Python Emission Localisation and Quantification (pyELQ)

Improving methane emission localisation and quantification through open sourcing

Bas van de Kerkhof, Matthew Jones, Rutger IJzermans

Definitions & cautionary note

Cautionary Note

The companies in which Shell plc directly and indirectly owns investments are separate legal entities. In this presentation "Shell", "Shell Group" and "Group" are sometimes used for convenience where references are made to Shell plc and its subsidiaries in general. Likewise, the words "we", "us" and "our" are also used to refer to Shell plc and its subsidiaries in general or to those who work for them. These terms are also used where no useful purpose is served by identifying the particular entity or entities. ''Subsidiaries'', "Shell subsidiaries" and "Shell companies" as used in this presentation refer to entities over which Shell plc either directly or indirectly has control. The term "joint venture", "joint operations", "joint arrangements", and "associates" may also be used to refer to a commercial arrangement in which Shell has a direct or indirect ownership interest with one or more parties. The term "Shell interest" is used for convenience to indicate the direct and/or indirect ownership interest held by Shell in an entity or unincorporated joint arrangement, after exclusion of all third-party interest.

Forward-Looking Statements

This presentation contains forward-looking statements (within the meaning of the U.S. Private Securities Litigation Reform Act of 1995) concerning the financial condition, results of operations and businesses of Shell. All statements other than statements of historical fact are, or may be deemed to be, forward-looking statements. Forward-looking statements are statements of future expectations that are based on management's current expectations and assumptions and involve known and unknown risks and uncertainties that could cause actual results, performance or events to differ materially from those expressed or implied in these statements. Forward-looking statements include, among other things, statements concerning the potential exposure of Shell to market risks and statements expressing management's expectations, beliefs, estimates, forecasts, projections and assumptions. These forward-looking statements are identified by their use of terms and phrases such as "aim"; "ambition"; ''anticipate''; ''believe''; "commit"; "commitment"; ''could''; ''estimate''; ''expect''; ''goals''; ''intend''; ''may''; "milestones"; ''objectives''; ''outlook''; ''plan''; ''probably''; ''project''; ''risks''; "schedule"; ''seek''; ''should''; ''target''; ''will''; "would" and similar terms and phrases. There are a number of factors that could affect the future operations of Shell and could cause those results to differ materially from those expressed in the forward-looking statements included in this presentation, including (without limitation): (a) price fluctuations in crude oil and natural gas; (b) changes in demand for Shell's products; (c) currency fluctuations; (d) drilling and production results; (e) reserves estimates; (f) loss of market share and industry competition; (g) environmental and physical risks; (h) risks associated with the identification of suitable potential acquisition properties and targets, and successful negotiation and completion of such transactions; (i) the risk of doing business in developing countries and countries subject to international sanctions; (j) legislative, judicial, fiscal and regulatory developments including regulatory measures addressing climate change; (k) economic and financial market conditions in various countries and regions; (l) political risks, including the risks of expropriation and renegotiation of the terms of contracts with governmental entities, delays or advancements in the approval of projects and delays in the reimbursement for shared costs; (m) risks associated with the impact of pandemics, such as the COVID-19 (coronavirus) outbreak, regional conflicts, such as the Russia-Ukraine war, and a significant cybersecurity breach; and (n) changes in trading conditions. No assurance is provided that future dividend payments will match or exceed previous dividend payments. All forward-looking statements contained in this presentation are expressly qualified in their entirety by the cautionary statements contained or referred to in this section. Readers should not place undue reliance on forward-looking statements. Additional risk factors that may affect future results are contained in Shell plc's Form 20-F for the year ended December 31, 2023 (available at www.shell.com/investors/news-and-filings/sec-filings.html and www.sec.gov). These risk factors also expressly qualify all forward-looking statements contained in this presentation and should be considered by the reader. Each forward-looking statement speaks only as of the date of this presentation, 19 November 2024. Neither Shell plc nor any of its subsidiaries undertake any obligation to publicly update or revise any forward-looking statement as a result of new information, future events or other information. In light of these risks, results could differ materially from those stated, implied or inferred from the forward-looking statements contained in this presentation.

Shell's Net Carbon Intensity

Also, in this presentation we may refer to Shell's "Net Carbon Intensity" (NCI), which includes Shell's carbon emissions from the production of our energy products, our suppliers' carbon emissions in supplying energy for that production and our customers' carbon emissions associated with their use of the energy products we sell. Shell's NCI also includes the emissions associated with the production and use of energy products produced by others which Shell purchases for resale. Shell only controls its own emissions. The use of the terms Shell's "Net Carbon Intensity" or NCI are for convenience only and not intended to suggest these emissions are those of Shell plc or its subsidiaries.

Shell's net-zero emissions target

Shell's operating plan, outlook and budgets are forecasted for a ten-year period and are updated every year. They reflect the current economic environment and what we can reasonably expect to see over the next ten years. Accordingly, they reflect our Scope 1, Scope 2 and NCI targets over the next ten years. However, Shell's operating plans cannot reflect our 2050 net-zero emissions target, as this target is currently outside our planning period. In the future, as society moves towards net-zero emissions, we expect Shell's operating plans to reflect this movement. However, if society is not net zero in 2050, as of today, there would be significant risk that Shell may not meet this target.

