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Localization and Quantification of Trace-gas Fugitive Emissions Using a Portable Optical Spectrometer

E. J. Zhang[1], C. C. Teng[2], T. G. van Kessel[1], L. Klein[1], R. Muralidhar[1], C. Xiong[1], Y. Martin[1], J. S. Orcutt[1], M. Khater[1], L. Schares[1], T. Barwicz[1], N. Marchack[1], S. Kamlapurkar[1], S. Engelmann[1], G. Wysocki[2], N. Sosa[1], W. M. J. Green[1]

[1]IBM Thomas J. Watson Research Center, Yorktown Heights NY 10598

[2]Dept. Of Electrical Engineering, Princeton University, Princeton NJ 08540

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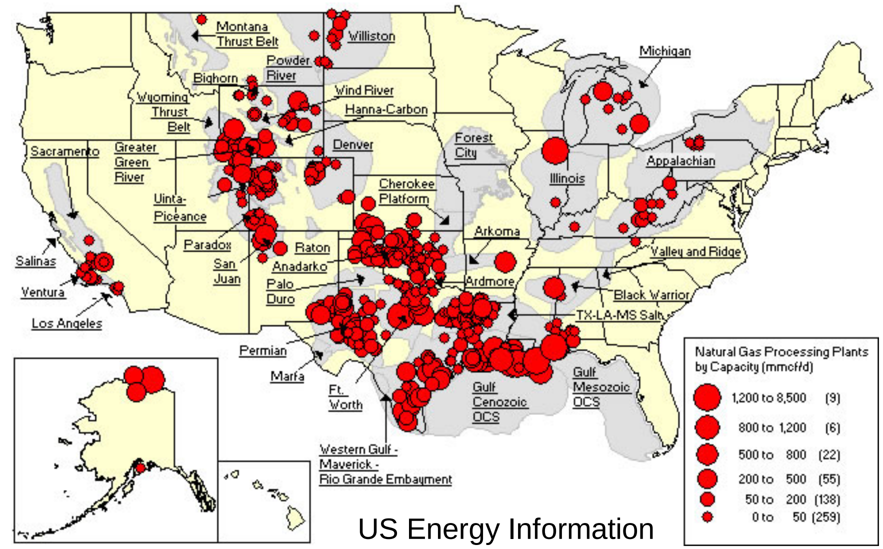
Presentation Outline

- Introduction
  - Motivation: CH_4 fugitive emissions monitoring
- Design and characterization of a portable TDLAS sensor
  - TDLAS sensor construction
  - Sensitivity analysis and chamber response time
- Field deployment at METEC CSU
  - Accuracy benchmark vs. MOX VOC sensors
  - AOA localization of CH_4 fugitive emissions
  - Source magnitude estimation (Gaussian plume / ML algorithms)
- Toward a next generation integrated photonic chip sensor
  - Initial results: on-chip evanescent field waveguide TDLAS
- Concluding remarks

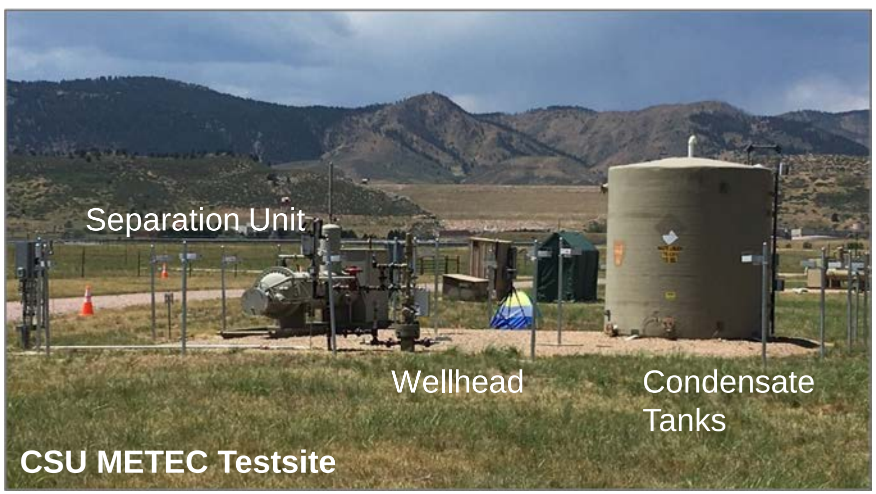
Motivation: CH_4 fugitive emissions monitoring

- > 500,000 active oil/gas wells in USA
- 570 × 10^9 ft^3 of CH_4 leakage in 2009, (59 % leaks during production phase)
- ~ 30% anthropogenic CH_4 emissions
- Radiative forcing of CH_4 is 37× greater than CO_2

Alvarez et. al., "Greater focus needed on methane leakage from natural gas infrastructure," Proc. Nat. Acad. Sci., 109 (17), pp. 6435-6440, (2012).



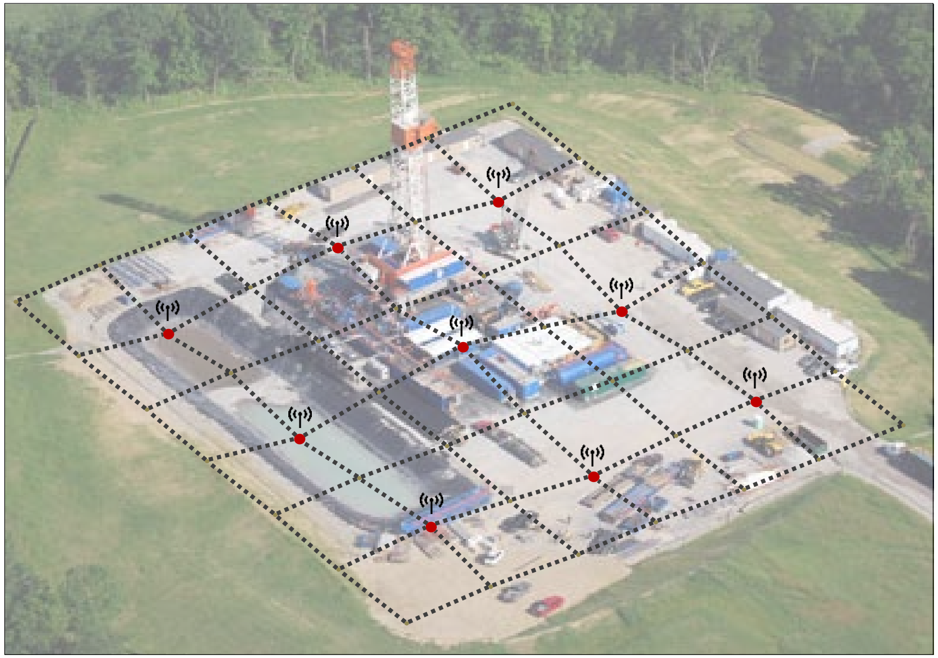
US Energy Information Administration



- CH_4 leakage rate on oil/gas well pad is 2-10% of total production!

