

Supplemental material

Emission scenarios on a potential shale gas industry in Germany and the United Kingdom

L. Cremonese¹, L. Weger^{1,2}, H. Denier Van Der Gon³, M. P. Bartels¹, T. Butler^{1,4}.

¹ Institute for Advanced Sustainability Studies (IASS), Potsdam, Germany.

² University of Potsdam, Potsdam, Germany.

³ TNO, Utrecht, the Netherlands.

⁴ Institut für Meteorologie, Freie Universität Berlin, Germany.

Corresponding author's email: L. Cremonese lorenzo.cremonese@iass-potsdam.de.

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1 Shale Gas Drilling Projections

1.1 Background information

The political discussion on a potential shale gas industry in Germany has been centered on the convenience of maintaining the domestic natural gas sector and know-how expertise in the country, as well as preserving a local production share of the domestic gas consumed. This is because natural gas production in Germany has been on the decline since the beginning of this century, decreasing from a previously stable production level of about 20 bcm (billion cubic meters) per year. For example, in 2016, roughly 7.2 bcm of natural gas was produced in Germany, which amounts to about 7% of its total consumption of natural gas (BVEG, 2018). Gas production saw an especially steep decline in the last five years mainly due to the majority of drilling projects being put on hold as a result of a revision of regulations placed on conventional fracking. In the UK, after experiencing a strong decline starting in 2000¹, offshore gas production has been stable at ~35 to 40 bcm per year, reaching 39.6 bcm in 2015, 58% of the total annual gas consumption of 68.1 bcm for that year (BP, 2017). Based on the historical data, we find it appropriate to develop projections targeting a shale gas output volume of about 10 bcm a year in Germany, and about 35 bcm in the UK.

In European countries where shale gas activity may take place in the future, it is plausible to expect engineering technologies capable to minimize the environmental footprint, similar or tighter than current ones. Therefore, these considerations are factored into our drilling and well specifications discussed here. In a 2012 report from the European Commission (Pearson et al., 2012), it was assumed that in the coming years a range between 15 and 36 wells per pad could be expected, each extending between 3,000 and 7,000 m horizontally. Based on this, we assume a value of 30 wells to be built per pad in our projections, with two groups of 15 wells running towards opposite horizontal directions and each extending for 2,500 m and in line with that reported by Acatech (2015), (Figure 2). This configuration can be achieved with a horizontal well-spacing of about 330 m, compatible with normal procedures performed in the US, as well as environmental standards (Díaz de Sousa et al., 2012; Harpel et al., 2012; Browning et al., 2013). The shale gas reservoir is reached from each well pad by three or ten vertical wells, according to the drilling settings choose in the emission scenarios. We assume that the vertical wells are drilled close to each other with a minimum distance of about 3 m, in accordance with industry practice to save space and reduce the environmental impact (DeMong and King, 2011).

1.2 Construction

The construction of the drilling projections is organized on a six-month (i.e., semester) basis. In the first semester, we assume that 100 wells in Germany and 140 in the UK start producing shale gas at a rate described by the production curve assigned to each basin. In the same semester, the same number of wells is under construction, and will constitute a new population that will enter the production phase in the following six-month period. In the second semester, two populations of producing wells determine the overall volume of gas produced, one at its first and the other at its

¹ Available at: <https://www.eia.gov/beta/international/analysis.cfm?iso=GBR>

second semester of activity. In parallel, a new set of wells is under drilling, entering the production phase in semester three. This pattern of well evolution proceeds until the targeted annual production is reached (i.e., circa 10 bcm for Germany and circa 35 bcm for the UK). At this point, we assume a new drilling rate in each country capable to maintain overall production constant (steady-state production). The average value of the drilling rates necessary to maintain production constant for the following three years is fed into the emission scenarios. For a given shale gas basin, a population of producing wells is defined as a cluster of wells at the same stage of production (i.e., same age).

The overall gas output is estimated as follows:

- To estimate the gas output for each population of producing wells in each basin, we refer to the production curves as explained in the main text;
- To reduce complexity, we assume that all the wells drilled over a semester enters production on the very first day of the following semester;
- The gas production rate changes over time, and consequently on a day-to-day basis. To reduce complexity in calculating monthly gas production, we applied gas production at day 15, which represents the median value for the month, to all the days of the month. The overall semester gas output is predicted by aggregating the gas produced over each month.

The volume of gas produced (V_p) by a given population of *producing wells* is calculated as follows:

$$V_p = \sum_{i=1}^6 P_{day15(i)} \times 30$$

where:

P_{day15} = gas production at day 15 based on the production curve;

i = month (6 for each semester);

30 = days of the month (average).

The national gas output (NG_o) for each country is estimated as follows:

$$NG_o = \sum_{b=1}^n \sum_{s=1}^m Vp_{(s)(b)}$$

where:

$Vp_{(s)}$ = volume of gas produced at semester (s);

m = age of the shale gas industry;

b = shale gas basin ($b=5$ for Germany and 1 for the UK).

1.3 Mishaps and adjustments

By developing the construction of the drilling projections on a semester-basis, it is not feasible to reach the same annual gas production in each well productivity case (see Figure S1). Due to the direct correlation between total gas produced and related emissions, a comparison of such drilling projections as originally calculated would be erroneous. To fix this incongruence, we operate in the following way. For each country, we select the productivity case that generates an annual gas

production closest to the targeted annual amount (see Section 1.1) as the reference case. All the parameters characterizing the reference case (i.e., total gas output, *wells under production* and *producing wells*, see the Methodology Section in the main text) are left unchanged. Differently, in order to obtain the same volume of gas as the reference case at the end of the supply chain for the other productivity cases, we linearly normalize their parameters based on their annual gas production offsets to the reference case. This operation is carried out for both countries. Such linear correction did not affect the qualitative significance of our emission results, and is required lest differing volumes of gas produced were largely responsible for emission discrepancies in the results (e.g., total CO₂ emissions are strongly correlated to the total methane flowing through the supply chain). Following the same approach, the gas combusted during the processing of the gas is also factored in to ensure the same CH₄ output at the end of the gas chain. Therefore, we add the amount of gas consumed at the processing stage at the beginning of the supply chain. In this way, we obtain a higher total amount of gas extracted by the producing well populations which accounts for the gas combusted during processing.

1.4 Results

In Table S1 we present the TRR_{basin} and EUR_{well} applied to the drilling scenarios. Our results are in line with EUR values of other shale gas basins in the US. For instance, the *Unterkarbon* P50 EUR_{well} of about 200 mcm (million cubic meters) is comparable to data from the Marcellus Shale play (WEO, 2015).

Table S1. TRR and EUR_{well} for all basins and productivity case considered in this study. TRR data are from BGR (2016) and BGS (2013).

	Productivity case	Unterkarbon	Mittelrhät	Posidonia Schiefer	Wealden	Fischschiefer	Bowland Basin
TRR _{basin} (bcm)	P25	220	30	270	30	0	2870
	P50	320	50	390	40	1	3760
	P75	480	70	570	60	2	5450
EUR _{well} (mcm)	P25	139	21	40	112	0	174
	P50	203	36	58	149	1	228
	P75	304	50	85	224	2	330

In Figure S1 we report results from the drilling projections for each country. The evolution of three parameters is shown: i) the drilling rates (number of wells drilled each semester, see main text, Methodology Section), ii) the total number of producing wells, and iii) the gas output for both countries under different well productivity scenarios. The total volume of gas produced is the amount as originally obtained by the drilling projections.