Forward-Looking non-GAAP measures

This presentation may contain certain forward-looking non-GAAP measures such as cash capital expenditure and divestments. We are unable to provide a reconciliation of these forward-looking non-GAAP measures to the most comparable GAAP financial measures because certain information needed to reconcile those non-GAAP measures to the most comparable GAAP financial measures is dependent on future events some of which are outside the control of Shell, such as oil and gas prices, interest rates and exchange rates. Moreover, estimating such GAAP measures with the required precision necessary to provide a meaningful reconciliation is extremely difficult and could not be accomplished without unreasonable effort. Non-GAAP measures in respect of future periods which cannot be reconciled to the most comparable GAAP financial measure are calculated in a manner which is consistent with the accounting policies applied in Shell plc's consolidated financial statements.

The contents of websites referred to in this presentation do not form part of this presentation.

We may have used certain terms, such as resources, in this presentation that the United States Securities and Exchange Commission (SEC) strictly prohibits us from including in our filings with the SEC. Investors are urged to consider closely the disclosure in our Form 20-F, File No 1-32575, available on the SEC website www.sec.gov.

Agenda

Background

Why are methane emissions worth reducing?

Why Methane Matters

- Methane is a powerful greenhouse gas; its impact on climate change over 20 years is more than 80 times greater than CO_2.
- Reducing emissions of methane is considered one of the most effective near-term actions to keep the more ambitious 1.5°C goal of the Paris Agreement within reach.
- Worldwide initiatives are taken to reduce global methane emissions.

- Shell has a target to maintain methane emissions intensity below 0.2% and achieve near-zero methane emissions by 2030.
- Shell has committed to the voluntary reporting framework OGMP2.0 under the flag of the United Nations Environmental Program, which aims to increase transparency and accuracy of methane emissions reporting.

METHANE GUIDING PRINCIPLES

AIMING FOR ZERO Methane Emissions Initiative

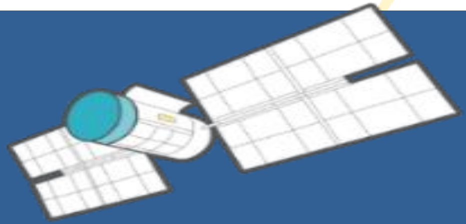
GMP Oil And Gas Methane Partnership 2.0

Some references

- Homepage | Global Methane Pledge
- Global Methane Tracker 2024 – Analysis – IEA
- The Oil & Gas Methane Partnership 2.0 (OGMP 2.0) | UNEP - UN Environment Programme
- Home - Aiming For Zero (ogci.com)
- Reduce Global Methane Emissions | Methane Guiding Principles
- Shell.com Methane

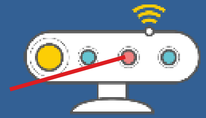
Overview of technologies for methane emission measurement