Cost-effective sensor network for localization and precise quantification (ppmv-level) of CH_4 on oil and gas production well-pads

Use-case for innovative sensor networks



An Intelligent Multi-Modal Methane Measurement System (AIMS)

Technological driver: ARPA-E MONITOR

- Cost-effective sensor network for continuous CH_4 leak quantification, localization, and repair
- No viable technology today: Alignment of performance with required cost point poses significant challenge

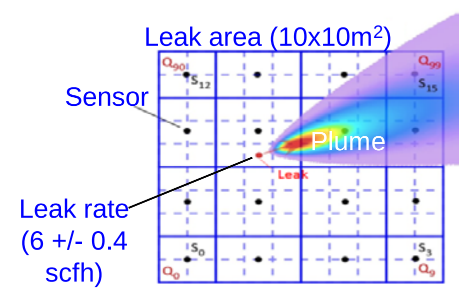
Opportunity driver: Application of physical analytics/IoT solutions to

- Significantly reduce fugitive CH_4 emissions across the oil and gas industry
- Improve production efficiency, safety, and compliance with emissions regulations
- Harness the full potential of natural gas as a clean fuel

Real-time sensor mesh network (IBM MMT System)

→ **Aggregate/push to Bluemix cloud (MQTT protocol)**

→ **Physical analytics:**
- source inference via inversion
- plume dispersion models
- machine-learned model blending



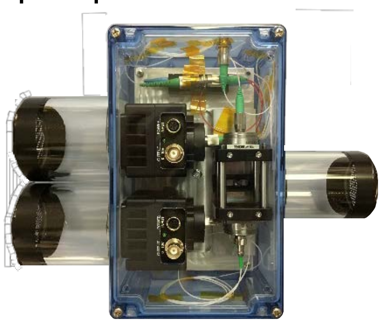
Use-case for innovative sensor networks

Metal-oxide (MOX):

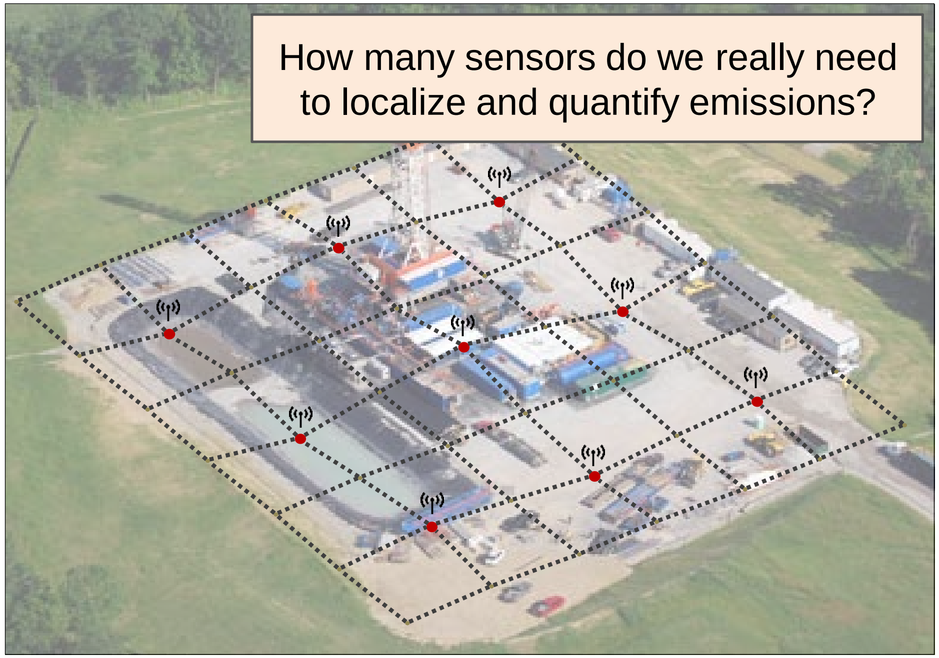
Figaro TGS2611

- Chemi-resistive sensor
- CH_4 adsorption (hot SnO_2)
- ppmv-level sensitivity
- ~10 USD / sensor
- Susceptible to other VOCs
- Ruggedized enclosure

Open-path TDLAS:



- Conventional NIR TDLAS
- < 5k USD / sensor
- **Intermediate SWaP-C compromise + benchmark IOS-TDLAS performance**



An Intelligent Multi-Modal Methane Measurement System (AIMS)

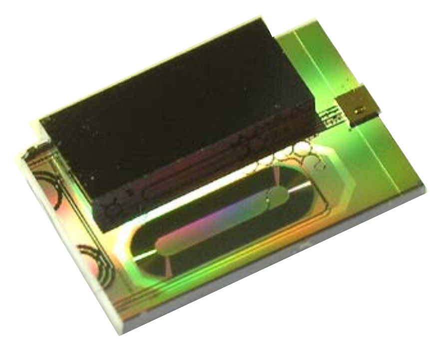
- Robust sensors to withstand harsh environments
- Low size, weight, power, and cost (SWaP-C)
- Species selectivity + sensitivity (DL < 10 ppmv)
- Lightweight data packaging on each WSN node for wireless connectivity and real-time analytics

Cavity-ringdown (CRDS):

Picarro G2308

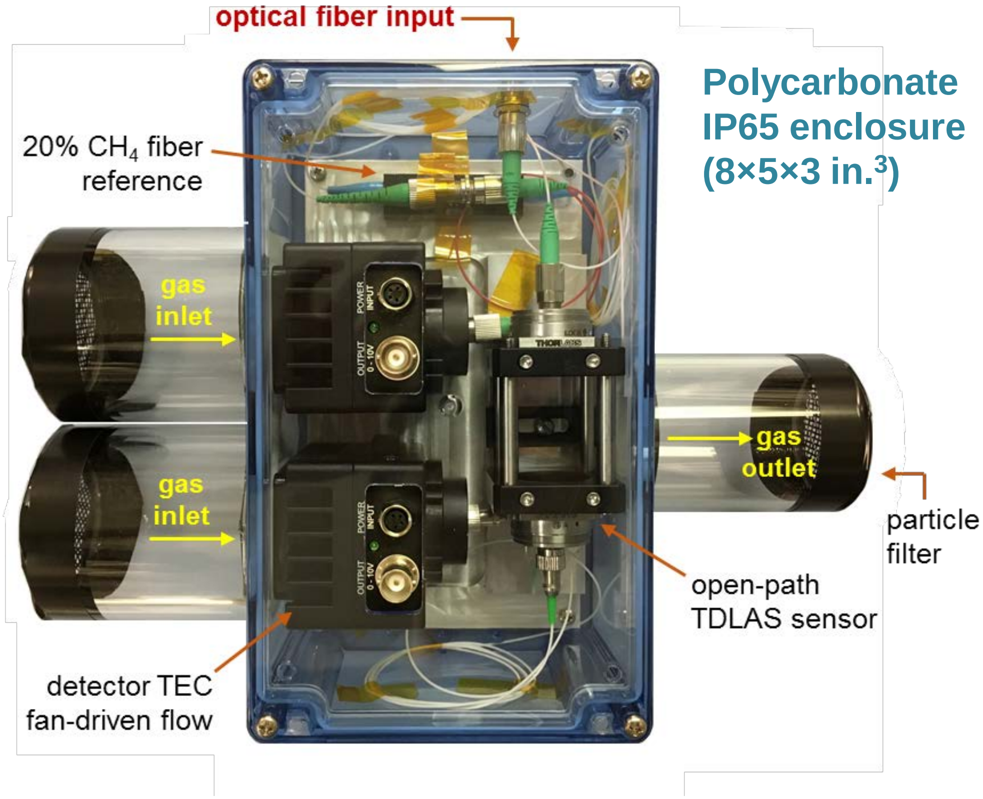
- Cavity-enhanced absorption
- < 10 ppbv sensitivity
- Dynamic range: (200 ppmv)
- 60 lbs, power: ~250 W
- Requires vacuum pump
- ~50k USD / sensor

