the remaining as complex.

Due to the lack of publicly available data regarding failure rates and operating conditions, the following assumptions were made to simulate those sites. These assumptions, along with their respective sources are outlined below:

- Stuck dump valve failure rate: provided by operators in the DJ basin.
- The probability of component leaks (pLeak) in all major equipment was set to 0.1%.
- All sites utilize gas pneumatics; emission factors were sourced from Allen et al. for the mid-continent region [50].
- Flares combustion efficiency was set to 97.5% when operating, 81.9% when malfunctioning, and 0% when unlit [51].
- All compressors were set to 100% load, and operating fraction to 95%. Their emission factors were extracted from the national study on gathering and compressor stations and scaled by their throughput [52].
- Each complex site was considered to have one water tank battery and one oil tank battery. The tank emissions were simulated mechanistically rather than using emission factors.
- The pressure release valve at the tank is designed to open when the pressure exceeds three times the expected volume of gas resulting from flashing. Additionally, the maximum gas flow rate at the flare has been established at three times the expected flashed gas volume from the oil tank, supplemented by half of the gas flashed at stage three of separation. When the flare reaches its maximum flow, the gas flow rate at the tank is also set to three times the expected flash from the oil tank, along with the gas flashed at stage three of separation.

3. Results

3.1 Production based Inventory

3.1.1. Current basin Emission Estimate

Using Tier 1 emission factors and associated uncertainties [12], the total methane loss calculated by the production-based bottom-up approach was estimated to be 607 Gg CH_4 y^{-1} with an upper and lower range of 66 and 1966 CH_4 y^{-1}, respectively (Table S1). This corresponds to a loss of 1.1% (range: 0.15% to 4.33%) of production. The Tier 1 emission factors for production originate from reports and studies made around 20 years ago [13,53–56]; there can be orders of magnitude between the maximum and minimum emission factors. The following sections will present the emission calculated from each source and the veracity of the emission estimate made in each.

3.1.2. Venting and Fugitives during Natural Gas and Oil Production

The emission factors presented for fugitive and venting at natural gas oil production sites was based on measurements made at 334 facilities across the US [16,45,55,56]. Emissions were quantified either using the EPA Method-21 [57], where a measured concentration is converted to an emission rate using a correlation equation, a GRI Hi-Flow sampler or using tracer flux, where SF_6 is released at the site and the CH_4 emission rate inferred from the ratio of downwind measured CH_4 and SF_6 concentrations.   Largest emissions were observed from gas-pneumatics, Kimray™ valves, flashing from crude tanks and compressors (Table 1) [16,17,55]. To understand if the emission factors used to generate the Tier 1 emission factor were still representative, we compared individual equipment emissions to contemporary field-based measurements [20,49].

Table 1. IPCC emission factors (EFs) based on those reported by the US EPA [13] for typical equipment on well pads [55]. Simple sites comprise wellheads only, complex sites have separators, heaters and smalll compressors [20].

Source	Fugitive EF (g CH_4 equip^{-1} h^{-1})	Vented EF* (g CH_4 equip^{-1} h^{-1})	Simple site (g CH_4 equip^{-1} h^{-1})	Complex site (g CH_4 equip^{-1} h^{-1})
Well heads	29		29	29
Separators	70			70
Kimray Valve		165		165
Heaters	73			73
Small Comp	339			339
Tanks		1,758		1,758
Dehydrator	114	102		216

Facility emission		g CH_4 site^{-1} h^{-1}	g CH_4 site^{-1} h^{-1}
Historic		29	2,706
Contemporary		40	5,200

*Estimated vented emissions for the Delaware Basin using published EFs [55], 2020 production rates [44] and site numbers [20]. Historic facility emission factors are based on measurement data from API (2004), while contemporary facility emission factors are based on measurements reported in Zhang et al. (2020) and Robertson et al. (2020).

Measured methane emissions from 55 out of 48,600 complex and 38 out of 97,000 simple sites in the Permian Basin were 40 and 5,200 g CH_4 h^{-1} , respectively [20,49]. A simple site comprises a wellhead or pumpjack only while a complex site has other equipment: separators, heaters, tanks, dehydrators and small compressors.   Using emission data used to generate the IPCC EFs [16,17,55], emissions from simple and complex sites are estimated at 29 and 2,706 CH_4 site^{-1} h^{-1}, respectively. Assuming the Permian basin is a reasonable proxy for the Delaware basin, the more recently measured emissions were from vented and fugitive emissions only (Table 1) and scaling up for the basin, the 'best-guess' IPCC Tier1 emission factor for natural oil and gas production underestimates emissions from venting and fugitives by factors of 1.2 and 1.4, respectively.