Source-level measurements



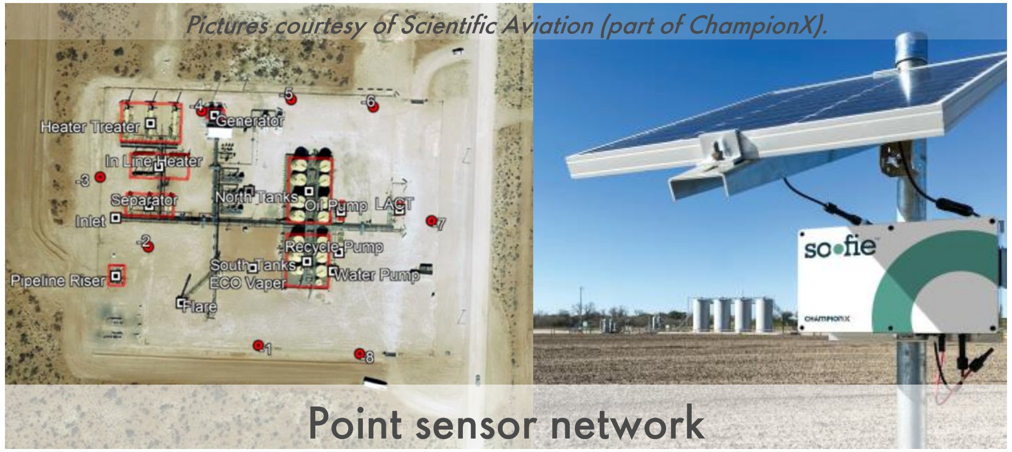
Satellites

Periodic surveys

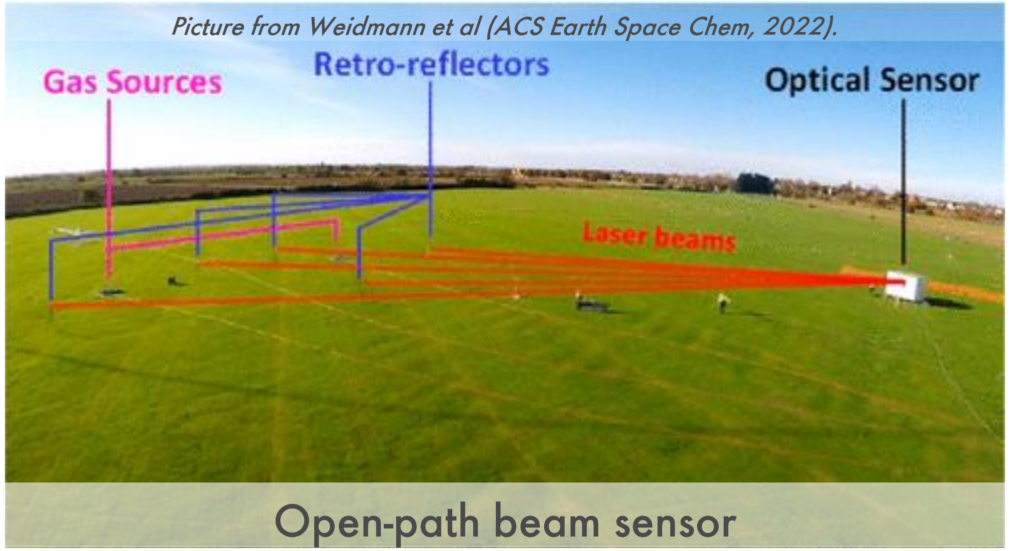


Continuous monitoring

Continuous monitoring technology



Point sensor network



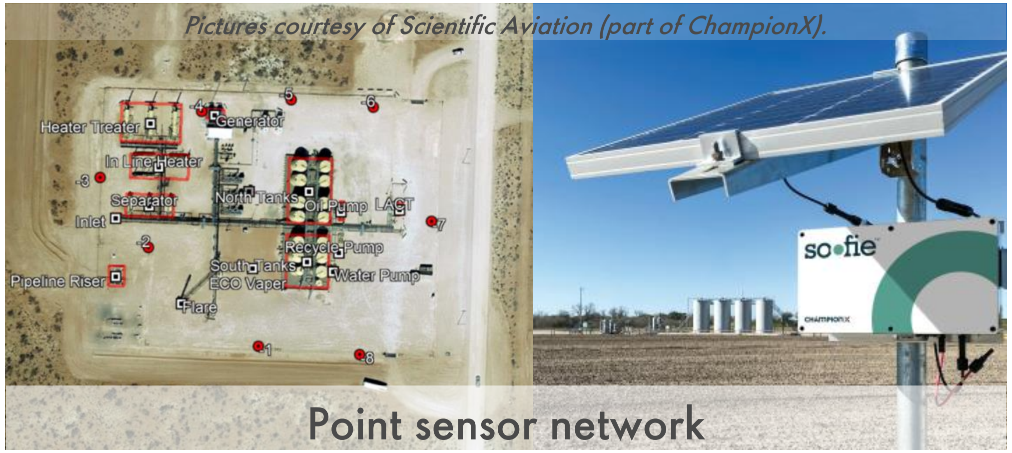
Open-path beam sensor


Infrared camera

Potential benefits of continuous monitoring systems:

- Early detection of unknown emissions (replacing or supporting Leak Detection and Repair campaigns)
- Quantification of time-varying emissions over long periods of time (continuous site-level measurement for OGMP2.0 L5)
- Demonstration of absence of emissions

Relevance of pyELQ for continuous monitoring technology

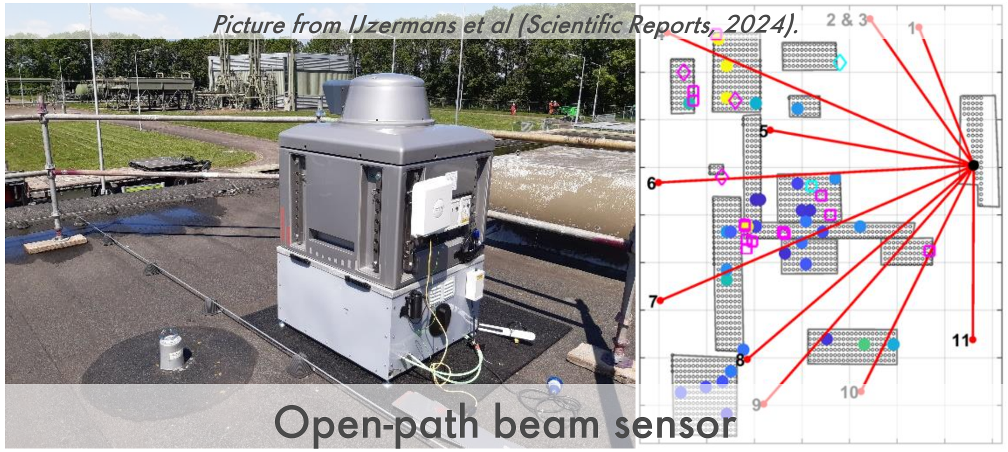


Pictures courtesy of Scientific Aviation (part of ChampionX).

