Analysis of NOx emissions and formaldehyde formation in U.S. oil and gas production regions using satellite data

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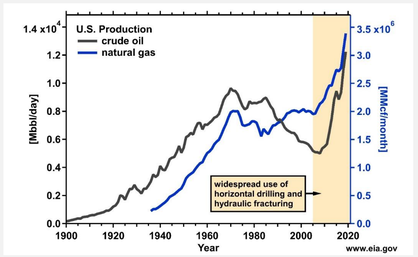
U.S. Oil and Gas Production

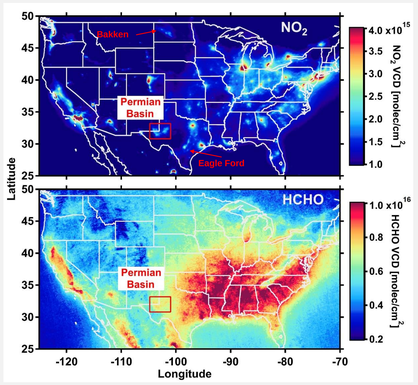
The development of horizontal drilling and hydraulic fracturing has led to a steep increase in the production of natural gas and crude oil from shale formations in the U.S. Associated with this industrial activity are emissions of ground-level ozone precursors such as nitrogen oxides (NOx = NO_2 + NO) and volatile organic compounds (VOCs).



Oil and gas operations are often in remote areas with little to no air quality measurements. Here we use NO_2 and formaldehyde (HCHO) observations from the TROPOMI satellite instrument to study NOx emissions and formaldehyde formation from VOC emissions.

TROPOMI

The TROPOspheric Monitoring Instrument (TROPOMI) measures both nitrogen dioxide (NO_2) and HCHO. In a previous study we have shown that NOx emissions from the Permian basin, Bakken and Eagle Ford are visible from space as increased NO_2 vertical column densities (VCDs) and that these VCDs scale with industrial activity (Dix et al., GRL, 2020). Currently, the Permian basin is one of the largest oil and gas production areas in the world.



TROPOMI tropospheric NO_2 and HCHO VCD averages for 05/2018 - 12/2019

Even though HCHO maps over the U.S. are dominated by HCHO formed from biogenic isoprene emissions, the distribution over the Permian basin looks very similar to the NO_2 signal and could indicate formation from VOCs emitted by oil and gas production.

Deriving NOx Emissions with the Divergence Method

Motivation:

The divergence method was developed and optimized for NOx point source detection (Beirle et al., 2019). Here we investigate its suitability to derive NOx emissions from remote area sources like well pad fields.

Method:

Apply continuity equation assuming steady state (principle of conservation of mass):

The **Divergence, D,** of the **Flux, F,** yields the **emission sources, E,** and the **sinks, S,** of **NO_2**:

D: = ∇F = E-S with

F = NO_2 VCD * wind speed

S = NO_2 VCD / tau with

tau, NO_2 lifetime, based on first order loss to OH around 1:30pm local time in a well mixed boundary layer

- Tau = 1/k*[OH] ; OH: parameterized as linear function of J(O1D) based on Rohrer et al., 2006
- J(O1D): function of Solar Zenith Angle based on Master Chemical Mechanism (MCM) (SZA < 60°)
- k(OH-NO2): function of pressure and temperature (100m above ground) based on MCM
- NOx/NO_2 = 1.32 (Beirle et al, 2019)

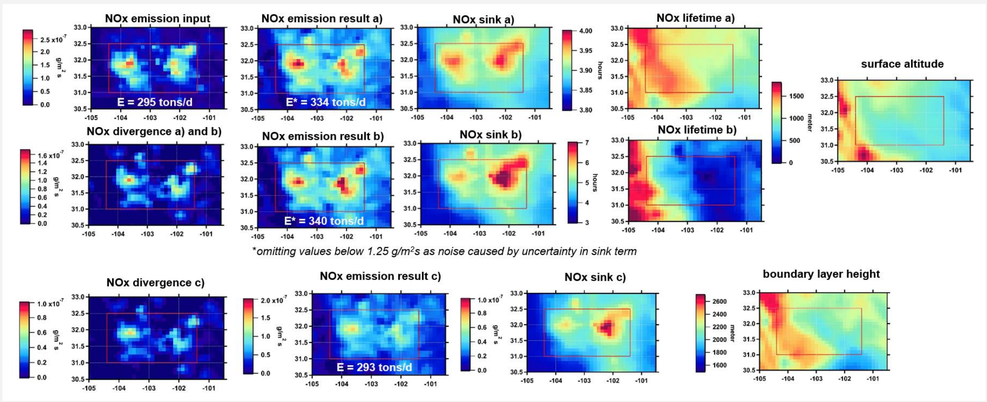
Simulation:

- WRF-Chem, the Weather Research and Forecasting Model coupled to Chemistry, provides synthetic data to test the suitability of the method for area sources.

