Modeling the impact of a potential shale gas industry in Germany and the United Kingdom on ozone with WRF-Chem

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Supplemental material

Table S1. **Namelist used in simulations with WRF-Chem**

&time_control	
start_year	= 2011,
start_month	= 05,
start_day	= 29,
start_hour	= 00,
start_minute	= 00,
start_second	= 00,
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auxinput4_interval = 360,

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auxhist3_interval = 1440,

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io_form_auxhist3 = 2,

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&domains

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time_step_fract_den              = 1,

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e_vert                           = 35,

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0.954,                           0.934,  0.909,    0.88,     0.845,

0.807,                           0.765,  0.719,    0.672,    0.622,

0.571,                           0.52,   0.468,    0.42,     0.376,

0.335,                           0.298,  0.263,    0.231,    0.202,

0.175,                           0.15,   0.127,    0.106,    0.088,

0.07,                            0.055,  0.04,     0.026,    0.013,

0.0,

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j_parent_start              = 1,
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parent_time_step_ratio      = 1,
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smooth_option               = 0,
/

&physics
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ra_lw_physics               = 4,
ra_sw_physics               = 2,
radt                        = 15,
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ifsnow                  = 1,
icloud                  = 1,
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mp_zero_out_thresh      = 1.e-12,
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maxens2                 = 3,
maxens3                 = 16,
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if_no_pbl_nudging_t = 0,

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if_zfac_t = 0,

k_zfac_t = 8,

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gt = 0.0003,

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dtramp_min = 60,

/

&dynamics

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km_opt = 4,

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kvdif                        = 0,
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scalar_adv_opt               = 2,
chem_adv_opt                 = 2,
tke_adv_opt                  = 2,
time_step_sound              = 4,
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v_mom_adv_order              = 3,
h_sca_adv_order              = 5,
v_sca_adv_order              = 3,
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spec_zone                    = 1,
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/

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photdt                          = 15,
chemdt                          = 10,
io_style_emissions              = 2,
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emiss_opt                       = 7,
chem_in_opt                     = 1,
phot_opt                        = 3,
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gas_ic_opt              = 1,
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wetscav_onoff           = 0,
cldchem_onoff           = 0,
vertmix_onoff           = 1,
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Text S1. conNO_x scenario development

In order to calculate the conNO_x scenario emission flux for emissions pre-processing, first the area over which to concentrate the NO_x emissions from drilling and fracking activities was calculated. Afterwards the NO_x emissions for drilling and fracking activities from the REm-U P25 scenario from Cremonese et al.

(2019), which make up 24% of total shale gas NO_x emissions for Germany and 18% for the UK, were divided by space and time values to get the emissions flux in units of kg m^{-2} s^{-1}. These calculations are described here.

Concentrated NO_x area

Displayed below are calculation steps (1-4) to convert number of wells pads (WP) in Germany (DE) and in the United Kingdom (UK) from concentrated NO_x activities to total area of concentrated NO_x emissions for the conNO_x scenario, adjusted to fit the pre-processing grid to which emissions are added. Note that, according to Cremonese et al. (2019)'s REm-U P25 scenario which are used as the basis for all simulations in this work, 166 and 206 wells are both drilled and fracked annually in DE and the UK, respectively. These values were averaged to 42 and 52 wells that are drilled and fracked over the JJA period respective to DE and the UK. In the conNO_x scenario one drilling and one fracking activity are applied per pad, so that a uniform emissions flux can be applied to the entire Concentrated NO_x area to reduce complexity (as opposed to say, half the concentrated NO_x area containing drilling activities only with one emissions flux and the other area containing fracking activities only with a different emissions flux). With one fracking and one drilling activity per pad, a total of 42 and 52 WPs are utilized in DE and the UK, respectively.

Calculation steps - Germany

1) $$42\ pads_{DE}\ \times 25\ km^2_{WP\ area} = 1050\ km^2 total\ area_{WP,DE}$$

2) $$1050\ km^2_{WP,DE}\ /\ 49\ km^2_{PP\ area} = 21.43\ \approx 20\ grid\ cells_{PP,DE}$$

3) $$20\ cells_{PP,DE}\ \times 49\ km^2_{PP\ area} = 980\ km^2 total\ area_{PP,DE}$$

4) $$980\ km^2 total\ area_{PP,DE}\ /\ 12250\ km^2 SG\ basin_{DE} = 8.0\%\ SG\ basin\ area$$

Calculation steps - United Kingdom

1) $$52\ pads_{UK}\ \times 25\ km^2_{WP\ area} = 1300\ km^2 total\ area_{WP,UK}$$