Point sensor network

Multiple deployments:

- Remote processing facility
- Large manned processing facility
- Well pad during well completion operations
- Data analysis done with pyELQ, in addition to vendor's own methods



Picture from IJzermans et al (Scientific Reports, 2024).

Open-path beam sensor

Multiple deployments:

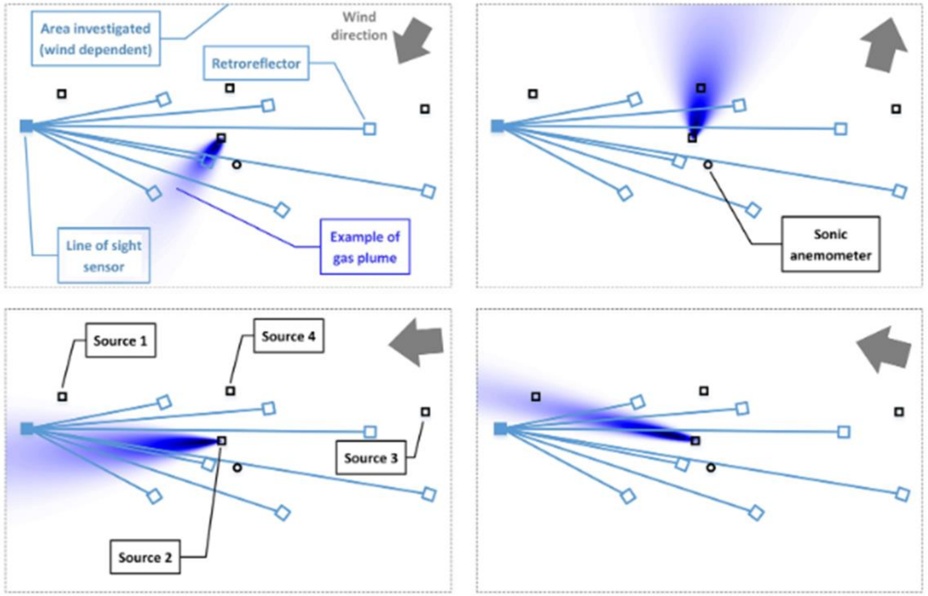
- Controlled release tests, in three campaigns
- Long-term deployment at medium-sized manned processing facility
- Data analysis done with pyELQ, results reported in IJzermans et al (Scientific Reports, 2024)

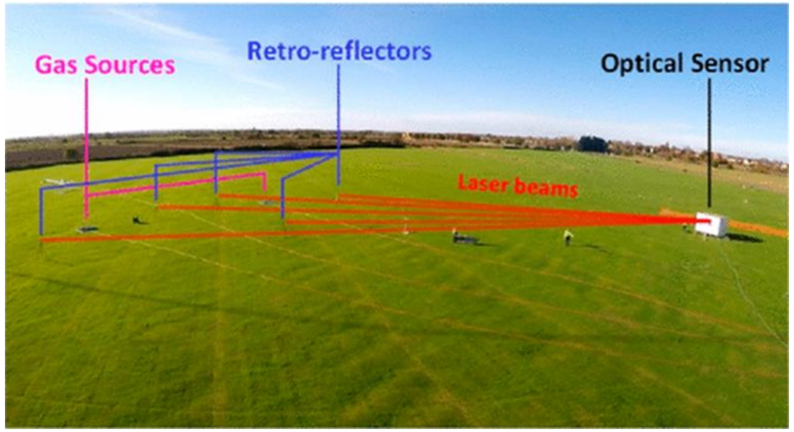
Technical details

The mathematics behind the code

Gaussian plume dispersion modelling

- To do inversion- need a model for mapping emissions at the source to concentration measurements at the sensor.
- We generally use the Gaussian plume model.
- Cross-section of the plume is a Gaussian density.
- Plume widens as it travels downwind, due to turbulent effects in the atmosphere.
- Figures taken from [Hirst et al, 2020]; [Weidmann et al, 2022].





Source emission rate

Concentration

$$c(x,y,z) = s \times a(x,y,z)$$

Plume coupling coefficient

Source height

$$a(x,y,z) = \frac{1}{2\pi u \sigma_h(x)\sigma_v(x)} \exp\left(-\frac{y^2}{2\sigma_h^2(x)}\right)\left[\exp\left(-\frac{(z-H)^2}{2\sigma_v^2(x)}\right) + \exp\left(-\frac{(z+H)^2}{2\sigma_v^2(x)}\right)\right]$$

Wind speed

Horizontal wind sigma

Vertical wind sigma

Bayesian Inversion

- The observed concentration values are represented using the following model:

$$\boldsymbol{y} = \boldsymbol{A}\boldsymbol{s} + \boldsymbol{b} + \boldsymbol{\epsilon}$$