3.1.3. Flaring

Reported amount of natural gas flared during production

The best estimate for flaring during gas and oil production is 0.08 and 3.36 Gg CH_4 y^{-1}, respectively (Table S1). Using a flare destruction efficiency of 0.98 [12,13,55], the best estimate can be used to calculate that 172 Gg CH_4 is sent to the flare each year, corresponding to 0.3% of total produced natural gas flared.   In 2019, 2% of the Texas total produced natural gas was reported to be either flared or vented [58]. If we assume venting is underestimated by a factor of 1.2 (Section 3.1.2), it follows that the amount of natural gas sent to flaring (both oil and gas) is underestimated by a factor of 4.2.   Additionally, the gas emitted from non-functioning/partially-function flares in the Permian basin has been measured and, combining the statistics of lit and unlit flares, result in a region-specific flaring destruction efficiency of 86.8% [51], approximately 11 percentage points lower than that assumed in current EPA reporting methods (GHGRP).

3.1.4. Transport

Gas Transmission

The Tier 1 annual emissions estimates for gas transmission for fugitives and venting, are estimated at 13 and 19 Gg CH_4 y^{-1}, respectively (Table S1). An aircraft based study reported total emissions of 0.12 Gg CH_4 h^{-1} from 517 gathering line leaks over 876,500 km of gathering lines in the

Permian basin [59].   If we assume constant emissions throughout the year of 6.5 Mg of CH_4 year^{-1} km^{-1}, the loss from the 11,520 km of gathering line in the Delaware basin [60] is estimated at 75 Gg CH_4 y^{-1} (Table 1).

Oil and condensate transport

Methane emission from oil and condensate occur as the liquid is brought to atmospheric pressure [55] and these emissions are typically characterized in either the vented or fugitive emissions.   We were unable to identify the root of the emission factor used by the IPCC in the sources identified but assume this is a combination of venting of flash gas produced as the oil stabilizes in tanks, 'working flash', and gas emitted from truck unloading of the tank when liquid product is transported from the production site.   At present, data on oil and condensate removal are unavailable, and in the absence of a better estimate we will continue to use the IPCC emission factor.

3.1.5. Maintenance

Tier 1 well servicing emissions are currently estimated at 15 Gg CH_4 y^{-1}. A recent study reported emissions from 432 well pads in the Denver-Julesburg Basin between 2020 and 2022 finding that on average, emissions from a well pads measured between 11 am to 4 pm were 17% higher than emissions measured between 4 pm and 11 am. We assume these emissions are the result of maintenance activities [8]. As well pad emissions have been reassessed to 781 Gg CH_4 y^{-1} (sections 2.1 and 2.2), we now estimate maintenance emissions at 133 Gg CH_4 y^{-1}.

3.1.6. Large Fugitives

The major shortcoming in the methods used to determine the EFs from fugitives is that they all use relatively time-consuming survey methods (high-flow sampling, tracer gas method and direct flow method) which only observe emissions from a small sample size of the emission population and are likely to miss the very large emitters [13,53–55,59,61,62]. Therefore, we assume large emitters are current unaccounted for in the IPCC emission inventory.

Recent studies using aircraft and satellites have identified very large emissions from oil and gas production, transmission and processing activities. Emissions observed and quantified by these methods have been estimated to account for 85% of the regional emissions [37,61,63,64]. At the altitudes flown by these platforms, it is impossible to distinguish between fugitive emissions and other sources already accounted for above (maintenance, flares and pipelines).