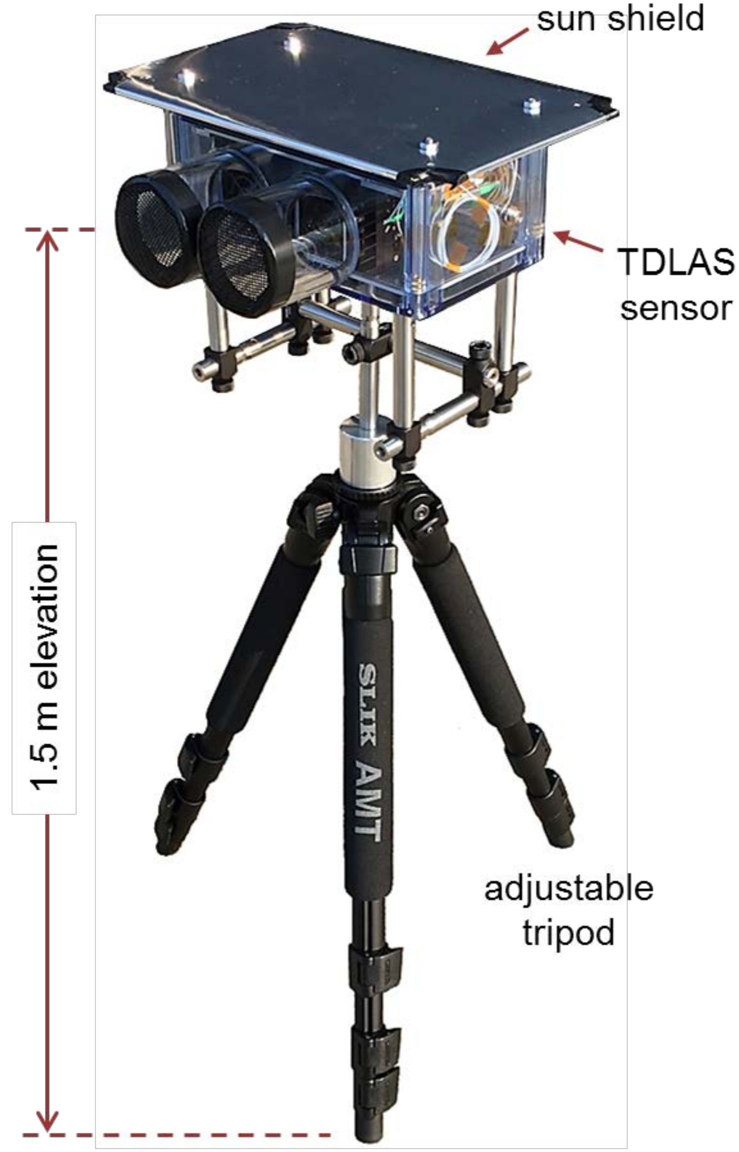
Integrated chip sensor:



- Integrated optical sensor TDLAS (IOS-TDLAS)
- Low-volume cost (< 250 USD)
- Sensitivity: 6.3 ppmv·$Hz^{-1/2}$

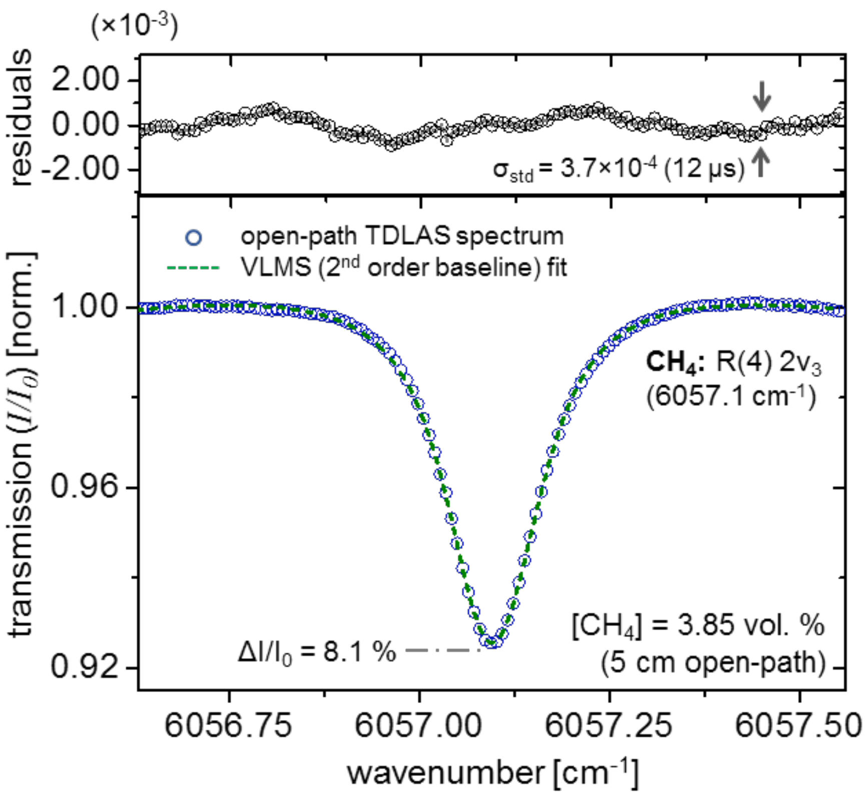
Portable TDLAS sensor construction

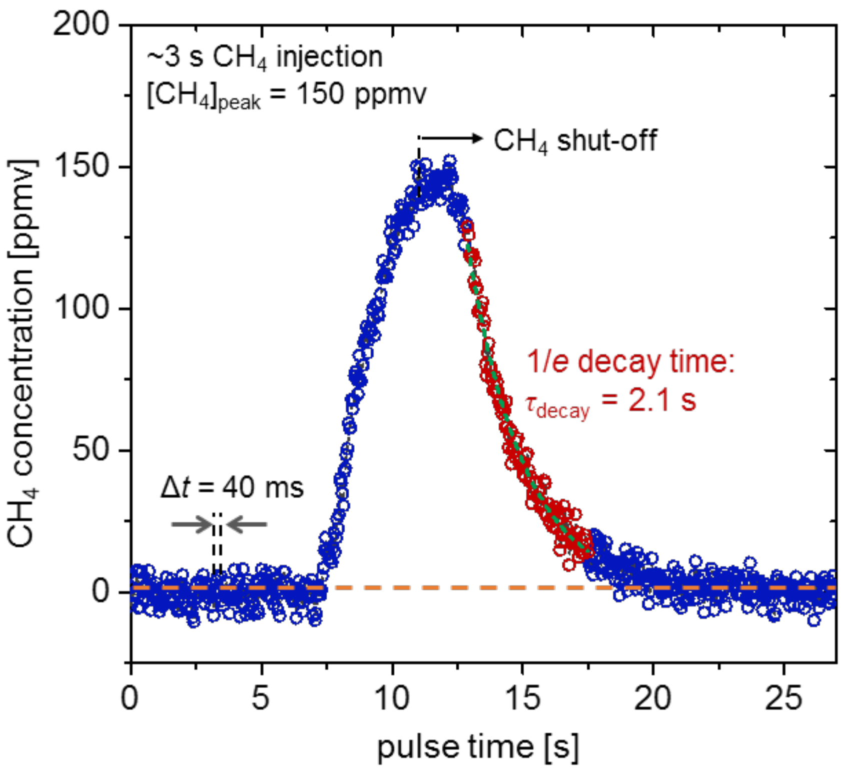




- 5 cm open-path fiber-coupled cell (TDLAS)
- Parallel (3 cm) 20 vol. % CH_4 (λ reference)
- Dual InGaAsP photodetector TEC fans for gas exchange in chamber