- Components are as follows:
  - $\boldsymbol{y} = (y_1, y_2, \dots y_n)'$ is the vector of concentration observations (units: ppm).
  - $A = (A_{11}, A_{12}, \dots, A_{21}, \dots A_{ij}, \dots)$ is the matrix of Gaussian plume coefficients (units: 1e6 hr/kg)
  - $\boldsymbol{s} = (s_1, s_2, \dots s_m)'$ is the vector of source emission rates (units: kg/hr).
  - $\boldsymbol{b} = (b_1, b_2, \dots b_n)'$ is the vector of atmospheric background methane concentrations (units: ppm, typically around 1.9 - 2 ppm).
  - $\boldsymbol{\epsilon} = (\epsilon_1, \epsilon_2, \dots \epsilon_n)'$ is the vector of measurement error terms (units: ppm).
- Main task of the inversion: separate the local “spiky” source contributions from the smooth/slowly-varying background contributions.
- **Bayesian inversion**: posterior distribution is product of likelihood and prior distributions

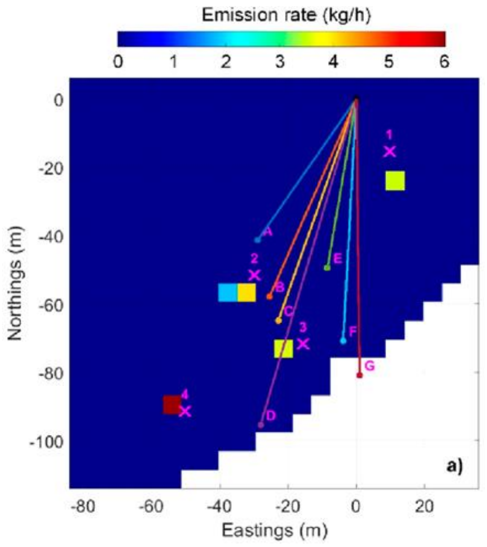
$$p(\boldsymbol{s}, \boldsymbol{b} | \boldsymbol{y}) \propto p(\boldsymbol{y} | \boldsymbol{s}, \boldsymbol{b}) \times p(\boldsymbol{s}) \times p(\boldsymbol{b})$$

- Can’t evaluate posterior parameter estimates directly- so we sample from the distribution using Markov Chain Monte Carlo (MCMC).

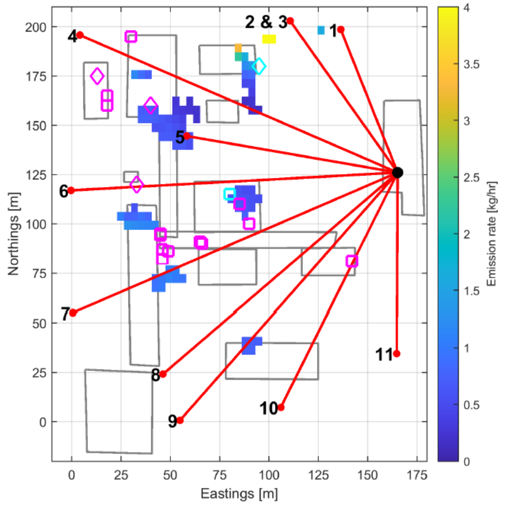
Inversion: source location information

- Two approaches to estimating source location implemented in the code:
  1. Fix source locations (e.g. on a grid at ground level), and switch off sources that don't fit the data well.
  2. Free source map, with locations estimated as part of the MCMC solver.
- In option 2, we use reversible jump MCMC to estimate number of sources & location simultaneously:
  - Create a new source in a random location (with a randomly-sampled emission rate).
  - Compute the prediction for the data with & without the extra source.
  - If adding the new source improves the fit to the data, we accept it (on average): otherwise, we reject.

  [With a similar process for removing sources.]