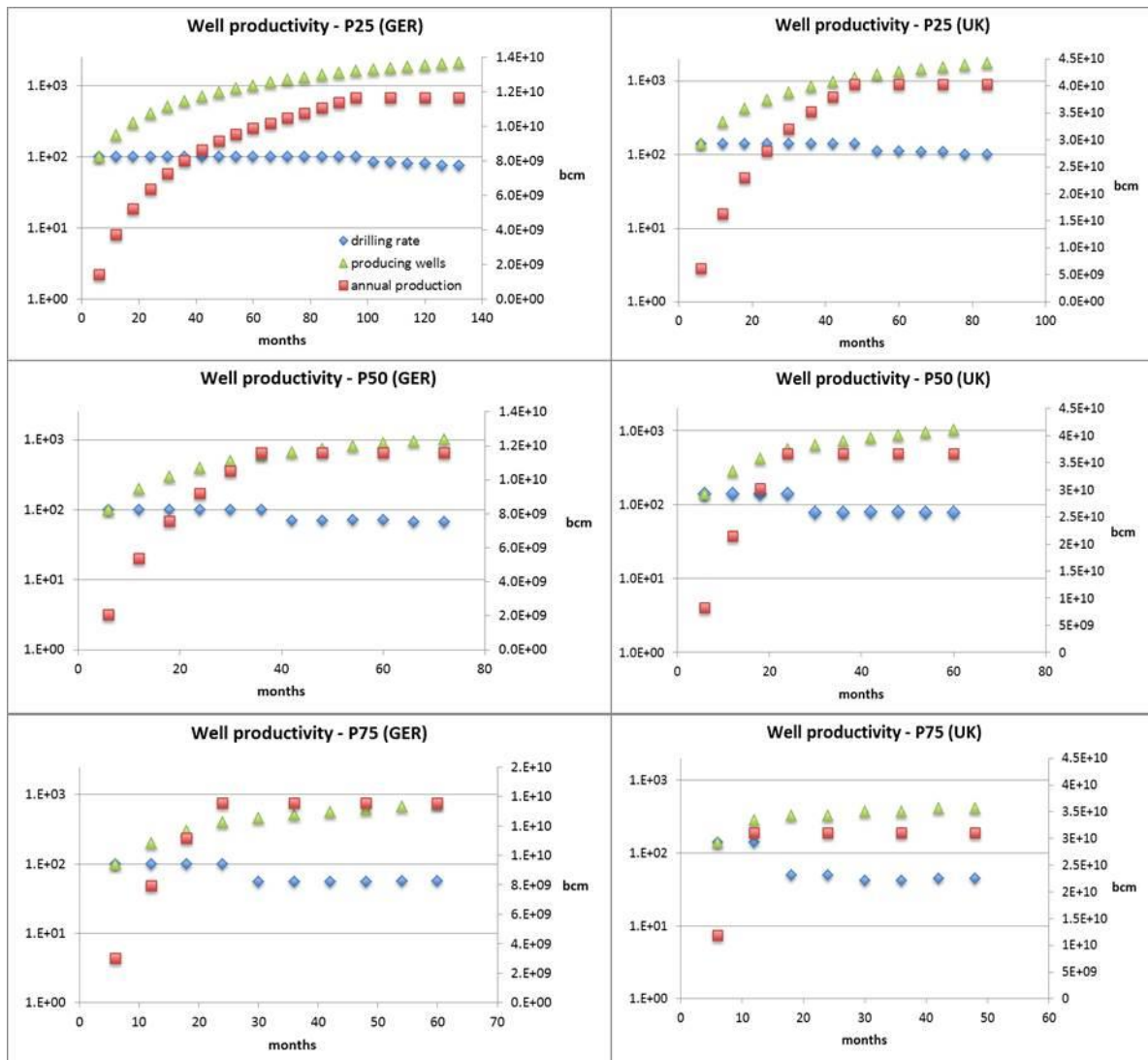


Figure S1. Drilling rate, producing wells and annual gas production for each scenario. The three productivity-cases (P25, P50 and P75) are shown for Germany (left) and the UK (right). For the drilling rate and number of producing wells refer to the left-hand y-axis on each figure.

2 Emission Scenarios

2.1 Gas composition

In the emission scenarios we consider two gas compositions defined as dry and wet compositions (low and high content of VOCs, respectively) representing the upper and lower boundaries of the shale gas compositional range. Concentrations are taken by data reported by Faramawy et al., 2016 (see Table S2). We also assume that no CO₂ is present in the raw wet gas although Faramawy et al. report a medium CO₂ concentration for the wet gas below 5%. This choice does not significantly affect our results since the volume of CO₂ emitted by all machineries and natural gas combustion along the production chain is by far higher than that lost from gas along the supply chain.

The emission scenarios exploring wet vs. dry gas production cases differ from each other only by the concentration of VOCs in the raw gas, respectively 15.4 and 4.0% v v⁻¹ (see Table S2). The drilling scenarios are built based on the CH₄ content in the gas, and not total raw gas production. This means that the well parameters defined by the drilling projections represent the amount of wells necessary to produce the desired amount of CH₄ for each country, with the volume of other compounds like VOCs or CO₂ to be added to assess the total volumes of raw gas. In other words, wells active in the wet- and dry-gas cases extract the same amount of CH₄, but produce different volumes of other pollutants according to the composition of the remaining fraction of the raw gas.

Table S2. Gas composition in the raw and dry natural gas. Data from Faramawy et al. (2016).

Pollutant	Formula	Wet raw natural gas (% Vol)	Dry raw natural gas (% Vol)
Methane	CH ₄	84.6%	96.0%
Carbon dioxide	CO ₂	0%	0%
Ethane	C ₂ H ₆	6.4%	2.0%
Propane	C ₃ H ₈	5.3%	0.6%
Butane	C ₄ H ₁₀	1.4%	0.1%
Pentane	C ₅ H ₁₂	0.2%	0.1%
Hexane	C ₆ H ₁₄	0.4%	0.1%
Heptane	C ₇ H ₁₆	0.1%	0.8%
Isobutane	C ₄ H ₁₀	1.2%	0.2%
Isopentane	C ₅ H ₁₂	0.4%	0.1%

2.2 Well pad construction

We assume a well pad area of 5 acres (about 2 hectares) to accommodate the cemented drilling pad, other equipment and trucks. We envisage the utilization of two machines for road construction and one for well pad preparation over two-week periods (NYSDEC, 2015, p. 295-296). Bulldozers,

backhoes and graders are needed to build access roads and clear the area where drilling and related activities take place. We assume a net engine power of 150 kW for bulldozers, 170 kW for excavators and 190 kW for graders. Emission factors (EFs) and other estimates are based on data from Helms et al.(2010) and NYSDEC (2015).