To disentangle emissions, we present data from the recent Colorado State University's C3 campaign, where data from Aviris NG and context cameras flown at 17,000 feet were used to quantify emissions from the Denver-Julesburg basin in the summer and fall of 2020. The aircraft survey detected 188 large recurring methane plumes, 65 of which did not originate from an oil and gas facility, 29 were from midstream facilities, 30 were matched to a production maintenance event and 11 may have been matched with a maintenance event. Removing of these plumes to generate an estimate for uncontrolled/undocumented emissions at production sites in the DJ basin, the remaining 24 plumes emit 5.0 Mg CH_4 h^{-1}. Assuming a gas production rate of 2,500 MMscfd (1,706 Mg CH_4 h^{-1}) in the survey area [65], large uncontrolled/undocumented emissions at production sites is estimated at 0.3% of natural gas production.   If we assume similar emission behaviour in the Delaware Basin, we estimate large fugitive emissions from the gas production in the Delaware Basin at 165 Gg CH_4 y^{-1}.

3.1.6 Measurement Informed 2020 Tier 1 BU Emission Estimate

Updating the EPA emission factors using measurement data, we estimate the 2020 emissions from the Delaware Basin at 1.2 Tg CH_4 y^{-1}, which corresponds to a loss of 2.2% of CH_4 produced in the basin (Table 1). The largest increases in emissions are the result of considering large emitters, i.e., the long tail of the emission distribution not currently considered. The next largest increases were emissions from flares and the gathering systems.

Table 2. Current and updated bottom-up (BU) Tier 1 (T1), Tier 2 (T2) and MAES emission estimates and percentage of natural gas (NG) produced using alternate EFs described in Sections 2 and 3. Category Source: Fl – Flaring, Fu – Fugitive and V – Venting.

Category	Current T1 (Gg CH$_4$ y^{-1})	Updated T1 (Gg CH$_4$ y^{-1})	Change (%)	Current T2 (Gg CH$_4$ y^{-1})	Updated T2 (Gg CH$_4$ y^{-1})	Change (%)	MAES (Gg CH$_4$ y^{-1})
Gas production (Fu)	140	196	+40	146	241	+65	
Gas Production (Fl)	0.1	3	+2900	1	10	+900	
Oil Production (Fu)	242	337	+39	54	484	+765	
Oil Production (V)	97	118	+21	0	136		
Oil Production (Fl)	3	92	+300	29	203	+600	
Large Fugitives (Fu)	-	165		**-**	**-**		
Production	*482*	*911*	*+89*	*230*	*1074*	*+367*	*880*
Servicing (Fl/V)	15	133	+786	1	215	+21400	
Gas Trans (Fu &V)	32	75	+134	57	128	+125	
Liquid Transport (Fu)	16	16	0	0	27		
Gas Processing (Fu)	62	86	+39	22	82	+272	
Gas Processing (Fl)	0	8		1	4	+300	
Oil Processing	0	0		4	17	+325	
Total (Gg CH$_4$ y^{-1})	**607**	**1,227**	**+102**	**315**	**1,546**	**+391**	
Normalized loss (%)	*1.1*	*2.2*	*+100*	*0.6*	*2.8*	*+367*	

3.2. Equipment based Emissions Inventory

3.2.1. Current basin Emission Estimate

Current CH$_4$ emissions from oil and gas operations in the Delaware basin generated using EPA Tier 2/3 emission factors and activity data [46,47] are estimated at 315 Gg CH$_4$ y^{-1} (Table 2). The largest emissions are calculated from fugitives from the 8,200 gas wells (146 Gg CH$_4$ y^{-1}) while emissions from the 37,486 oil wells are much smaller (83 Gg CH$_4$ y^{-1}). Maintenance is estimated at 1 Gg CH$_4$ y^{-1}, transmission at 57 Gg CH$_4$ y^{-1} and processing at 27 Gg CH$_4$ y^{-1}. The current bottom-up emission estimate from the Delaware basin reported to the GHGI using EPA Tier2/3 emission factors is estimated at a gas normalized rate of 0.6%.

3.2.3. Flaring

As with the Tier 1 emission estimates from flaring, we assume that the current emissions are based on a flare destruction efficiency of 98%. Again, we adjust the emissions for a Permian basin based destruction efficiency of 86.8% [51] across all flaring activities. For oil production, this affects associated gas flaring, flaring from large and small tanks, and miscellaneous production flaring. For gas production sites, flare destruction efficiency affected tanks with flares. There were also some small changes to emissions from flaring in the gathering/boosting and processing activities. Considering a less efficient flare makes the most impact for emissions from associated gas flaring and 'Miscellaneous Production Flaring' activities, with an estimated additional 140 Gg CH$_4$ yr^{-1} emitted from associated gas flaring alone. By considering flares less efficient than EPA suggests that the EPA currently underestimates CH$_4$ emissions from flaring activities by 186 Gg CH$_4$ y^{-1} (Table 2).