CH_4 spectra and chamber response time





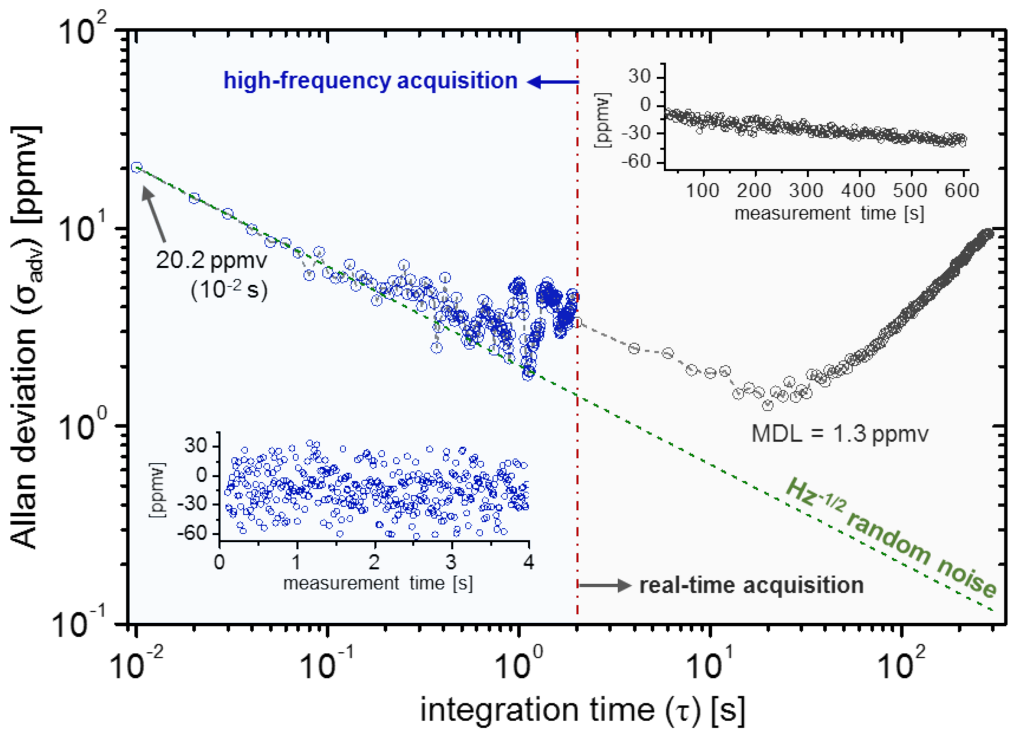
$2\nu_3$ CH_4 R(4) spectra at 6057.1 cm^{-1} (1651 nm)

- Alignment optimized + AR lens for fringe reduction
- Voigt nonlinear regression with 2nd order baseline
- 2 ms spectral acquisition (500 Hz laser ramp)
- Residual deviation: α_{min} = 6.5×10^{-7} cm^{-1}·$Hz^{-1/2}$

Chamber response time

- ~3 s release (1.0 vol. %) → 150 ppmv CH_4
- 40 ms measurement resolution
- 90% to 10% → 2.1 s (1/*e* decay time)
- Typical CH_4 peak: ~20 s (field measurements)

Laser ramp-rate for optimized sensitivity

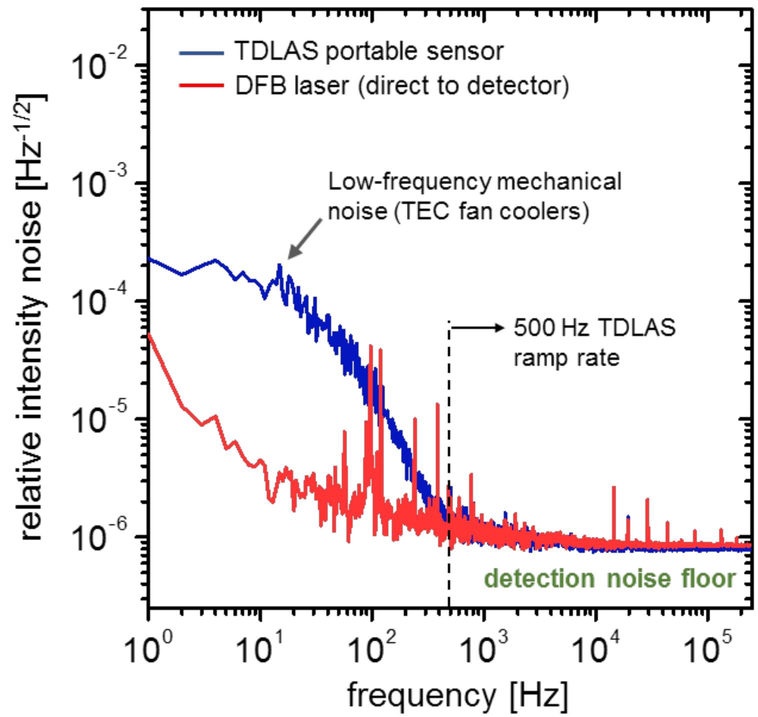


Detection sensitivity:

σ_{adv} = 2.0 ppmv · $Hz^{-1/2}$

Min. fractional absorption:

$(\alpha L)_{min}$ = 4.5×10^{-6} $Hz^{-1/2}$



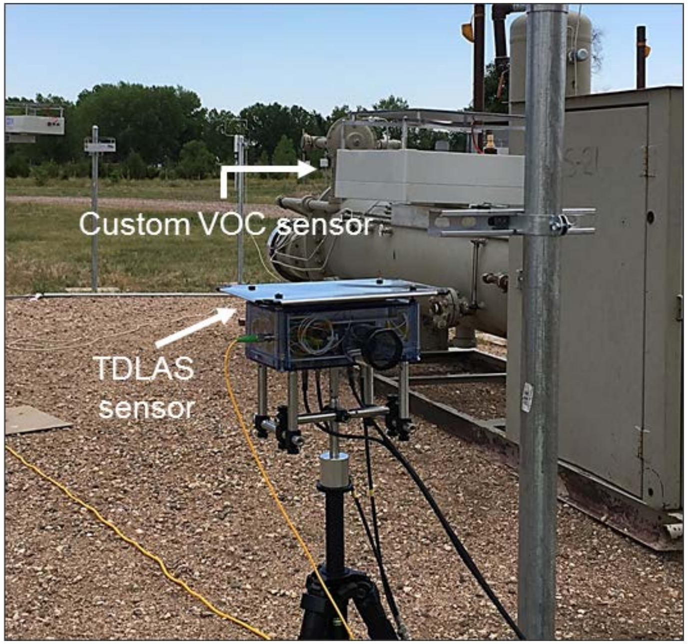
TDLAS sensor Allan-deviation and RIN analysis:

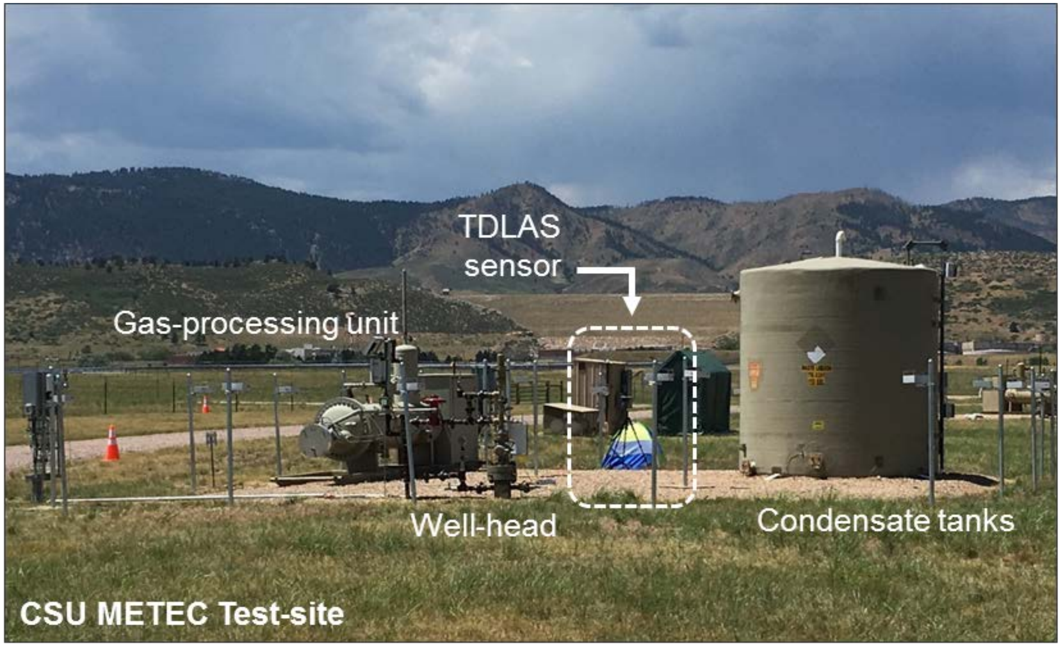
- High-frequency (2 ms) and real-time (2 s) operation
- Low-frequency noise (< 500 Hz) due to fan-cooled TECs for InGaAsP photodetectors
- Laser f_{ramp} = 500 Hz to avoid low-frequency noise
- NEP = 7.2×10^{-10} W·$Hz^{-1/2}$ (100 kHz) → sensor operates at 2.2× detection noise floor

Field deployment at the METEC facility (CSU)

Methane Emissions Technology Evaluation Center (METEC) field deployment:

- 5-day deployment (July 17-21, 2017): 16.6 hours CH_4 data
- 4.4 hours control, 12.2 hours blind (1.9 hours CH_4 data)
- Blind measurements: TDLAS sensor not always downwind
- TDLAS sensor co-located with a customized VOC MOx sensor for accuracy benchmark



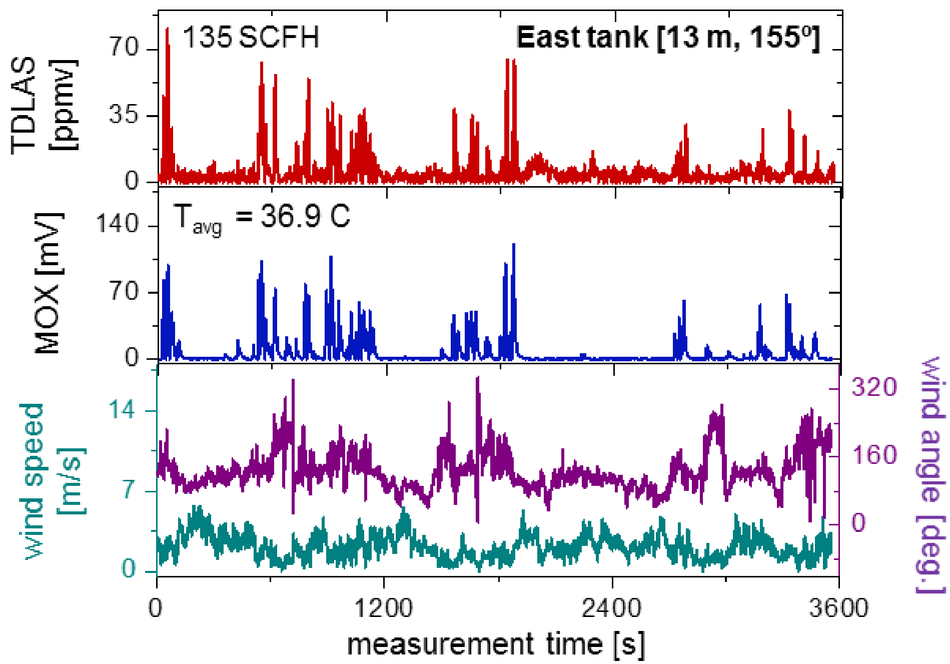


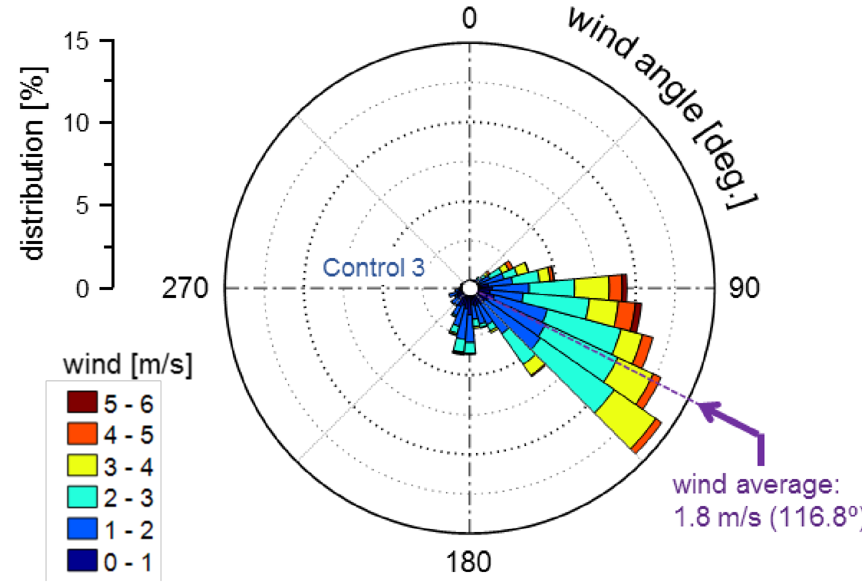
Experimental Configuration:

- Control: 68 SCFH – 135 SCFH
- Blind: 0 SCFH – 40 SCFH
- Concurrent anemometer measurement