Road preparation: 2 bulldozers, 2 excavators, 2 graders; Load Factor (LF; this parameter indicates the time share the machinery is in operation): 50%. Well pad configuration: 2 bulldozers, 1 excavator; LF: 50%.

Total emissions for each productivity case, emission scenario and country are calculated as follows:

$$E(i) = \#_{wellpads} \times EF(i)_{machines} \times \#_{machines} \times LF \times h_{operations} \times kW_{machine}$$

Where (i) is the specific pollutant.

Table S3. Values for REm and OEm applied to well pad construction.

REm-U	REm-L	OEm-U	REm-L
Road construction: 2 bulldozers, 2 excavators, 2 graders, 2-week operation Wellsite configuration: 2 bulldozers, 1 excavator, 1-week operation LF: 0.5 EF: stage IIIB/IV ²	Road construction: 2 bulldozers, 2 excavators, 2 graders, 2-week operation Wellsite configuration: 2 bulldozers, 1 excavator, 1-week operations LF: 0.5 EF: stage IV	Road construction: 2 bulldozers, 2 excavators, 2 graders, 2-week operation Wellsite configuration: 2 bulldozers, 1 excavator, 2-week operations LF: 0.5 EF: stage IIIB/IV	Road construction: 2 bulldozers, 2 excavators, 2 graders, 2-week operation Wellsite configuration: 2 bulldozers, 1 excavator, 1 week operation LF: 0.5 EF: stage IV

2.3 Trucks and water supply

In this section we estimate the emissions generated by truck movements and electricity need to provide the well pads with materials required for i) well pad construction, ii) drilling the borehole, and iii) fracking activities. We consider the employment of trucks with a capacity of 20 m³ for liquid transport (i.e., mainly chemicals and waters) and 30 m³ for solids (i.e. drilling mud, sand, cement and proppants). A total number of 480 truck movements per well pad are assumed based on data reported from NYSDEC 2015 (p. 6-305). In our scenarios, the cement pad holding drilling operations is 30 x 30 m in REm and 10 x 30 m in OEm, half-meter thick and composed by a cement-sand-water mixture in the ratio 1:4:1.

Emissions associated with the trucks employed are based on the HBEFA report (IVT, 2015) considering an average speed of 40 km h⁻¹. The vehicle market in Europe and its emissions standard share is based on the KBA report (p. 27).³ Here the % of each emission category is calculated only considering Euro II, III, IV, V (together with EEV, see Footnote 5 at p. 42 of the same report), and VI. "Sonstige", as it is not categorized, is excluded from our analysis. The trucks we consider, when loaded, belong to the group "12001 and more kg". Here values refer to trucks half-loaded. Because

² Emission standards for Nonroad Engines in the EU. More information available at: <https://www.dieselnet.com/standards/eu/nonroad.php#s3>. Accessed 15 April 2019.

³ Report available at: http://www.kba.de/SharedDocs/Publikationen/DE/Statistik/Fahrzeuge/FZ/2016/fz13_2016_pdf.pdf?blob=publicationFile&v=2. Accessed 15 April 2019.

our trucks are completely loaded on the way to the well site but mostly unloaded on their return, emissions related to 50%-loaded trucks can be fairly adopted. We estimate each truck drives about 100 km (including both ways), and the volume of water necessary for each fracking stage is kept constant at 2,000 m³.

PM produced by tyre, brake, road wear combined and re-suspended material from truck movements are added to the emission scenarios according to EFs reported by the EMEP/EEA (2016) and Denier Van Der Gon et al. (2018). The share of km driven in highways vs. urban/rural roads is chosen at 70 and 90% in the high and low boundaries respectively. PM EFs fall to zero values during rain events and when the road surface is wet. To include this consideration into our scenarios we estimate the number of rainy days in Germany (186 d y⁻¹) and the UK (163 d y⁻¹), averaging it from major cities located in or close to the reservoir areas (Statista, data for 2008 and 2017 respectively, available online).

Most of the energy required to move a water mass is spent to lift the water, while in a horizontal tract the only resistance opposing the movement in the pipeline system is composed by frictional forces. In our case, distances and changes in altitude are unknown. Assuming that frictional forces are negligible, we estimate that (on average) our masses of water is lifted to a height of 50 m on their way to the production site. This assumption would therefore include cases where the water (e.g., from natural reservoirs like lakes, rivers, etc.) is delivered downhill without additional energy required, and cases where the energy required is higher (i.e., transporting the water uphill). Energy requirements are calculated using the following equation (CottonInfo, 2015). To calculate the electricity required to pump 1 MI (1,000 t) of water, we apply the following equation:

$$Electricity = \frac{2.275 \times TDH}{EF_{pump} \times EF_{drive} \times EF_{motor}}$$

Where:

- TDH: vertical difference between water source and delivery;
- Eff_{pump}: efficiency of the pump (between 0.5 and 0.9, we choose 0.8);
- Eff_{drive}: Efficiency of drives (between 0.95 and 1, we choose 1);
- Eff_{motor}: Motor efficiency 0.9 (average from electrical motors).

Accordingly, the power requirement for 1 MI is 190 kWh in our scenarios.

Total emissions for each productivity case, emission scenario and country are calculated as follows:

$$E(i) = (\#_{truck} \times EF(i)_{truck} \times km_{truck}) + (kWh \times EF(i)_{electr.})$$

Where:

- (i) is the specific pollutant;
- The electricity consumption is required for pipelining drilling and fracking waters.

Table S4. Values for REm and OEm applied to trucks utilization and water recycling.

REm-U	REm-L	OEm-U	OEm-L
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Stage length: 60 m Water piped: 0% Truck EFs: Mixed Euro 3/6 Well construction: 10 verticals Drilling water recycled: 50% Fracking water recycled: 50% Wear: PM _{2.5} and PM ₁₀ from upper 95% confidence interval Road type: Highway:Urban:Rural= 0.7:0.2:0.1	Stage length: 300 m Water piped: 100% Truck EFs: Mixed Euro 3/6 Well construction: 10 verticals Drilling water recycled: 50% Fracking water recycled: 50% Wear: PM _{2.5} and PM ₁₀ from lower 95% confidence interval Road type: Highway:Urban:Rural= 0.9:0.05:0.05	Stage length: 60 m Water piped: 0% Truck EFs: Euro 6 Well construction: 3 verticals Drilling water recycled: 90% Fracking water recycled: 90% Wear: PM _{2.5} and PM ₁₀ from upper 95% confidence interval Road type: Highway:Urban:Rural= 0.7:0.2:0.1	Stage length: 300 m Water piped: 100% Truck EFs: Euro 6 Well construction: 3 verticals Drilling water recycled: 90% Fracking water recycled: 90% Wear: PM _{2.5} and PM ₁₀ from lower 95% confidence interval Road type: Highway:Urban:Rural= 0.9:0.05:0.05
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2.4 Drilling

We envisage four drilling machines at each site: three in constant use and one as a back-up, so the assigned LF is 0.75 (as discussed with experts in the field) instead of 0.6 as reported by other authors (e.g., Pring et al., 2015). Four diesel electricity generators, 1000 kW each, are assumed to be installed at each well pad in REm, while in OEm electricity is always provided by the national grid power. Although the distance between remote wellsites and the electricity network might make this case rather unrealistic, a higher population density in Europe compared with the US must be accounted for (Kavalov and Pelletier, 2012). The time needed to complete the drilling operations is based on the drilling speed reported by Pring et al. (2015) and the total length of the wellbores, different in OEm and REm (3 and 10 vertical wells, respectively). Aggregation of several horizontal wells onto a single vertical well as implemented in our scenarios – enabled by recent engineering innovation - is a practice that has shown to control emissions (Robertson et al., 2017).