2) $$1300\ km^2_{WP,UK}\ /\ 49\ km^2_{PP\ area} = 26.53\ \approx 25\ grid\ cells_{PP,UK}$$

3) $$25\ cells_{PP,UK}\ \times 49\ km^2_{PP\ area} = 1225\ km^2 total\ area_{PP,UK}$$

4) $$1225\ km^2 total\ area_{PP,UK}\ /\ 17052\ km^2 SG\ basin_{UK} = 7.2\%\ SG\ basin\ area$$

Here we walk through the steps to calculate the concentrated NO_x area, for each country. In calculation step 1 the number of WPs is multiplied by the WP area used in Cremonese et al. (2019) (5kmx5km=25km^2) to calculate total WP area for concentrated NO_x emissions. In step 2, the WP area from step 1 is divided by the pre-processing (written as 'PP' in subscript) grid cell size (7kmx7km=49km^2, Kuenen et al. 2014) to adjust to the pre-processing grid, and subsequently rounded to produce a simple quadrilateral area. In step 3 the total concentrated NO_x area adjusted to the pre-processing grid is calculated. Finally in step 4 the percentage of shale gas (written as 'SG' in subscript) basin area consisting of concentrated NO_x emissions is calculated, based on the size of the shale gas basins of these two countries. Note that the shale gas basin area is based on the raster grid used in our simulations.

Concentrated NO_x time

According to Cremonese et al. (2019)'s REm-U P25 scenario, the time required to drill one well is 392 h, or approximately 16.33 days. On the other hand, the time required to frack one stage is 2.5 h, where there are a total of 41.7 stages per well. Because only one stage can be drilled at a time per well, this amounts to a total of 104.17 hours, or rather 4.34 days. In order to reduce complexity and have one emissions flux, all concentrated NO_x emissions are averaged over one period of time, based on the time required to carry out the longer activity, i.e., drilling. Since it is necessary to apply daily values in emissions pre-processing, this period of time is rounded up to 17 days.

Placement of Concentrated NO_x emissions based on sensitivity studies

In the sensitivity study to select the location for the concentrated NO_x emissions, the following steps were performed, for both Germany and the United Kingdom:

1. Shale gas basin mask netCDF file was converted from the emissions pre-processing grid to a mask adapted to the output grid, to analyze WRF-Chem output data in the shale gas regions only.
2. Areas classified as 'urban or built up land' in the USGS dataset were removed from the mask. This was done so as not to include areas which would be unrealistic for potential locations to add concentrated drilling and fracking activities.
3. The j, k, lat, lon, and $MDA8_{Diff,max}$ (scenario minus base) values were recorded per grid cell for each grid cell of the mask, and for each day of the simulation period. $MDA8_{Diff,max}$ is described in **Equation S1** below.
4. This data was obtained for two scenarios: SG1-wet gas, and SG1-wet gas *without* added shale gas NO_x emissions. Note that both scenarios contain added shale gas VOC emissions.
5. There are several shale gas basins for Germany, and so this data was filtered by removing coordinates and their corresponding values for German shale gas basins which were not large

enough to accommodate the concentrated NO_x area, i.e, Unterkarbon basins located in the Baltic Sea (near Rügen) and by the Ruhr Valley (see Cremonese et al. 2019) for depiction of basins and corresponding basin names). This was not performed for the UK, since it contains one large, continuous basin, i.e., the Bowland.

6. $MDA8_{Diff,max}$ values: SG1-wet gas (no NO_x) values were subtracted from SG1-wet gas (aptly referred to here as $MDA8_{Diff,max,NOx}$), to see what the effect of added NO_x emissions from shale gas was on MDA8 per grid cell and per day.
7. The top 30 highest $MDA8_{Diff,max,NOx}$ values for both Germany and the UK were recorded.
8. Of these top 30 values for each country, cells which formed a continuous area were filtered for. Note that in Germany a continuous area of about 4 grid cells was filtered for, and for the UK an area of about 5 grid cells, based on the size of the concentrated NO_x activities and the resolution, i.e., size of each grid cell of the output grid.
9. Based on these steps, a rough area that may be especially sensitive to concentrated NO_x emissions for increased MDA8 production was determined. Note that it was not possible to determine the exact area because of inherent and unavoidable differences between the output grid and pre-processing grid. That is to say, because the output grid and pre-processing grid contain differing horizontal resolutions, the grid cell lat/lon coordinates likewise differ.
10. After having determined a rough continuous area which displays a heightened sensitivity to added NO_x emissions for increased MDA8 production in the output grid, the closest lat and lon coordinates of the pre-processing grid matching the coordinates of the output grid were determined.
11. After determining this, a new mask was created for the concentrated NO_x area, for each country, adapted to the pre-processing grid. The mask was located roughly in the same area as the output grid.
12. Again, due to slight differences and discrepancies in coordinates as a result of converting from one grid to the other, the concentrated NO_x mask was checked against the shale gas basin mask of each country to ensure that the NO_x mask was roughly within the shale gas region; the mask was adjusted as necessary.