Goal: single-sensor source AOA and magnitude estimation

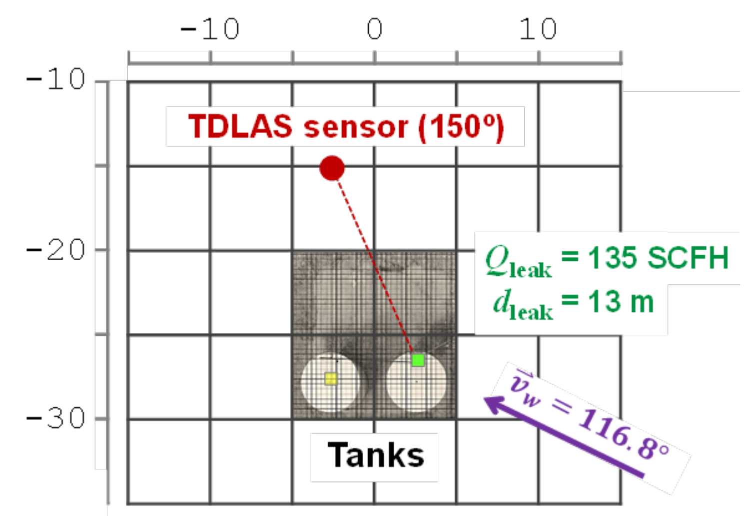
Control experiment: tank CH_4 release





Concurrent TDLAS / MOX / anemometer data:

- Downwind placement of TDLAS sensor (150° LoS)
- 1 hour measurement, 2 s time-resolution (TDLAS/MOX)
- East tank thief hatch (13 m, 135 SCFH) control CH_4 leak
- Good visual correspondence between TDLAS/MOX units
- Real-time acquired temperature (MOX unit thermistor)



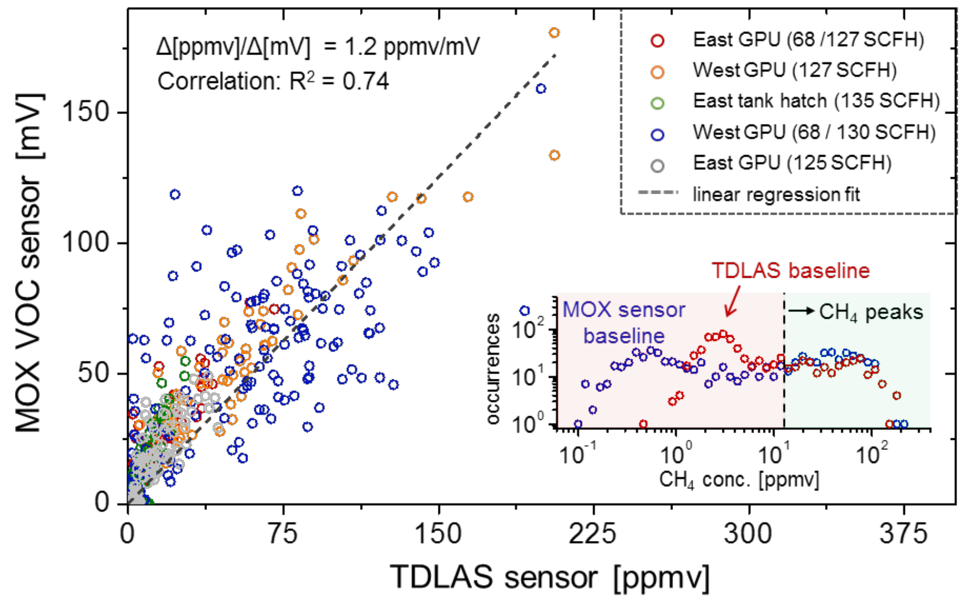
CH_4 retrieval and TDLAS/MOX comparison

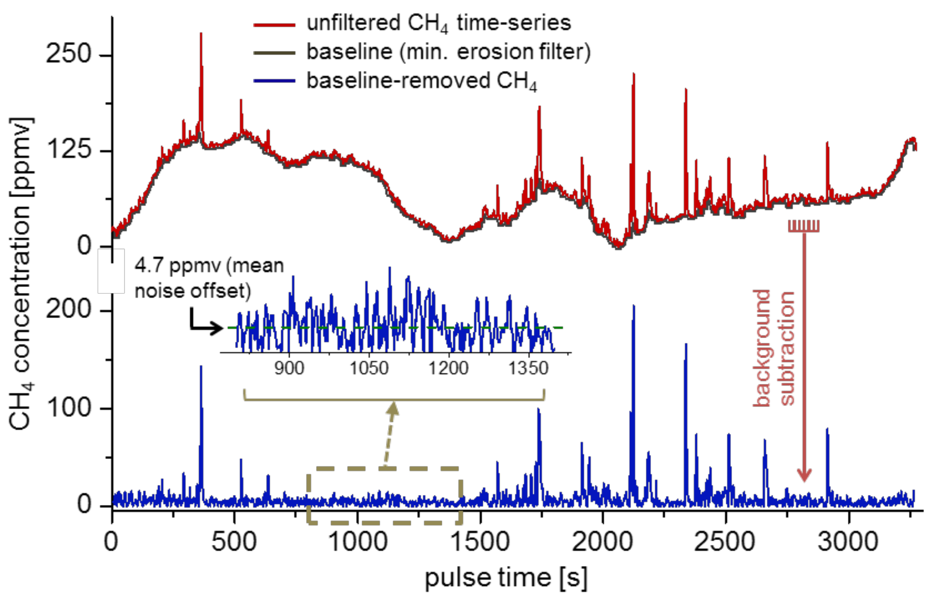
Real-time CH_4 retrieval:

- 500 Hz line-scan rate, VLMS (2 s resolution)
- Account for temperature dependent:
  - i. transition line-strength $S_{\eta\rightarrow\eta'}(T)$
  - ii. air-broadening coefficient $\delta\nu_L(p,T)$
- Post-analysis baseline erosion:

$$[CH_4](t_i) \rightarrow [CH_4](t_i) - \min_{t_i \in B_i}[CH_4](t_i)$$

$$B_i = \left\{ \lfloor t_i/T_B \rfloor \cdot T_B \le t < \left(\lfloor t_i/T_B \rfloor + 1 \right) \cdot T_B \right\}$$