Total emissions for each productivity case, emission scenario and country are calculated as follows:

$$E(i) = \#_{wells\ under\ construction} \times EF(i)_{drilling} \times \#_{machines} \times LF \times h_{operations} \times kW_{machine}$$

Where (i) is the specific pollutant.

Table S5. Values for REm and OEm applied to the drilling stage.

REm-U	REm-L	OEm-U	OEm-L
Diesel-powered generators EF: Stage IV-IIIb 10 horizontal wells each vertical well wells each horizontal	Diesel-powered generators EF: Stage IV-IIIb 10 horizontal wells each vertical well wells each horizontal	Electric drilling 3 horizontal wells each vertical well wells each horizontal	Electric drilling 3 horizontal wells each vertical well wells each horizontal

2.5 Fracking

We assume a total pump power capacity required for each fracking stage between 35,000 and 45,000 hp with a LF of 0.5% (Roy et al., 2014). Electric pumps are not expected here due to the large amount of energy required that is not available from the national power grid under usual settings. Based on a fracking stage length between 60 and 300 m extrapolated from the literature and experts, we obtain a range of fracking stages for each 2,000 m-long horizontal well between 8.3 and 41.6

Total emissions for each productivity case, emission scenario and country are calculated as follows:

$$E(i) = \#_{wells\ under\ construction} \times EF(i)_{pumps} \times \#_{machines} \times LF \times h_{operations} \times kW_{machine} + \#_{stages}$$

Where (i) is the specific pollutant.

Table S6. Values for REm and OEm at the fracking stage.

REm-U	REm-L	OEm-U	OEm-L
41.6 stages wells ⁻¹ Fracking operations: 2.5 h EF: 50% stage IV – 50% stage IIIB	8.3 stages well ⁻¹ Fracking operations: 1.5 h EF: 50% stage IV – 50% stage IIIB	41.6 stages well ⁻¹ Fracking operations: 2.5 h EF: 50% stage IV	8.3 stages well ⁻¹ Fracking operations: 1.5 h EF: 50% stage IV

2.6 Well completion

To estimate CH₄ loss during the well completion stage, we refer to the findings reported by Allen et al. (2013). In their study, empirical data from a large population of wells resulted in an average emission of 1.7 Kt of CH₄ per well completion activity, significantly below the results shown by the EPA GHG Inventory 2016, Annex 3, Table A-134 (EPA, 2016), where volumes range between 3.2 and 36.8 Kt according to the technique adopted. Nevertheless, another EPA report (EPA, 2014a) states that a reduction of total emissions between 95 and 98% can be achieved through Reduced Emission Completions (REC also called “green” completion). We assume no existing limitations for REC such as absence of nearby pipelines or low pressure of the gas, also considering that this gas can be combusted in small site-turbines to produce electricity on-stage, a technology which is already deployed in Europe.

Total emissions for each productivity case, emission scenario and country are calculated as follows:

$$E = \#_{wells\ under\ construction} \times loss_{well\ site}$$

Table S7. Values for REm and OEm applied to well completion activities.

REm-U	REm-L	OEm-U	OEm-L
3.3 t CH ₄ event ⁻¹ (high-boundary 95% confidence interval)	1.0 t CH ₄ event ⁻¹	1.7 t CH ₄ event ⁻¹	0.7 t CH ₄ event ⁻¹ (low-boundary 95% confidence interval)

2.7 Production sites

Emissions of CH₄ and other pollutants at the production sites are chosen according to results from Omara et al. (2016). Here the CH₄ leakage rate average is estimated at 0.23% of total production, with a maximum of 0.40%. Production at wellsites analyzed by Omara et al. presents production volumes similar to our shale gas industry (between 40 x 10⁶ cf d⁻¹ in Germany P50 and 130 x 10⁶ cf d⁻¹ in UK P50 scenarios). Moreover, the study focused on the Marcellus play, a predominantly gas-producing area with several horizontal wells per pad at new sites. As reported by Marchese et al. (2015) and Mitchell et al. (2015), in the production sector compressor leaks are responsible for almost 90% of total CH₄ emissions. Substituting diesel with electric compressors would eliminate uncombusted fugitive CH₄ (Marchese et al. 2015 Supporting Information; Mitchell et al., 2015 Supporting Information). Nevertheless, in OEm (where we envisage the extreme case where all the sites are provided with electricity from the national grid) we assume an emission decrease by only 90% with respect to REEm to account for accidental leaks from valves and joints.

Emissions reported by Omara et al. were measured during production activities including liquids unloading operations, the emissions of which are calculated separately in our scenarios. Therefore, to avoid double-counting, we reduce the volume of CH₄ from producing wells by the amount estimated during liquids unloading (see Section 2.9).

Total emissions for each productivity case, emission scenario and country are calculated as follows:

$$E = gas_{produced} \times leakage_{rate_{production\ site}}$$

Table S8. Values for REEm and OEm applied to the production sites stage.

REEm-U	REEm-L	OEm-U	OEm-L
Diesel compressors Gas loss: 0.40%	Diesel compressors Gas loss: 0.23%	Electric compressors Gas loss: 0.04% (10% of REEm-U)	Electric compressors Gas loss: 0.02% (10% of REEm-L)

2.8 Wellhead compressor exhaust

Wellhead compressors help to increase productivity from mature reservoirs where the natural gas pressure is not high enough to ensure economic production. We assume the engagement of 3 diesel compressors in REEm (where 3 horizontal wells are connected to the same vertical well), and an electric compressor of 750 kW OEm, where the number of aggregated horizontal wells is 10 for each vertical well. The occurrence of wellhead compressors is assumed to be 25% of total producing sites (NYSDEC, 2015). Also for this stage of the shale gas supply chain, diesel compressors in REEm are substituted with electric ones in OEm.

Total emissions for each productivity case, emission scenario and country are calculated as follows:

$$E(i) = \#_{producing\ wells} \times \%_{wells} \times EF_{(i)} \times h_{operations} \times kW_{compressor}$$

Where:

(i) is the specific pollutant;

% wells is the share of wells we estimate are equipped with wellhead compressors.

Table S9. Values for REm and OEm applied to wellhead compressor exhaust.