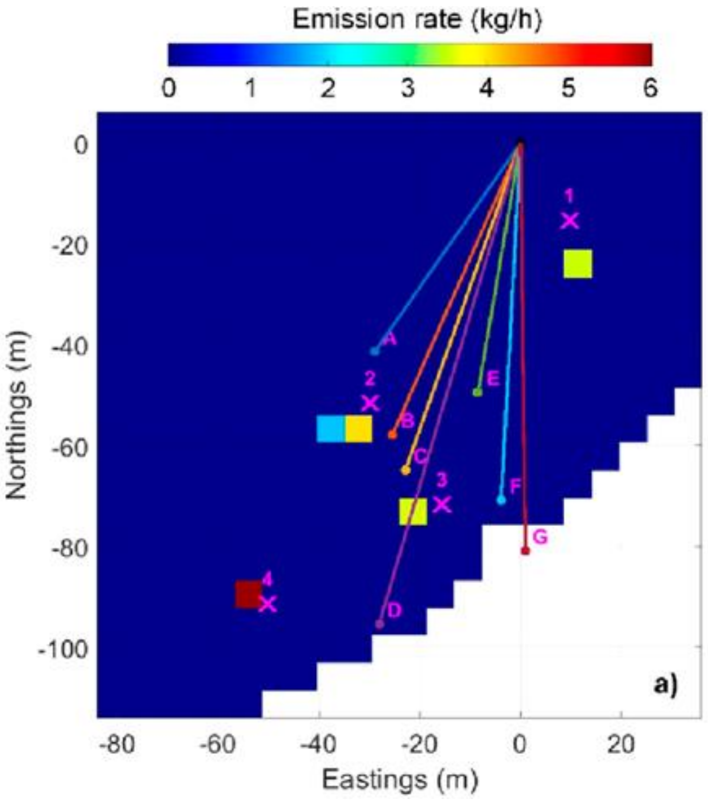
Gridded solution



Free (RJ) solution

Results in controlled release tests: open-path beam sensor

- Test with controlled releases at an empty airfield in the UK, with MIRICO prototype open-path beam sensor (Weidmann et al (ACS, 2022)).
- Four different, but simultaneously emitting methane sources of 3-5 kg/h were successfully detected, located and quantified, without a priori knowledge of number of sources, source location and magnitude – even for sources outside of the area covered by the beams.

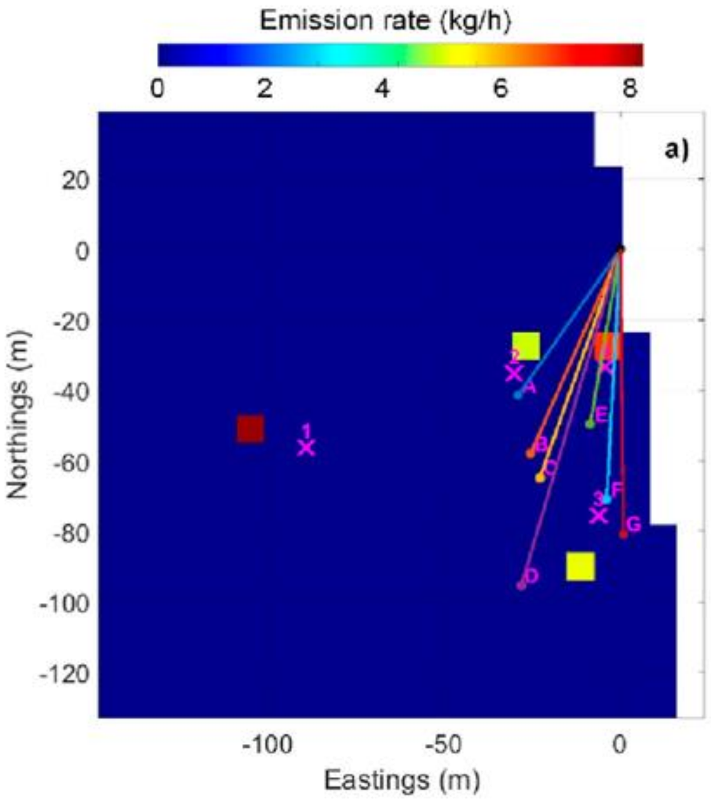


"known-known" case

source	actual rate(kg/h)	inferred rate(kg/h)	inferred to actual relative difference (%)
1	5.11 ± 0.12	3.5 ± 0.5	−31
2	5.03 ± 0.04	5.9 ± 0.9	+17
3	5.06 ± 0.06	3.6 ± 0.3	−29
4	5.06 ± 0.03	6.1 ± 0.5	+20

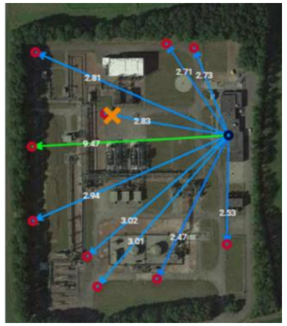
"unknown-unknown" case

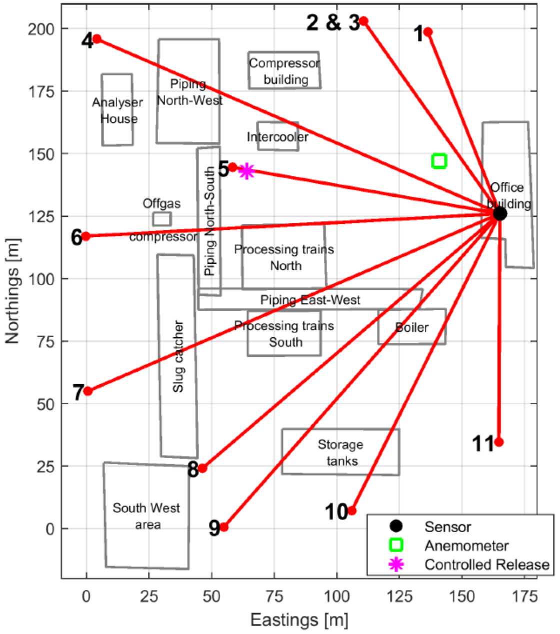
source	actual rate (kg/h)	inferred rate (kg/h)	inferred to actual rate relative difference
1	5.03 ± 0.04	8.7 ± 0.7	+73
2	5.03 ± 0.05	5.0 ± 0.3	−1
3	5.02 ± 0.07	5.2 ± 0.4	+4
4	5.04 ± 0.14	7.1 ± 0.5	+41