Equation S1

In order to provide statistical data (Table S2) on maximum difference in MDA8, the maximum of the difference in MDA8 between the scenario and base case at time t is calculated for every x y coordinate over region R (ΔMDA8).

$$\Delta MDA8(t) = \max(MDA8_{scenario}(t,x,y) - MDA8_{Base}(t,x,y)) \forall\ xy\ \in R$$

Table S2. **Summary of ΔMDA8 statistical data over the whole domain in μg m^{-3}, over JJA**

	SG1			SG2			SG3		
Statistical data	dry gas	wet gas	conNO$_x$	dry gas	wet gas	conNO$_x$	dry gas	wet gas	conNO$_x$
Minimum	0.3	0.4	0.4	0.3	0.6	0.8	0.6	1.8	1.6
Q1	0.8	1.1	1.4	1.0	1.6	1.8	1.4	5.0	5.0
Median	1.2	1.4	2.1	1.3	2.5	2.9	2.1	6.7	6.3
Q3	1.6	2.0	3.2	1.8	3.2	4.0	2.7	10.2	9.7
Maximum	3.7	4.5	9.5	3.9	6.5	9.6	4.8	28.3	23.3
Average	1.4	1.6	2.6	1.5	2.6	3.2	2.2	8.0	7.5

Table S3. **Stations per country and exceedance data per country with respect to the EU threshold, over JJA**

		SG1				SG2				SG3			
Country		dry gas		wet gas		dry gas		wet gas		dry gas		wet gas	
	Σ[a]	Σ[b]	%[c]	Σ	%	Σ	%	Σ	%	Σ	%	Σ	%
France	386	27	7	32	8	30	8	41	11	40	10	67	17
Italy	244	17	7	20	8	18	7	23	9	21	9	37	15
Germany	234	4	2	4	2	4	2	6	3	5	2	16	7
Spain	129	1	1	2	2	1	1	3	2	3	2	5	4
Austria	111	2	2	4	4	4	4	4	4	4	4	6	5
U. Kingdom	80	1	1	3	4	3	4	5	6	5	6	15	19
Poland	61	1	2	1	2	1	2	2	3	2	3	2	3
Czech Rep.	60	0	0	0	0	0	0	2	3	2	3	5	8
Belgium	42	0	0	0	0	0	0	2	5	2	5	5	12
Hungary	17	0	0	1	6	0	0	1	6	1	6	2	12
Sweden	12	0	0	0	0	0	0	0	0	0	0	0	0
Netherlands	15	0	0	0	0	0	0	0	0	0	0	1	8
Slovakia	11	0	0	0	0	0	0	0	0	0	0	1	9
Denmark	7	1	14	1	14	1	14	1	14	1	14	2	29
Serbia	6	1	17	1	17	1	17	1	17	1	17	1	17

[a]Number of stations with valid measurements per country. Only country stations which are located within the model domain are included in the analysis.

[b]Number of stations that experience exceedances per country.

[c]Percentage of stations per country that have an exceedance.