REm-U	REm-L	OEm-U	OEm-L
Diesel compressors (300 kW) EF: stage IIIB/IV.	Diesel compressors (300 kW) EF: stage IIIB/IV.	Electric compressor (750 kW) - CH ₄ accidental leaks are not accounted since they are already at losses at production sites	Electric compressor (750 kW) - CH ₄ accidental leaks are not accounted since they are already at losses at production sites

2.9 Liquids unloading

Liquids unloading is an engineering practice that is required during gas production when the liquids co-produced with the gas clog the well and restrict or obstruct the free flow of gas. The frequency of this practice depends on the natural tendency of the well to produce liquids, which is strictly related to the geology of the target formation and the age of the well. Allen et al., 2015 SI (Table S5.2) reports that liquids unloading is performed at ca. 80% of the wells analyzed in their study, covering a population of different ages and nature (for both fracked and non-fracked wells). Plunger lifts are used to remove the liquids accumulated in the well and restore gas production, a valuable alternative to large VOC emissions during the blowing down of the well (EPA, 2014b). Both manual and automated plunger lifts are very effective in preventing emissions, although the former relies on onsite manual performance and is therefore less reliable than the automated one. It is important to note that the population of wells in our dry gas scenario does not require this procedure since dry gas is inherently low in VOCs. Since wells considered in our study are all relatively young (maximum 8-10 years old), we assume that between 5 and 10 liquids unloading activities take place at each well per year (Allen et al. 2015).

In OEm we assume implementation of automatic plunger lifts, which may become standard if strict regulations are in place. In REm, manually triggered plunger lifts are considered. Wells without plunger lifts have not been considered in our scenarios since this would not respect sufficient environmental standards. Uncertainties here are given by the low- and high-boundaries for emissions shown in Figure 5 of Allen's paper.

Total emissions for each productivity case, emission scenario and country are calculated as follows:

$$E(i) = \#_{producing\ wells} \times EF(i)_{wellsite} \times \text{annual events}$$

Where (i) is the specific pollutant

Table S10. Values for REm and OEm applied to liquids unloading.

REm-U	REm-L	OEm-U	OEm-L
Manually triggered plunger lifts Liquids unloading per well: 10 events y ⁻¹ CH₄ emissions: 351 m ³ well ⁻¹	Manually triggered plunger lifts Liquids unloading per well: 5 events y ⁻¹ CH₄ emissions: 195 m ³ well ⁻¹	Automatic triggered plunger lifts Liquids unloading per well: 10 events y ⁻¹ CH₄ emissions: 59 m ³ well ⁻¹	Automatic triggered plunger lifts Liquids unloading per well: 5 events y ⁻¹ CH₄ emissions: 14 m ³ well ⁻¹

2.10 Gathering facilities and pipelines

Gathering is defined as the pipeline system connecting the wellhead compressor with the processing plant. Along this path several facilities and devices are employed to ensure a regular and safe flow of the gas, such as gathering compressors, separators for CO₂, water and condensate, and others. Here, emissions from gathering facilities and pipelines are calculated separately. Mitchell et al. (2015) provides data on CH₄ losses from this connecting system which we critically apply to assign appropriate EFs to the emission scenarios.

2.10.1 Gathering facilities

In order to define the amount of gas lost at gathering facilities (for leaks from pipelines, see below), we refer to a selection of stations analyzed by Mitchell et al. (2015), in which the gas throughput is comparable to the gas collected at gathering plants as described in our study (ranging between 12.7 to 217 t y⁻¹). The 25 and 75 FLER (Facility-Level Emission Rate) %tile averages of this selected population of plants is assigned in OEm (657 t facility⁻¹) and in REm (1110 t facility⁻¹) scenarios. Due to the fact that the number of electric compressors in operation is unknown since they were not listed by Mitchell et al. during sampling campaigns, and that some plumes were not correctly measured or systematically captured (as discussed in Mitchell's paper), there is the possibility that the data source to which we refer are overall biased slightly low.

As observed in the US gas plays and reported by Marchese et al. (2015) and Mitchell et al. (2015), gathering facilities generally collect gas from 10 to 100 horizontal wells. We assume that this parameter is regulated under state law and therefore we apply two different cases in our emission scenarios: 1) gas collected from 30 wells at gathering facilities in REm; and 2) gas collected from 80 wells in OEm.

2.10.2 Emissions from supplementary devices at facilities

Based on data reported in Marchese et al. (2015, SI), we assign the number of compressors, pneumatic controllers, pneumatic pumps, chemical pumps and Kimray pumps at each gathering station. Pneumatic devices are mechanically powered by the high-pressure of the gas, and are implemented anytime electricity supply cannot be provided. EFs for these devices are assigned according to data reported by Helms et al. (2010).

Other parameters that we associate with these devices are reported in Table S11.

Table S11. Number and operational characteristic of devices at gathering stations.

Device	Number facility ⁻¹	Loading factor (LF) ⁴	kW
compressors	35	60%	127 ⁵
pneumatic controllers	69	10%	0.03 ⁶

⁴ Report available at: <http://www.ourenergypolicy.org/wp-content/uploads/2014/04/epa-devices.pdf>. Accessed 15 April 2019.

⁵ Mitchell et al., 2015.

⁶ See ref. 5.

pneumatic pumps	5	10%	1.7 ⁷
chemical pumps	12	10%	1.7 ⁸
Kimray pumps	1755	10%	3.7 ⁹

We assume that in REm all compressors are run via diesel engines, while controllers and pumps are pneumatic or activated by the national power grid (therefore assuming that connection to the national power grid is always possible). In OEm, all machines and controllers are supplied by the national power grid. As noted earlier, electric compressors have the potential to eliminate gas leaks. Emission ranges will therefore be representative for all types of compressors: diesel (highest emission case), electric (lowest emission case), and natural gas-powered (intermediate emission case).

Total emissions for each productivity case, emission scenario and country are calculated as follows:

$$E(i) = \#_{gathering\ plants} \times [(losses_{gathering\ plant} + (\#_{devices} \times kw_{device} \times h_{operations} \times LF_{device} \times EF_{(i)})]$$

Where (i) is the specific pollutant.

Table S12. Values for REm and OEm applied to gathering facilities.

REm-U	REm-L	OEm-U	OEm-L
CH₄ loss at facility: 1110 t Wells connecting to facilities: 30 EFs compressors: Stage IIIB/IV	CH₄ loss at facility: 657 t Wells connecting to facilities: 30 EFs compressors: Stage IIIB/IV	CH₄ loss at facility: 5% of REm-U, plus emissions from electrical grid power Wells connecting at facilities: 80	CH₄ loss at facility: 5% of REm-L, plus emissions from electrical grid power Wells connecting at facilities: 80

2.10.3 Gathering pipelines

In order to assign gas emissions from gathering pipelines, we select data reported by Marchese et al. (2015, SI) in which they model the CH₄ loss rate in the US natural gas supply chain. Results show a gas leak of 0.035%, a value similar to the one reported by the EPA GHGI. We differentiate REm and OEm based on the fact that in the former more above-ground wellheads are planned (10 wellheads per well pad vs. 3 in OEm). In the absence of better data, we assume an arbitrary emission reduction in OEm by 15% when compared to REm that accounts for the reduced number of wellheads present on each well pad.

Total emissions for each productivity case, emission scenario and country are calculated as follows:

$$E = gas_{produced} \times leakage\ rate_{gathering\ pipeline}$$

⁷ See ref. 5.

⁸ Data available at: <https://www.itc.es/>. Accessed 15 April 2019.