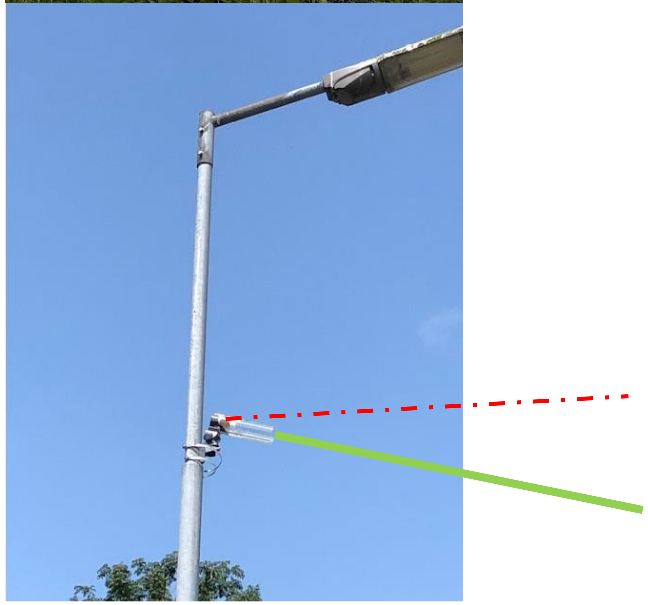


Test in oil & gas facility: open-path beam sensor (1/2)

- Test with MIRICO's first commercial open-path beam sensor at a gas compression and distribution facility
- Results reported in [IJzermans et al (Scientific Reports, 2024)]