Settings for WRF-Chem and TROPOMI:

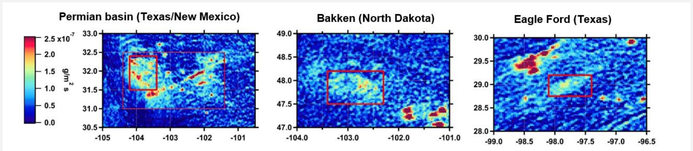
	WRF-CHEM (2018/06 – 2018/08)	TROPOMI (2018/05 – 2020/12)
NO_2	a) WRF-Chem Boundary Layer (BL) VCD average b) WRF-Chem BL VCD average c) WRF-Chem BL VCD average normalized by BL height	tropospheric VCD
Tau	a) as described above b) same as a), but using WRF-Chem OH at 100m above ground c) as described above	as described above

WRF-Chem simulation results:



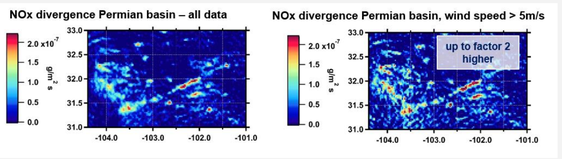
*omitting values below 1.25 g/m²s as noise caused by uncertainty in sink term

TROPOMI NOx emission results:

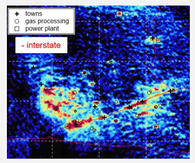


NOx emission [tons/day]		
	This work (% difference to FOG)	FOG
Permian basin	97 (+15%)	84
Eagle Ford	28 (-15%)	34
Bakken	73 (+22%)	60

Comparison with the Fuel-based Oil and Gas (FOG) NOx emission inventory (Negron et al., 2018).



The divergence term can be increased by up to a factor of 2 when filtering for high wind speeds.

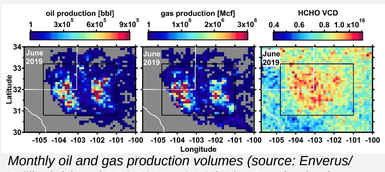


Filtering for and/or determining of other NOx sources within the Permian basin area is possible.

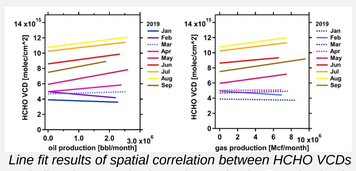
HCHO formation over the Permian basin

Motivation:

We detect elevated HCHO columns over the Permian basin during summer. Here we use TROPOMI HCHO observations in combination with WRF-Chem and MCM simulations to study if the satellite measurements are indicative of VOC emissions from oil and natural gas production.



Monthly oil and gas production volumes (source: Enverus/ Drillinginfo) and TROPOMI HCHO in the Permian basin.



Line fit results of spatial correlation between HCHO VCDs and oil and gas production volumes for the Permian basin.

The line fits show a positive correlation between April and September, as increases in photochemical activity yield HCHO amounts discernable from space. Lack of correlation in winter indicates a smaller contribution of direct HCHO emissions.

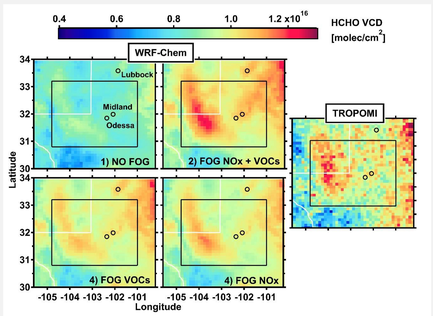
Method:

HCHO formation is investigated using 1) WRF-Chem and 2) 0D MCM Box modeling

Settings for WRF-Chem and 0D modeling:

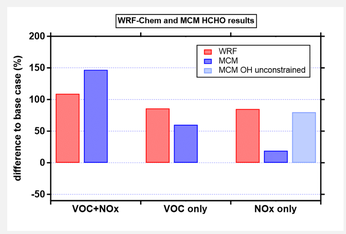
1) Base case: biogenic and anthropogenic NOx and VOC emissions
2) Base case + FOG: NOx emissions based on fuel consumption and scaled VOC emissions (Francoeur et al., 2021)
3) Base case + FOG VOC only *or* 4) + FOG NOx only

WRF-Chem results:



Comparison of HCHO WRF-Chem simulations with TROPOMI HCHO VCDs for July 10 - August 16, 2018. TROPOMI HCHO observations are best matched by including FOG NOx and VOC emissions.

Preliminary 0D modeling results:



Comparison of HCHO yields between WRF-Chem and 0D modeling. Initially the 0D model is run with OH constrained. The increased HCHO yield under high NOx conditions requires unconstrained OH to allow for radical recycling.

Conclusion

- Application of the divergence method on synthetic WRF-Chem data shows that the divergence method works in principle for area sources.
- Derived NOx emission results are affected by the definition of the NOx lifetime and by the effect of changing boundary layer heights on NO_2 VCDs.
- Application to TROPOMI data shows good agreement with the FOG inventory.

- TROPOMI HCHO observations are best reproduced by WRF-Chem runs with FOG NOx and VOCs emissions, indicating that HCHO formation from oil and natural gas VOC emissions can be significantly detected from space.
- Preliminary 0D modeling results indicate findings comparable to the WRF-Chem simulations, but further analysis is needed to investigate the effects of the different mechanism (explicit VOC reactions in MCM and grouped VOC reactions in WRF-Chem) and to asses the importance of individual VOCs for HCHO formation.

References and Acknowledgements

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Acknowledgements:

NASA ACMAP program, Colorado Energy Research Collaboratory
NOAA Cooperative Institute Agreement, Rocky Mountain Institute