⁹ Data available at: https://kimray.com/Downloads/Marketing/Electric_Glycol_Pump/SSEG-001_Electric_Glycol_READER.pdf. Accessed 15 April 2019.

Table S13. Values for gas leakage rate for applied to gathering pipelines for REm and OEm.

REm-U	REm-L	OEm-U	OEm-L
Gas leakage: 0.035%	Gas leakage: 0.035%	Gas leakage: 0.030%	Gas leakage: 0.030%

2.11 Processing

2.11.1 Gas emissions

To determine natural gas and air pollutant emissions at natural gas processing stations we refer to the study by Mitchell et al. (2015) and to the AP-42 Report from the EPA¹⁰. The amount of gas produced at each well pad ranges between 12.7 and 217 t h⁻¹ in our study, making it reasonable to assume that the amount of gas processed at each facility of our scenarios is comparable to data discussed in Mitchell et al. (here the gas amount ranges between 100 and 780 t h⁻¹). Based on these similarities, we assign the same leakage rate suggested by Mitchell’s study at processing plants: 0.046% and 0.079% in OEm and REm, respectively.

By substituting diesel-engine compressors with electric ones in OEm, it would completely eliminate CH₄ leaks from these devices (Marchese et al. 2015 Supporting Information; Mitchell et al., 2015 Supporting Information) as well as most VOC emissions onsite: according to Marchese et al. (2015) venting and combustion from compressors represent 90% of all emissions (Table S5 in SI, Marchese et al.). Since we cannot rule out that emissions-reducing compressors (e.g., electric) were also deployed at the processing stations investigated by Mitchell et al., we only assume emission reductions of 50% in REm to avoid potential double counting.

2.11.2 Energy requirement

Different electricity-producing gas turbine typologies may be employed at processing plants (e.g., simple or with abatement measures for NO_x and CO like water-steam injection or heat-recovery systems). According to the AP-42 Report from EPA, simple cycle gas turbines are often used in the petroleum industry due to the low price and large availability of gas. In order to cover different turbine typologies, in our scenarios we assume implementation of uncontrolled gas turbines in REm and water-steam injection turbines in OEm. The latter is technologically more advanced and requires high quantities of fresh water which may make its adoption challenging in some areas. Therefore, its adoption is more consistent with an optimistic scenario. The AP-42 report indicates a gas combustion efficiency value for simple cycle turbines between 15 and 42%, while between 38 and 60% for combined cycle gas turbines. Very similar values are assigned to turbines for oil and gas applications by Siemens.¹¹ Accordingly, in our REm and OEm we apply turbines with a range of efficiency spanning from 30 to 60%.

In our scenarios, we estimate that 164 kWh of energy is required to process 1,000 m³ of natural gas based on Müller-Syring et al. (2016) and consultants from the oil and gas industry. Assuming turbine

¹⁰ Report available at: <https://www3.epa.gov/ttnchie1/ap42/ch03/final/c03s01.pdf>. Accessed 15 April 2019.

¹¹ An overview on different gas turbines available on the market is available at: <https://www.siemens.com/global/en/home/products/energy/power-generation/gas-turbines/refining-petrochemical.html>. Accessed 15 April 2019.

efficiencies of the range reported above, the amount of gas combusted on site ranges between 2.8 and 5.6% of total gas processed in the different scenarios.

Total emissions for each productivity case, emission scenario and country are calculated as follows:

$$E(i) = (\text{leakage rate}_{\text{processing plants}} \times \text{gas}_{\text{processed}}) + (\text{gas}_{\text{combusted}} \times EF_{(i)})$$

Where:

(i) is the specific pollutant;

gas_{combusted} depends on turbine efficiencies.

Table S14. Values for REem and OEem applied to gas processing.

REm-U	REm-L	OEem-U	OEem-L
Gas leakage: 0.079% Uncontrolled gas turbines with combustion efficiency of 30%.	Gas leakage: 0.046% Uncontrolled gas turbines with combustion efficiency of 40%.	Gas leakage: 0.039% Water-steam injection turbines with combustion efficiency of 50%.	Gas leakage: 0.023% Water-steam injection turbines with combustion efficiency of 60%.

2.12 National power grid

Power from the national electric grid is required in our scenarios to supply energy for operations at different stages. The amount of power required varies according to the technology involved in the different scenarios. EFs for the national electric grid are calculated according to emissions produced by the different energy carriers (mainly coal and natural gas) and to their share of energy generated. The German Environmental Agency (UBA) provides detailed and updated EFs for the national power grid¹², while data available for the UK are limited to CO₂ and CH₄. We therefore decide to apply EFs for Germany to both countries (data for Germany 2015, see Table S17), given the very similar gCO₂-eq. kWh⁻¹ values associated with both countries (540 gCO₂-eq. kWh⁻¹ for Germany and 528 gCO₂-eq. kWh⁻¹ for the UK in 2016, see Section *Emission Intensity* in the manuscript) and the negligible relative component that the power sector exerts on total CO₂ and CH₄ emissions (see discussion in the Sensitivity Analysis Section). The two countries examined have a similar energy mix: ca. 40% of the power generated is produced via nuclear and renewables, while the remaining share differs in gas and coal utilization: respectively 12 and 45% in Germany, while 42 and 22% in the UK.

Table S15. EFs for the national power grid applied for Germany and the UK. Data in g kWh⁻¹.

Pollutant	value
NO _x	0.454
PM ₁₀	0.016
PM _{2.5}	0.014
CO	0.227
CO ₂	534.000
N ₂ O	1.816
CH ₄	0.167
VOCs	0.018

¹² Emission factors are available at: <https://www.umweltbundesamt.de/themen/luft/emissionen-von-luftschadstoffen/spezifische-emissionsfaktoren-fuer-den-deutschen>. Accessed 15 April 2019.

3 Sensitivity analysis

We carry out a sensitivity analysis (SA) for the scenarios presented in our manuscript to gain insight into the effects and implications that the input parameters of the system (i.e., independent variables) exert on final emissions (i.e., dependent variable). This procedure enables us to quantitatively characterize the sensitivity of the output values when each single input variable changes, so as to determine the influence of the input and therefore the accuracy it requires when defining the values' boundary. The SA is also a method to assess the robustness and limitations of the model, which in turn provides guidance on interpretation of results and restrictions of the results' applicability. The SA is carried out by systematically varying each input parameter while keeping the others constant, and observing the effect that this variation has on the output. The SA is run for the REm-P50 case for Germany, and investigates the following pollutants: CO₂, CH₄, VOCs and NO_x. We vary parameters that are constant through the scenarios, as well as variables that define and differentiate the scenarios. This is because the choice about variability of these coefficients is finalized at a later stage, and is also partially based on the SA results. A selected group of variables and parameters are increased from the lower end (REm-L) to the upper end of their uncertainty range (REm-U) to observe the variation generated on total emissions for each pollutant. When no range is described due to lack of data (i.e., kilometers driven by trucks), a flat increase of 50% is imposed. Results show a large impact variance associated with single emitting stages across the production system, and this distribution is characteristic and special for each pollutant. Variables which are shown to significantly affect final overall emissions undergo further investigation. Hereby we analyze variables and parameters based on two different aspects: on the one hand we measure the impact (in %) that a variation of the independent variables within its uncertainty range has on total emissions (i.e., effective impact, Table S16). On the other, we normalize this impact per single unit of variation of the independent variable, in order to define the "power" of a variable to affect final total emissions independent of the range of variability we impose (i.e., potential impact, Table S17). While through the first approach we obtain a sense of the real influence that each variable has in our study, the second one provides us with a qualitative assessment of the strength that such variables possess in affecting overall results.