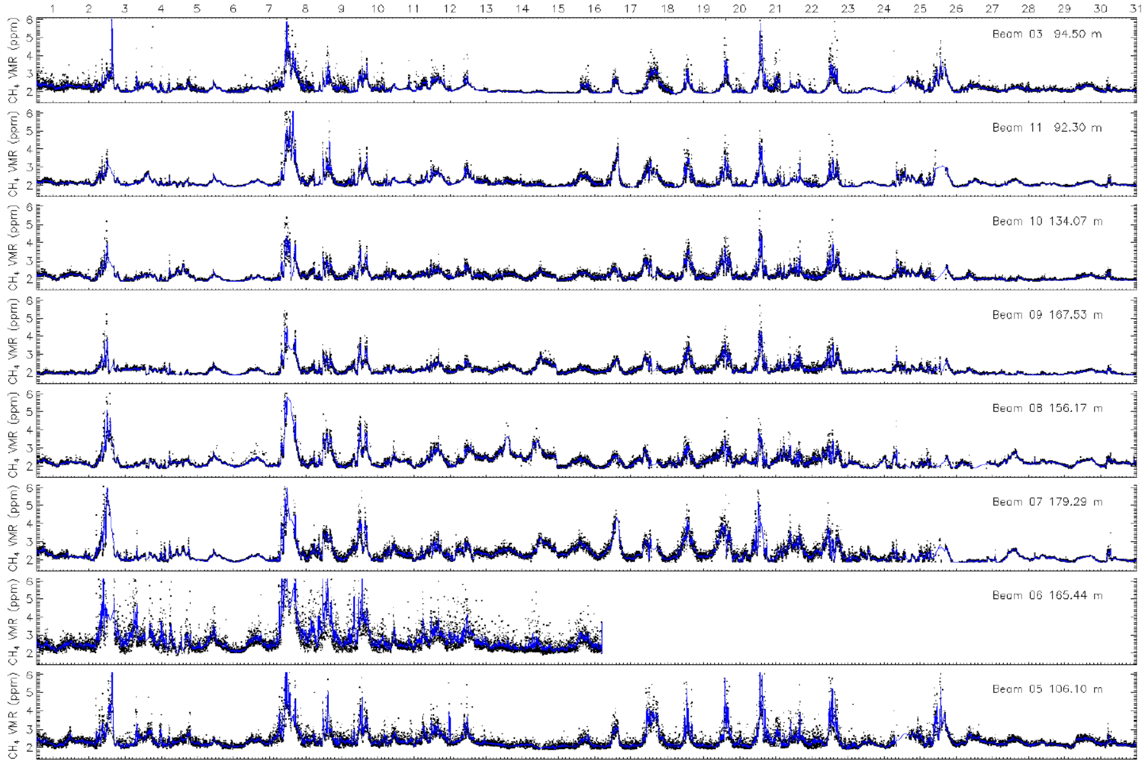




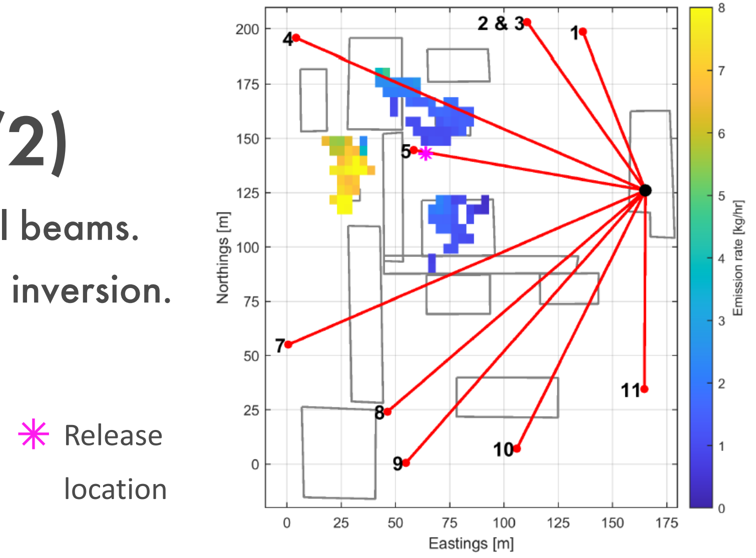


Test in oil & gas facility: open-path beam sensor (2/2)

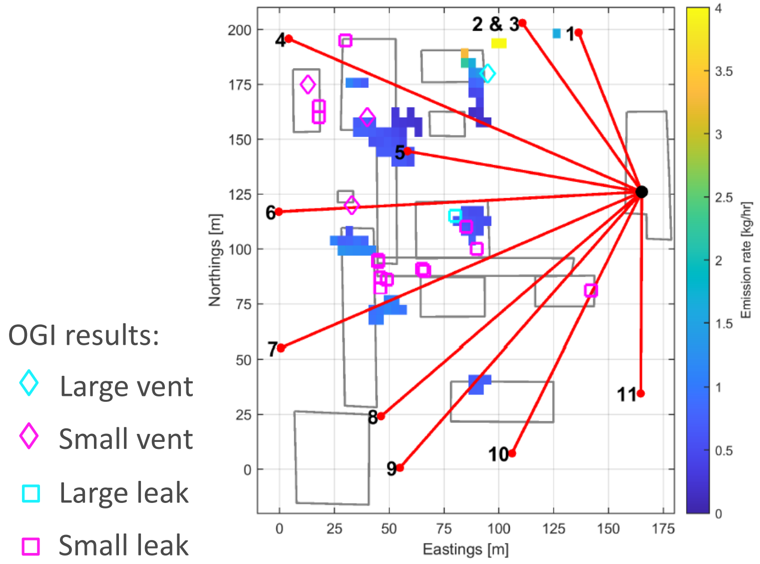
- Continuous (~2 min frequency) measurement of path-averaged CH_4 concentration along all beams.
- Peaks during the nighttime in background concentrations - probably related to temperature inversion.
- Data analysis performed on suite of short-term controlled releases (4x ~60 minutes).
- Persistent sources identified with data analysis over long time series; confirmed with OGI.



Time series for 1 month of methane concentration measurements.



Controlled release, 5 kg/h.



Persistent sources, ~5 kg/h total.

Open-sourcing pyELQ

Open-sourcing pyELQ through LFE

- pyELQ was open-sourced in SEDE Open on 14 February 2024. Link here: https://github.com/sede-open/pyELQ
- Motivation (why LFE):
  - Increase awareness of the functionality outside of Shell
  - Encourage collaboration with others working in the industry
  - Facilitating continuous improvement in the capabilities available for methane emissions quantification
  - Help to create transparency around approaches to methane emissions quantification
  - Potential value of these algorithms is “bigger” when open sourced

Code quality

- All code on Github: https://github.com/sede-open/pyELQ
- pyproject.toml
- PEP 8 coding standard with (automated) tools black and isort
- Docstrings in Google format, including typehinting
- Github actions: automate workflows, PR templates
- SonarQube, Mend, Github Advanced Security
- GH pages: https://sede-open.github.io/pyELQ/
- Packaging and upload to PyPi: https://pypi.org/project/pyelq-sdk/

Q&A

Back-up slides

Potential improvements to the code base

Allow combining fixed and variable source locations within the same solution (*New features/models*).	Allows users to specify fixed locations for known sources at a site, and then allow a free source map to fit any unknown source locations.
Implement options in the openMCMC back end for using jax.numpy package for calculations (*Improvements to existing functionality*).	JAX is a python package that can auto-generate gradients for functions (without them having to be implemented separately) and allows compilation of functions to give potential substantial speed-ups. Implementing JAX options for some of the functions (e.g. Gaussian plume, normal distribution) will give extra functionality, and reduce implementation time for other functionality that we want to add in future- for example: • Gradient-based sampling for source location (enables better source location sampling, less likely to get stuck). • Gradient-based sampling of plume dispersion parameters. • Maximum likelihood initialization routines.
Dispersion modelling with obstacles in the flow field (*New features/models*)	Add an extra dispersion model to the code- better able to handle non-constant wind directions, and to handle obstacles (e.g. buildings) in the flow field.