3.2.3. Venting and Fugitives During Production

Current emission factors

Emission factors for high, intermittent and low bleed pneumatic devices, as presented in the GHGI additional information [46], were based on measurements made in 1995 [17,18,55]. Emissions factors for produced water are not based on measurement and result from process simulation modelling conducted by the Energy Environmental Research Center, 1995 [55]. For uncontrolled tanks, the EPA Tier 2/3 emission factor is presented as 74 kg CH_4 bbl^{-1} of crude oil [46], but there are no references given for the origin of this emission factor (Supplementary Materials Section S2). For controlled tanks, the reduction in emission is only based on the operator's estimate of VRU recovery and amount of gas sent to flare.

Most of the other emission factors used for petroleum system production were taken from the API workbook [66], GRI/EPA report [56], a consensus of an industry review panel, or was assumed to be zero due to lack of data [46,47] (Table S4). In summary, the most reliable emission factors were based on measurements of equipment and industrial practices 27 years ago, while the least reliable are assumed to be zero as they had not been measured.

Suggested changes to emission factors

To investigate if current (27-year-old) emission factors for petroleum systems (oil wells) are representative of emissions from equipment in present day, we compared the emission factors used to calculate operator's GHGRP reports against measurements data. The key shortcoming of the 1996 datasets is the relatively small sample size and the unlikelihood of those sampling campaigns to encounter very large emitters. To account for very large emitters, we take data from a recent study that used a Monte Carlo simulation approach to aggregate production equipment's missions in the Barnett Shale production region in Texas [67]. We assume given the proximity of the Barnett shale to the Delaware basin that there are common practices that could give an indication of how reliable the current EPA emission factor data are.

The equipment with the largest change in emission factor are the pneumatic devices (increase ~ factor four) and the oil well heads (increase in ~ factor of 10) (Table 3). Emission factors presented in Zavala-Araiza et al., (2017) for chemical injection pumps and compressors are very similar to those published in 1995. It is more difficult to tell how emission factors compare for produced liquids as data published by Zavala-Araiza et al., 2017 presents the units as kg CH_4 $MMbbl^{-1}$ of oil and produced water.

Table 3. Current emission factors used to derive EPA GHGI reports and data from recent measurement studies accounting for large emitters [67].

Source	2021 EPA EF	Units	Suggested EF	Units
Large Tanks w/VRU	2	kg/MMbbl	28	kg/site
Large Tanks w/o Control	38	kg/MMbbl	639	kg/site
Small Tanks w/o Flares	99	kg/MMbbl	1,679	kg/site
Pneumatic Devices, High Bleed	4,066	kg/device	12,128	kg/device
Pneumatic Devices, Low Bleed	161	kg/device	481	kg/device
Pneumatic Devices, Int Bleed	1,556	kg/device	4,643	kg/device
Chemical Injection Pumps	1,518	kg/pump	1,577	kg/pump
Oil Wellheads	117	kg/well	1,314	kg/well
Compressors	703	kg/compressor	876	kg/compressor
Produced Water	14,198	kg/MMbbl	736	kg/Site

Current activity data

For the Delaware basin, activity data for petroleum systems (oil wells) are calculated as basin-specific values calculated from year-specific GHGRP subpart W data reported by operators [46,47].

<u>Suggested changes to activity data</u>

Largest differences between the 2021 activity data derived using EPA methodology [46,47] were the number of pneumatic devices in the basin. The current EPA approach suggests that there are only one pneumatic device per well head while a measurement study suggests 2.7 devices per wellhead [50]. Well pad equipment count estimates were based on Delaware basin-based field campaign equipment counts [20,49].

Table 4. 2021 activity data, as calculated by EPA methodology, and suggested activity data derived from recent publications.