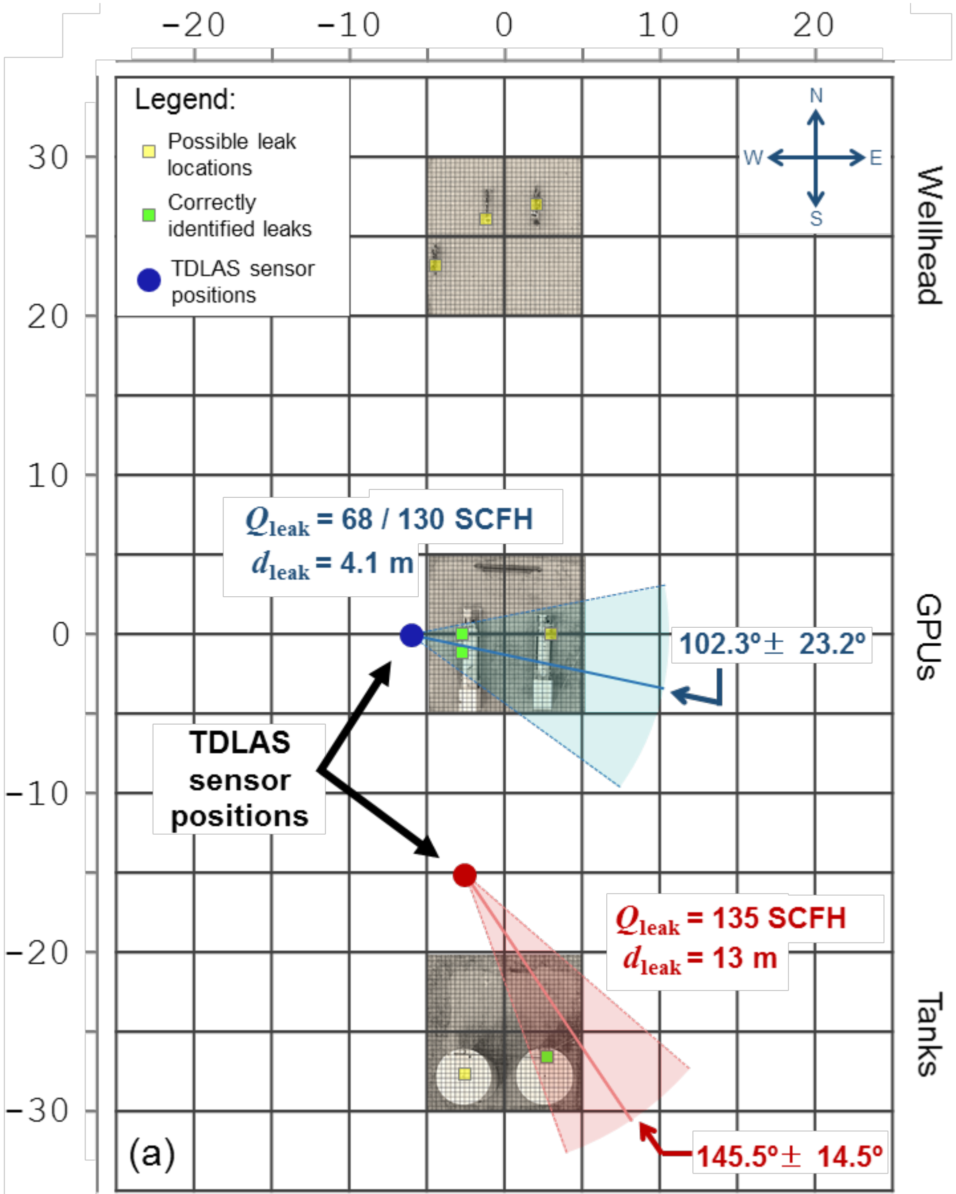




TDLAS / MOX sensor comparison:

- 5 Control experiments (4.4 hours), spans leak rates 68 – 135 SCFH
- TDLAS sensor placed downwind from leak
- Good R^2 correlation (0.74); non-ideal orientation
- Erosion noise floor peak: ~ 3 ppmv (consistent with Allan-deviation sensitivity)
- TDLAS/MOX sensor agrees for $[CH_4] > 12$ ppmv

Determining emission source location

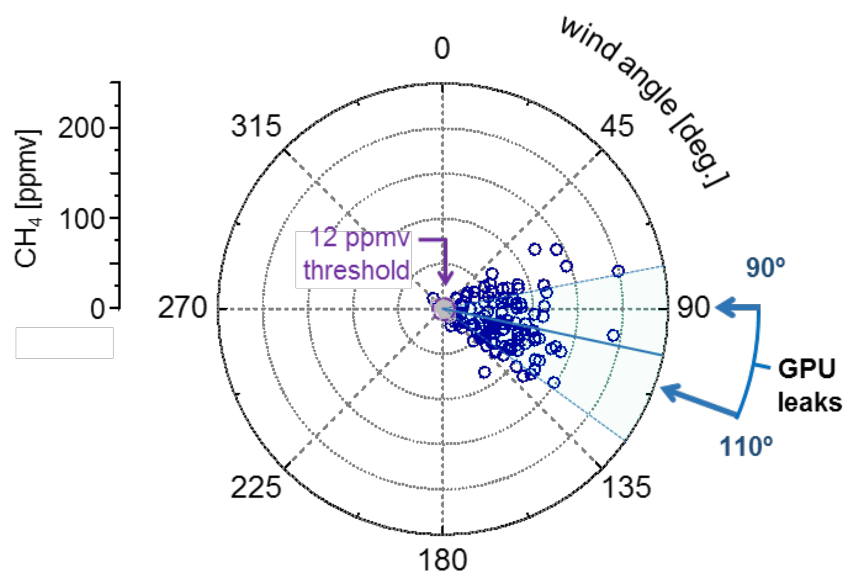


Leak angle-of-arrival (AOA) localization:

- Bin data in 20 s intervals; 12 ppmv threshold
- Correlate wind angles with CH_4 concentrations

$$\langle \alpha_{AOA} \rangle = \frac{\sum_i [CH_4](t_i) \cdot \varphi_i}{\sum_i [CH_4](t_i)}, \quad \varphi_i = \tan^{-1}\left(\frac{\boldsymbol{v}_x}{\boldsymbol{v}_y}\right)$$

- Single-sensor can only determine AOA, need ≥ 2 sensors for true localization



Summary of METEC field test results

Experiment	Leak duration	Leak component	Flow rate (SCFH)	Leak location [distance, angle]	Average wind-velocity $\langle v_w \rangle$	Leak AOA $\langle \alpha_{AOA} \rangle \pm \delta\alpha_{AOA}$
Control 1	3554 s	East GPU (Pad 3)	68/127	9.0 m (90°)	1.96 m/s (137.2°)	102.3° ± 22.0°
Control 2	1757 s	West GPU (Pad 3)	127	4.1 m (90°,110°)	2.60 m/s (125.6°)	109.9° ± 24.1°
Control 3	3553 s	East tank (Pad 3)	135	13.0 m (155°)	1.77 m/s (116.8°)	145.5° ± 14.5°
Control 4	3552 s	West GPU (Pad 3)	68/130	4.1 m (90°,110°)	1.58 m/s (97.0°)	102.3° ± 23.2°
Control 5	3459 s	East GPU (Pad 3)	125	9.0 m (90°)	2.80 m/s (61.6°)	82.6° ± 13.2°
Blind 1	3442 s	Tank (Pad 1)	36.1	3.4 m (60°)	0.58 m/s (68.9°)	76.3° ± 53.6°
Blind 2	3470 s	Wellhead (Pad 2)	4.4	6.9 m (125°)	1.41 m/s (124.8°)	119.3° ± 25.2°

Calculated source angle-of-arrival (AOA) for single-sensor "localization":