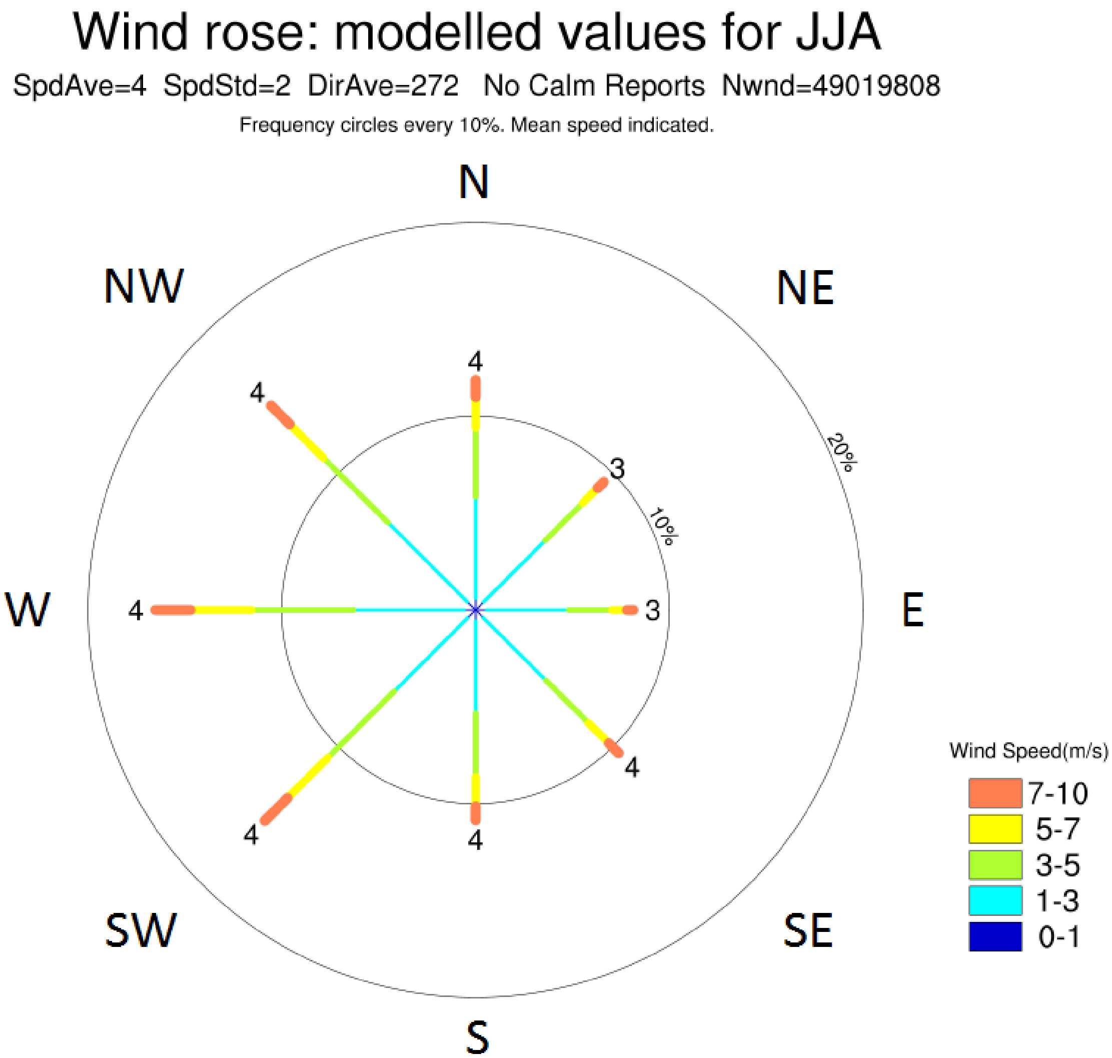

Figure S1. **Wind rose diagram of hourly modeled values over domain for JJA.** The length of each directional bar indicates the frequency (percentage of time) that wind blows from the respective direction, where each concentric circle represents a different frequency. The colors indicate the percentage of time that wind blows from a particular direction at a certain speed, in units of $m \cdot s^{-1}$. The number at the end of each directional bar indicates the average wind speed from that direction. Overall statistics for the entire data sample are included in the title, where SpdAve = wind speed average; SpdStd = standard deviation of the wind speed average; DirAve = directional average; Nwnd = number of modelled values. No calm reports means that there were no modeled data points where the wind speed was at exactly 0.