Source	2021 Activity Data	Unit	Suggested activity data	Units
Large Tanks w/VRU	213	MMbbls	21,932	Sites
Large Tanks w/o Control	145	MMbbls	14,915	Sites
Small Tanks w/o Flares	6	MMbbls	639	Sites
High Bleed	257	Pneumatics	849	Pneumatics
Low Bleed	14,706	Pneumatics	48,625	Pneumatics
Intermittent Bleed	15,647	Pneumatics	51,738	Pneumatics
Separators	1.05	Sep/well	1.24	Sep/well
Heater/Treaters	0.17	Heater/well	1.00	Heater/well
Headers	2.77	Header/well	0.67	Header/well
Compressors	0.10	Comp/well	0.64	Comp/well

<u>Updated emission estimate</u>

By considering the changes to the emission factors and the activity data, we suggest that the EPA's current approach underestimates emissions from fugitive and vented emissions from oil and gas production sites by a factor of four. We update the total emissions from gas (241 Gg CH_4 y^{-1}) and oil productions sites (484 Gg CH_4 y^{-1}) to 726 Gg CH_4 y^{-1} with the largest emissions resulting from accounting for a larger number of pneumatic devices that emit more than previously estimated.

3.2.4. Flaring/Venting of Associated Gas

Following the Tier 1 approach, we estimate the destruction efficiency of flares in the Delaware basin at 86.4% [51]. The amount of associated gas that is vented in the Delaware basin is one of the largest uncertainties in the inventory.   The EIA suggest that 2% of produced gas is either vented or sent to flare [58], while a recent study based on satellite observations suggest the up to 3.7% of gas is vented/flared [27]. Taking an integer middle-estimate of 3% of gas is either vented or flared, suggests that emissions from venting in the Delaware basin are 136 Gg Ch_4 y^{-1}, but this value is highly uncertain (+400%, -100%)

3.2.5. Maintenance

As with the Tier 1 approach and in the absence of direct studies on maintenance events, the contribution from maintenance was taken as 17% of the total emissions from a well pads, which results in emissions of 121 Gg Ch_4 y^{-1} (Table 1)

3.2.6. Transport

Currently, it is estimated that 4 Gg CH_4 y^{-1} is lost from the natural gas gathering system. As described in Section 3.1.4, an estimated 6.5 Mg of CH_4 $year^{-1}$ km^{-1} is lost from the 11,520 km of gathering line in the Delaware basin resulting in emissions of 75 Gg CH_4 y^{-1} (Table 1). Adding this

difference to the emissions to the compressor, tank and engine emissions in the EPA estimate results in emissions of 128 Gg CH_4 y^{-1} (Table 1).

3.2.7. Measurement Informed Tier 2/3 BU Emission Estimate of Oil and Gas Activities

Updating Tier 2/3 emission factors and activity data published by the EPA, we estimate the 2020 emissions from the Delaware Basin at 1.5 Tg CH_4 y^{-1}, which corresponds to a loss of 2.8% of CH_4 produced in the basin.   The largest increases in emissions are the result of change in size of fugitives from oil production (+431 Gg CH_4 y^{-1}), maintenance (+214 Gg CH_4 y^{-1}), flared oil production (+174 Gg CH_4 y^{-1}), and vented gas from oil production (+136 Gg CH_4 y^{-1}). The change to emissions from fugitive gas from oil production results from changes to both the emission factor and the activity data, especially from gas pneumatics (+250 Gg CH_4 y^{-1}), chemical injection pumps (+49 Gg CH_4 y^{-1}), compressors (+34 Gg CH_4 y^{-1}), and controlled/uncontrolled tanks (+11 Gg CH_4 y^{-1}).   The most speculative estimates presented by this study are the emissions from maintenance events and vented gas from oil production. At present we have no understanding of how uncertain the estimate from maintenance is but suggest the uncertainty in emissions from vented gas is between +400% and -100%.

3.3 MAES Inventory Model

MAES was run for 365 days with 300 Monte Carlo iterations for 25,381 simple sites and 12,691 complex sites. After accounting for 17% of emissions attributed to maintenance activities, the mean CH_4 loss for the simple and complex sites was estimated at 0.19% [0.15%, 0.24%] and 4.40% [4.21%, 4.59%], respectively, at a 95% confidence interval. The higher normalized loss in complex sites is mainly due to vented and combusted emissions from additional equipment on site such as compressors, tanks, and flares. For the Delaware basin, production sites are estimated to emit 0.88 Tg CH_4 y^{-1} [0.83, 0.93].