CO₂ total emissions are largely influenced by variation in the utilization and performances of the numerous engines employed along the production chain, so that variables related to these during drilling, at wellhead compressors, at gathering facilities and during processing (i.e., efficiency of gas turbines during processing) strongly affect final emissions (Figure S2). Results show that, although the number of gathering facilities can strongly affect final CO₂ outputs, the very restricted variability within the OEm and REm range boundaries significantly limits its effective contribution. It is anyway worth noting that the range of this parameter varies significantly in the OEm and REm, so that its overall relevance in these emission cases is very different. A wide range characterizing the fracking stage time interval is responsible for an overall contribution up to 6.1% despite a low normalized potential (up until 2.6%). Gas turbine efficiency during processing is by far the key parameter capable of raising total emissions by 16.6% when varying within its uncertainty range. Likewise, it displays high normalized sensitivity. Figure S3 evidences how parameters controlling CH₄ emissions differ substantially from the results for CO₂. Gas losses at production sites and gathering facilities markedly dominate total emissions, each raising the final output by 31.6% and 32.7% respectively when varying within their corresponding uncertainty ranges. The normalized impact of the number

of gathering facilities necessary to streamline the gas register contribution on final emissions very similar to the ones displayed by CH₄ emissions at the same stage (both circa 41.6%), although its narrow confidence range preclude significant effects on total emissions. Gathering pipelines and processing activities (gas lost and turbine efficiency) show a normalized impact below 10% and an effective impact below 5%. As expected, VOC emissions (Figure S4) closely resemble CH₄ results: these two pollutants are (for the most part) linearly correlated, as they are co-emitted through natural gas losses. NO_x are emitted by hundreds of diesel engines employed across the gas production chain, so that the utilization of all these at each stage of gas production affect total emissions to different extents (Figure S5). Its highest impacts observed on total emissions are from the time interval of fracking operations, followed (in order) by gas turbine efficiency at processing stations, volume of water per fracking stage, as well as fracking stage length and drilling time operations. The influence of these stages on total NO_x emissions ranges from 8.3% to 19.3% per stage, while their normalized impacts range from 16.6% (drilling operations) up to 66.3% (gas turbine efficiency). Once again, the parameter “# gathering facility” has a considerable normalized impact but a negligible real influence on overall emissions. As observed for CO₂, the fracking stage length has an effective impact of 11.1% despite a much lower normalized potential.

Production site preparation and ancillary operations during drilling and fracking do not have any relevant repercussions on total emissions of the pollutants examined here. Similar results are evidenced by operations of liquids unloading as well as parameters associated with trucks such as kilometers driven, emission standards, and others. CH₄ and VOCs potentially lost during well completion operations or at the liquids unloading stage have a very irrelevant contribution to total volumes, although their effects at the local level may be more pronounced. EFs from the electrical power grid do not show any appreciable contribution to total volume for all pollutants, although showing a minimal effect on NO_x emissions (3.6% of effective impact against 7.1 of potential impact).

Table S16. Effective impact of independent variable variations on total emissions. The table summarizes the effect of variations of single pollutants within their range boundaries and at different stages of gas production on final emissions. The variation applied is reported in the final column.

Stage	Parameter	CO ₂	CH ₄	VOCs	NO _x	Variation
Well pad developmet	Duration of operations	<0.1%	-	-	<0.1%	REm-L to REm-U
Truck traffic	Driving distance	0.1%	-	-	0.1%	50%
Drilling	Duration of operations	3.7%	-	<0.1%	8.3%	50%
Fracking operations	Length fracking stage	5.2%	-	<0.1%	11.1%	REm-L to REm-U
	Vol. water per fracking stage	0.1%	-	-	11.1%	50%
	Duration of operations + # stages	0.8%	-	<0.1%	19.3%	REm-L to REm-U
Well completion	Emissions CH ₄ per well	-	0.5%	0.5%	-	REm-L to REm-U
Production sites	loss (% of production)	-	31.6%	31.6%	-	REm-L to REm-U
Wellhead compressors	# Compressors	4.2%	-	<0.1%	2.0%	50%
Liquids unloading	Absolute emissions	-	-	-	-	REm-L to REm-U
Gathering facilities	# facilities	0.5%	0.6%	0.6%	0.4%	REm-L to REm-U
	Absolute emissions	-	28.8%	28.8%	-	RmM-L to REm-U
	Gas leaked (pipelines)	-	3.3%	3.3%	-	50%
Processing	Gas leaked (% of gas processed)	-	6.1%	6.1%	-	REm-L to REm-U

	Gas turbine efficiency	16.6%	1.4%	1.4%	16.6%	REm-L to REm-U
Electricity	EF electricity	2.4%	<0.1%	0.01%	3.6%	50%

Table S17. Potential impact of independent variable variations on total emissions. The table summarizes the effect of normalized variations of single pollutants at different stages of gas production on final emissions. The variation applied is reported in the final column.

Stage	Parameter	CO ₂	CH ₄	VOCs	NO _x	Variation
Well pad developmet	Duration of operations	<0.1%	-	-	<0.1%	REm-L to REm-U
Truck traffic	Driving distance	0.3%	-	-	0.3%	50%
Drilling	Duration of operations	7.4%	-	<0.1%	16.6%	50%
Fracking operations	Length fracking stage	1.3%	-	-	2.8%	REm-L to REm-U
	Vol. water per fracking stage	0.1%	-	-	22.2%	50%
	Duration of operations + # stages	1.2%	-	<0.1%	28.9%	REm-L to REm-U
Well completion	Emissions CH ₄ per well	-	0.5%	0.5%	-	REm-L to REm-U
Production sites	loss (% of production)	-	42.7%	42.7%	-	REm-L to REm-U
Wellhead compressors	# Compressors	8.3%	-	<0.1%	4.0%	50%
Liquids unloading	Absolute emissions	-	-	-	-	REm-L to REm-U
Gathering facilities	# facilities	35.2%	41.6%	41.6%	29.0%	REm-L to REm-U
	Absolute emissions	-	41.5%	41.6%	-	REm-L to REm-U
	Gas loss (pipelines)	-	6.5%	6.5%	-	50%
Processing	Gas leaked (% of gas processed)	-	8.5%	8.5%	-	REm-L to REm-U
	Gas turbine efficiency	66.4%	5.5%	5.4%	66.3%	REm-L to REm-U
Electricity	EF electricity	4.9%	<0.1%	<0.1%	7.1%	50%