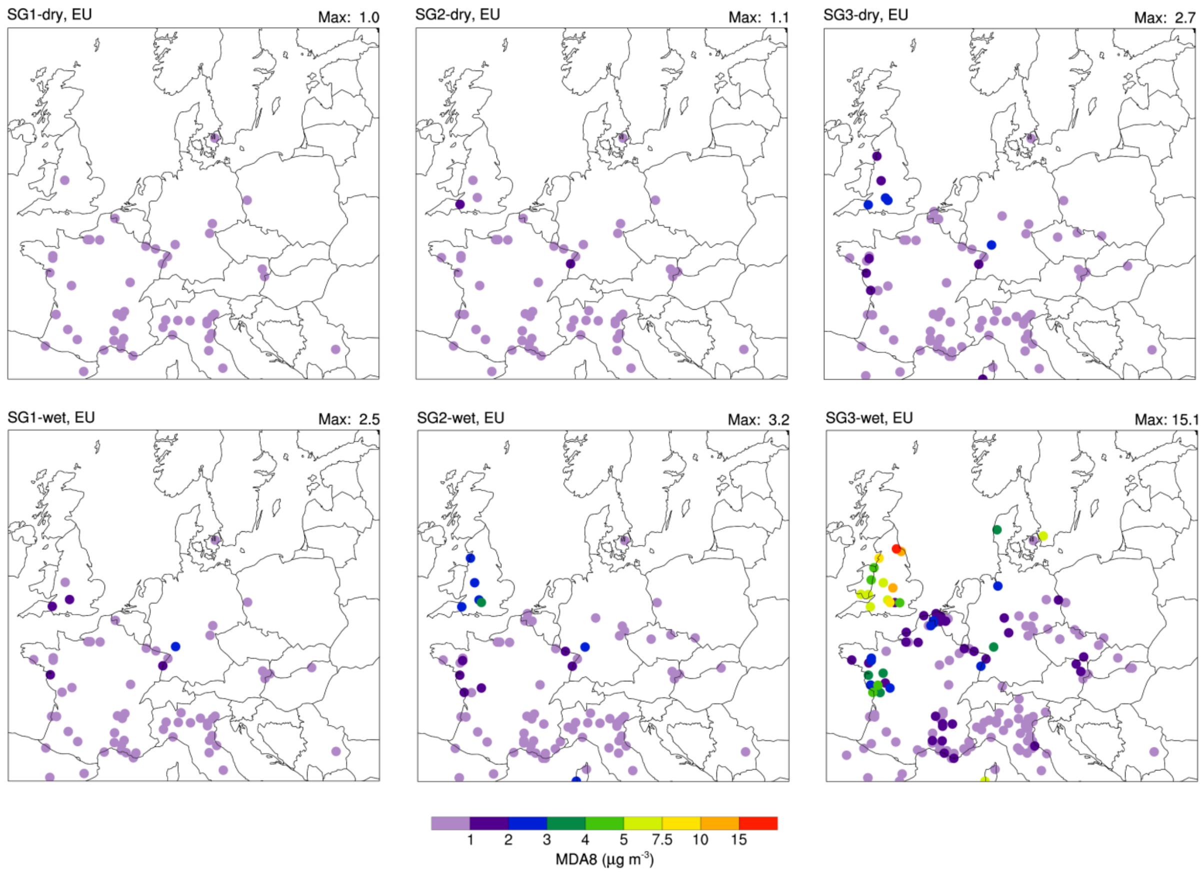

Figure S2. **Spatial depiction of exceedances and corresponding exceedance magnitude.** Exceedance magnitude is defined as the difference between the shale gas scenarios and base case when an exceedance occurs, and is an indicator of the robustness of shale gas emissions on an exceedance. Exceedances are displayed as filled dots at the station locations where they occur, in μg m^{-3}, over JJA, applying the EU guideline for O_3 as the threshold (120 μg m^{-3}). For stations which experienced more than one exceedance, the maximum exceedance magnitude is shown. The top left-hand corner of each plot indicates the particular scenario, and the top right-hand corner displays the maximum exceedance magnitude value experienced over the domain and simulation period.

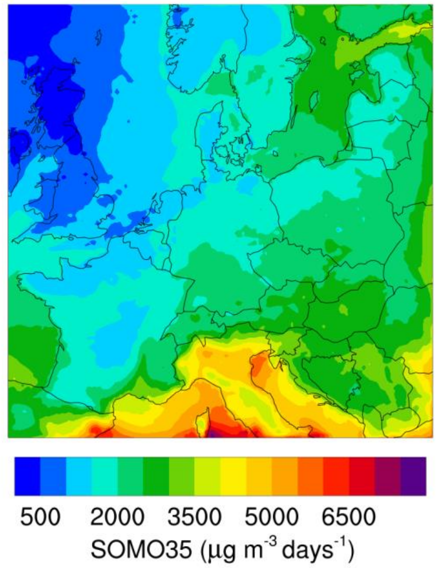

Figure S3. **Surface plot of SOMO35 (annual Sum of Ozone Means Over 35 ppb, daily maximum 8-hour) for base case simulation, in µg/m^3·days, over JJA**. SOMO35 is an indicator of accumulated O_3 exposure.

References

Cremonese L, Weger LB, Denier van der Gon HAC, Bartels M, Butler TM. 2019. Emission scenarios of a potential shale gas industry in Germany and the United Kingdom. *Elem Sci Anth* **7**(1): 18. doi:10.1525/elementa.359.