While these estimates are based on the assumptions specified in Section 2.3, improving the accuracy of the estimate is contingent on collecting additional information from operators or public databases including: facility production rates, on-site equipment, maintenance activities, and the classification of facilities into prototypical sites. In addition to site-specific data, regional characteristics, including failure rates, duration, and size of large emissions, exert a significant influence on the basin-scale emission estimate. In 2022, an aerial survey measured methane emissions from 7,474 production sites in the Permian basin [68]. However, this dataset could not be used as input to MAES as facility configuration and production rate information were not collected, and often times measured emissions are significantly higher than the average production set for a facility. This limitation underscores the need for more comprehensive information and collaboration with operators to achieve more robust results in a basin model.

3.4 Non-Oil and Gas Activities

Methane emissions from non-O&G anthropogenic sources within the Delaware basin are taken from the EPA's 2012 Gridded Methane Emissions Inventory and estimated at 31 Gg CH_4 y^{-1} with the majority of emissions (81%) from agricultural sources in New Mexico to the north and west of the basin and the remainder from the waste sector [19,20,26].

4. Discussion

This study presents the results of three approaches that can be used to generate a bottom-up emission inventory for oil and gas operations in the Delaware basin. The first method, a Tier 1 approach, used "developed world" emission factors that are based on oil and gas production rates to generate methane emissions. Using 2020 oil and gas production values [44] and IPCC emission factors [12], the total methane loss calculated by the production-based bottom-up approach was estimated to be 607 Gg CH_4 y^{-1} with an upper and lower range of 66 and 1,966 CH_4 y^{-1}, respectively. When the emission factors were changed to accommodate region-specific measurement studies

[20,26,37,49,61,63,64] we estimate emissions at 1.2 Tg CH_4 y^{-1}, corresponding to a loss of 2.2% of CH_4 produced, and largest increases in emissions are a result of large emitters, emissions from flares, and emissions from gas transmission.

The second methods used individual emission factors and activity data for major pieces of production, gathering, boosting and processing equipment to make region specific (Permian basin), Tier 2/3, emission estimates. Both emission factors and activity data were taken from the EPA appendices for petroleum systems [46] and natural gas systems [47]. Using these data, the 2020 methane emission from oil and gas activities in the Delaware basin are estimated at 315 Gg CH_4 y^{-1}, or 0.6% of production. Incorporating measurement studies to make the emission factors both contemporary and regionally specific [27,49–51,59,67] results in an emission estimate of 1.5 Tg CH_4 y^{-1}, 2.8% of production, with the largest increases resulting from a change in size of fugitives from oil production (+430 Gg CH_4 y^{-1}), maintenance (+214 Gg CH_4 y^{-1}), flared oil production (+174 Gg CH_4 y^{-1}), and vented gas from oil production (+136 Gg CH_4 y^{-1}).

Even though some contemporary studies were used to update both Tier 1 and Tier 2/3 approaches [49,51,59], the methods for calculating the production based and equipment based inventory estimates are quite different but arrive at similar estimates. The Tier 1 emission estimate was most affected by the inclusion of large emitters based on observations of Zimmerle et al. (in review). Similarly, the Tier 2/3 estimate was most affected by accounting for super emitting production sites observed by Zavala-Araiza et al., (2017). The IPCC Tier 1 and EPA Tier 2/3 bottom-up inventories did not account for these emissions as both derived emission factors using data derived from measurement data published in 1996 which did not observe any super emitters on their relatively small (334 facilities across the US) measurement campaigns [17,18]. Realistic emission factors can only be derived by observing and accounting for the long tail distribution through simulation [67] or by observing thousands of sites at a time using aircraft or satellite-based platforms [37,61,63,64].

One important point of note is the uncertainty that comes with using a Tier 1-based approach. Using IPCC recommended data, the initial emission estimate bounds were 66 Gg CH_4 h^{-1} to 1,966 Gg CH_4 h^{-1} with a 'best-guess' estimate of 607 (- 89%, +223%) Gg CH_4 h^{-1}. Without additional measurements, this estimate range is almost meaningless and any data reported to the IPCC using Tier 1 emission factors should be treated as highly uncertain. The main shortcoming of the EPA Tier 2/3 emission factors is that it comes without an uncertainty bound, which could be mistaken for an assertion of precision and accuracy. As our findings suggest, these emission factors are potentially wrong as they do not account for the long-tail emissions common to most oil and gas emissions distributions.