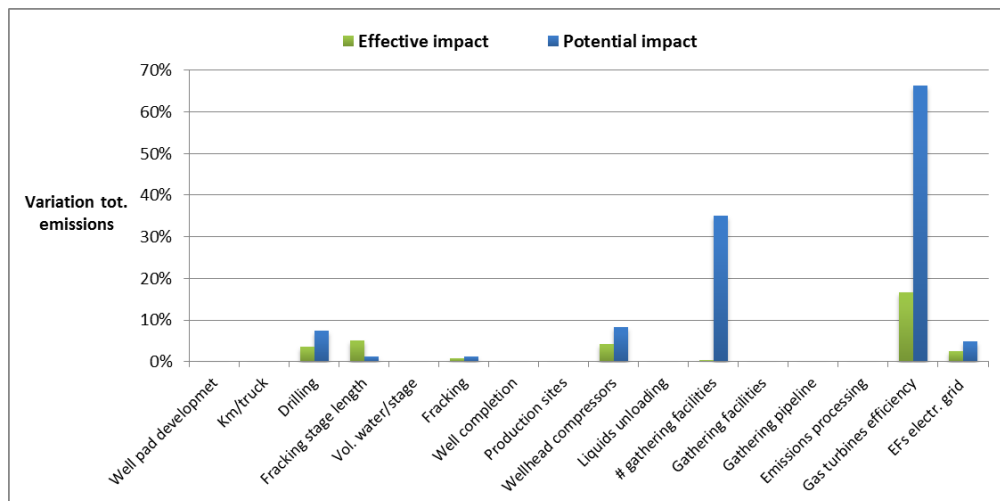


Figure S2. Sensitivity analysis results for CO₂. Visualization of the effective and potential impacts on final CO₂ emissions through variation of parameters at each stage of the upstream gas chain.

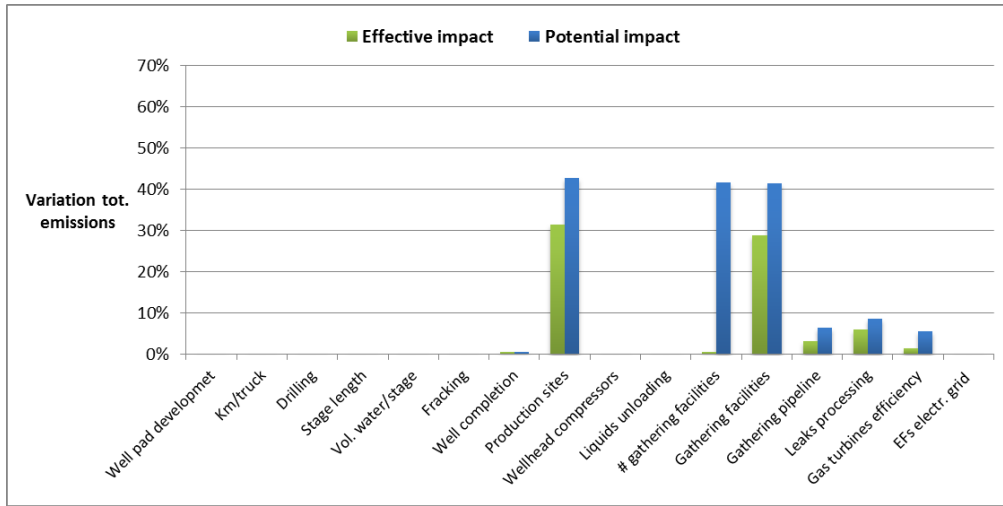


Figure S3. Sensitivity analysis results for CH₄. Visualization of the effective and potential impacts on final CH₄ emissions through variation of parameters at each stage of the upstream gas chain.

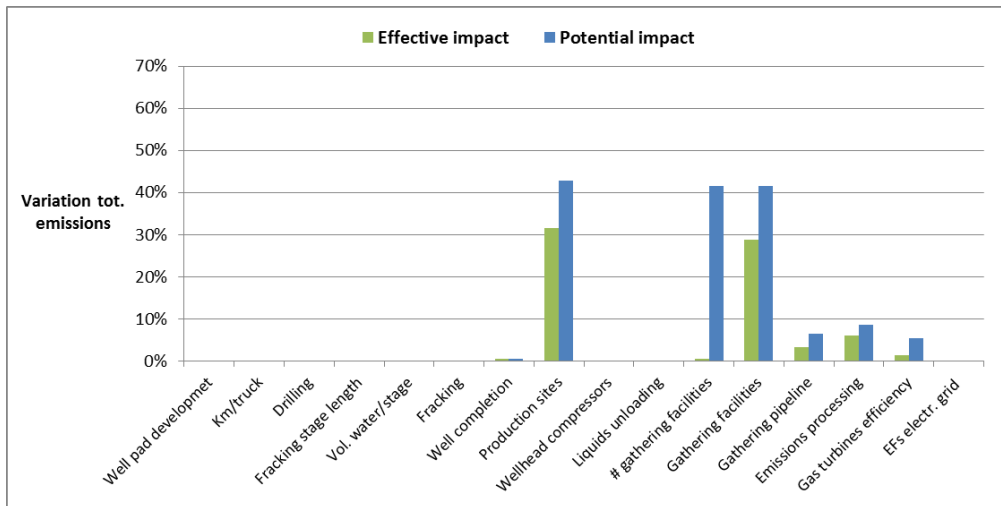


Figure S4. Sensitivity analysis results for VOCs. Visualization of the effective and potential impacts on final VOC emissions through variation of parameters at each stage of the upstream gas chain.

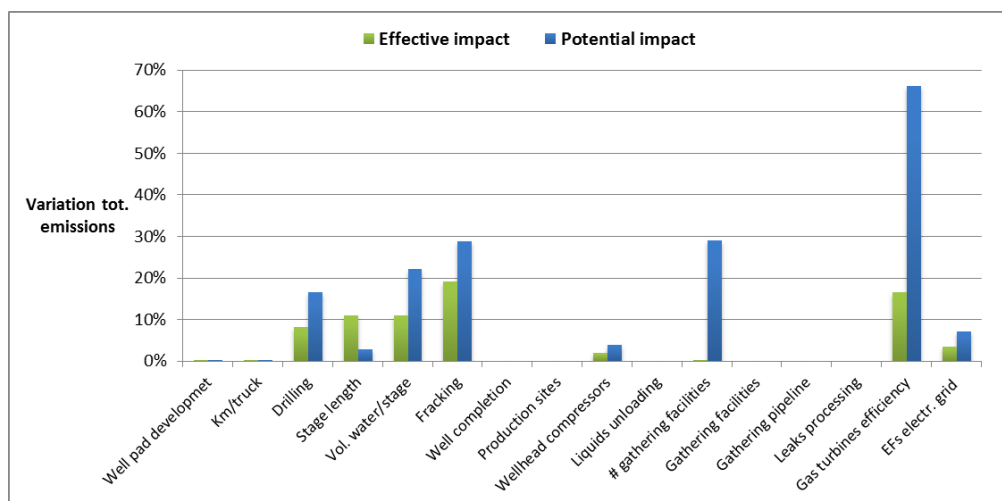


Figure S5. Sensitivity analysis results for NO_x. Visualization of the effective and potential impacts on final NO_x emissions through variation of parameters at each stage of the upstream gas chain.

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