While we acknowledge that approaches used in this study are subject to large and some data sources may not be exactly geo-located, the study illustrates that even a simple reassessment of bottom-up inventories using contemporary and near(er) region-specific observations will help close the gap between top-down and bottom-up inventory estimates.

The third method used – MAES – is a simulation tool that uses traditional and mechanistic models to estimate methane emissions at a facility and basin scale. The estimated CH_4 emissions for production activities in the basin according to the MAES models is 880 Gg CH_4 y^{-1}. Even though more data are required to run MAES than Tier 1 (production rates) and Tier 2/3 (equipment on sites), methane (and other species') emissions can be calculated across time frames, ranging from instantaneous emissions (easier for comparison against aerial survey measurements) to annual emissions (such as those documented in the GHGRP inventories). Additionally, this method provides a better estimate of the ethane-methane ratio of emitted gas, which varies substantially between source types, even within one site. Therefore, the cost of acquiring detailed information for MAES input is rewarded by the spatiotemporal variability of emission estimates that allows the BU emissions to be compared by measurements made by a range of TD methods.

2020 top-down estimates of oil and gas emissions in the Delaware include gas-normalized rates of 2.5% to 3.5% using tall tower measurements [26] and 4.6 % using TROPOMI satellite data [27]. These top-down estimates are much nearer the adapted Tier 1 (2.2%) and Tier 2/3 (2.8%) estimates

calculated in this study than emissions calculated using the stock emission factors provided by the IPCC and the EPA. Here we strongly suggest that bottom-up inventories are better informed by measurement activities to generate more regionally representative emission factors/activity data that more closely account for regional changes in operational activities and conforming to regional emission regulations.

5. Conclusions

To mitigate the gaps between BU and TD methods, we believe that the following topics deserve critical attention and further development:

- Dynamic EFs: current EFs are often outdated and do not account for variations in gas composition, equipment throughput, and equipment operational states. It is crucial to update and expand the EF structure to accommodate these nuances.
- Temporal Variability in Emissions: emissions vary significantly over time due to weather, seasonal patterns, timing of maintenance activities, and age of production activity. These fluctuations are often linked to human behaviour such as the willingness to perform equipment repairs in cold weather, requests from government agencies to reduce maintenance during the summer to mitigate ozone formation from co-emitted VOCs, or the introduction of additional operating equipment during winter such as heaters. However, a deeper investigation is needed to understand and quantify the underlying causes. Reconciliation exercises must take this factor into consideration.
- Data Collection Frequency: temporal mismatches in data collection can lead to discrepancies in reconciling emissions. The more frequent top-down measurements are employed, the better the BU model can be informed about failures/abnormal emissions.
- Granular Facility-level Data Collection: more data is needed regarding equipment count and ratings, performance, operating pressure and temperature, and oil and gas production for more accurate BU models.
- Data Quality/Reliability: in past projects, we have encountered challenges related to the quality and reliability of data. For instance, in aerial measurements, we observed significant fluctuations in methane rates over short time intervals (1 or 2 minutes) even when there were no substantial changes in facility operations. Such variations can often be attributed to factors like the facility's topography, which can introduce biases in wind speed assumptions used for emission rate estimation, or inherently wide uncertainties in the aerial system's estimation method. Additionally, inaccuracies can arise in bottom-up models when incorrect reporting numbers are employed, such as a common EF for 4SLB engines with and without pre-chambers, as still suggested by the EPA.
- Customized Approach for Different Facilities in Basin-wide Models: while configuring specific settings for thousands of facilities may be challenging and often cost-prohibitive, we can categorize sites into distinct classes known as Prototypical Sites (PS). Each PS should represent a group of similar facilities, with differences that do not significantly impact their emissions profiles. This classification of all facilities from a basin into PS can improve model accuracy and reduce the computational efforts required for BU simulation.
- Collaboration and Data Sharing: the previous point highlights the critical need for collaboration between measurement studies and operators. Data sharing and collaboration involving government, academia, and industry stakeholders are indispensable to improving BU and TD models and addressing the reconciliation challenge.
- Policy Updates: With advances in technology and site configuration, it is imperative to constantly update databases and guidelines through research, collaboration, and field measurements. Similarly, policies must evolve to align with recent trends and changes.

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