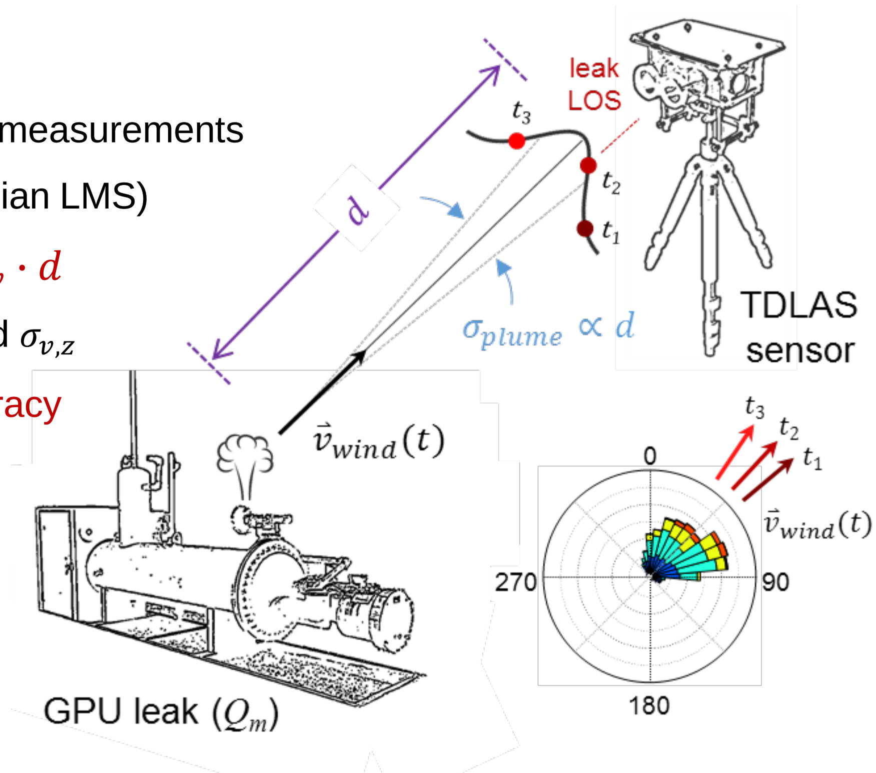
- Total 6.3 hours control + blind CH_4 release (85 % CH_4, 10.2 % C_2H_6, 0.7 % C_3H_8)
- AOA consistent with known source-detector line-of-sight (LoS), and downwind of CH_4 leak
- Single-sensor cannot distinguish between two leaks along a single LoS → choose placement wisely
- Can we estimate the source magnitude from a single sensor?
- Extract the shape of the plume for modeling (multiple sensors)

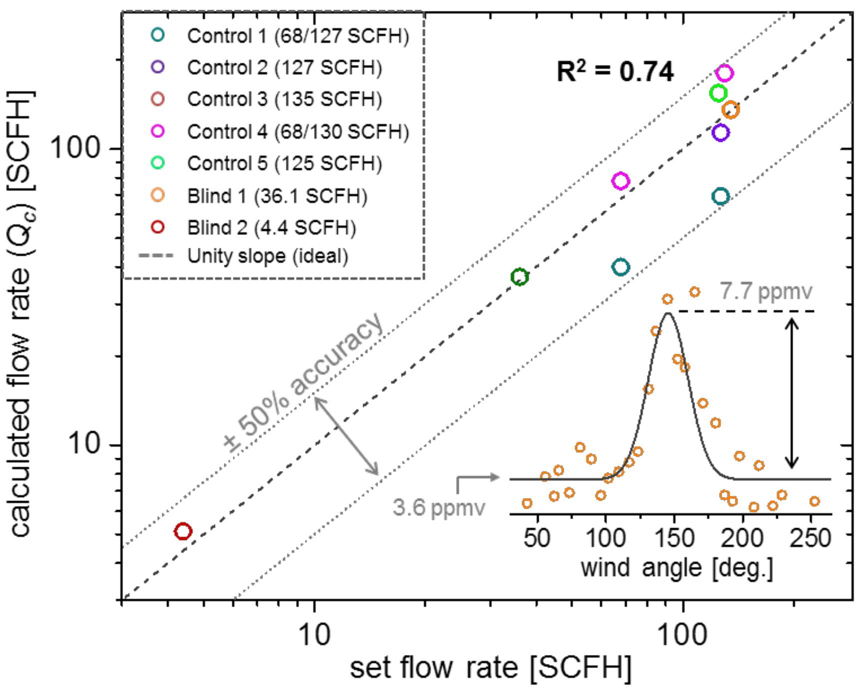
Need plume profile information
→ **use wind variability**

Single-sensor source magnitude estimation

Parametrized Gaussian plume model:

- Plume reconstruction from $\vec{v}_w$ variation in short-term measurements
- Identify nominal LoS CH_4 peak concentration (Gaussian LMS)
- d << D_L (Lagrangian integral dist. ~ 10^2 m) → $\sigma = \sigma_v \cdot d$
- Optimization (i.e. "calibration") of dispersions $\sigma_{v,y}$ and $\sigma_{v,z}$
- Training data shows Q_c agreement within 50 % accuracy



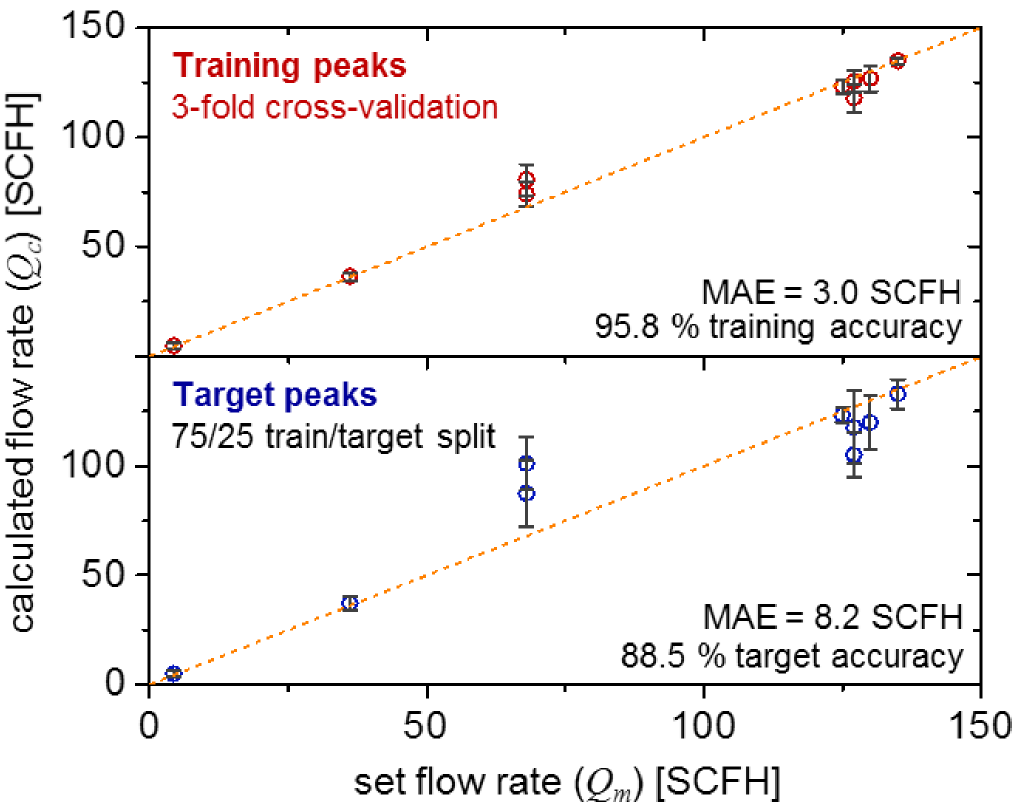


$$Q_c = \kappa \cdot (2\pi \cdot \sigma_{v,y} \cdot \sigma_{v,z}) \cdot \frac{[CH_4](\mathbf{r}_s) \cdot \langle |\mathbf{v}_w| \rangle \cdot d^2}{\zeta(z_s, H, \sigma_{v,z} \cdot d)}$$

$$\zeta = \exp\left[-\frac{(z-H)^2}{2(\sigma_{v,z} \cdot d)^2}\right] + \exp\left[-\frac{(z+H)^2}{2(\sigma_{v,z} \cdot d)^2}\right]$$

Calculated emissions flux (Q_c)

Source estimation using ML models



- Random-forest model accuracy: ± 8.2 SCFH (target MAE) → 88.5 % Q_c accuracy
- Top features (d, $[CH_4]$, $\vec{v}_w$) consistent with GP model:

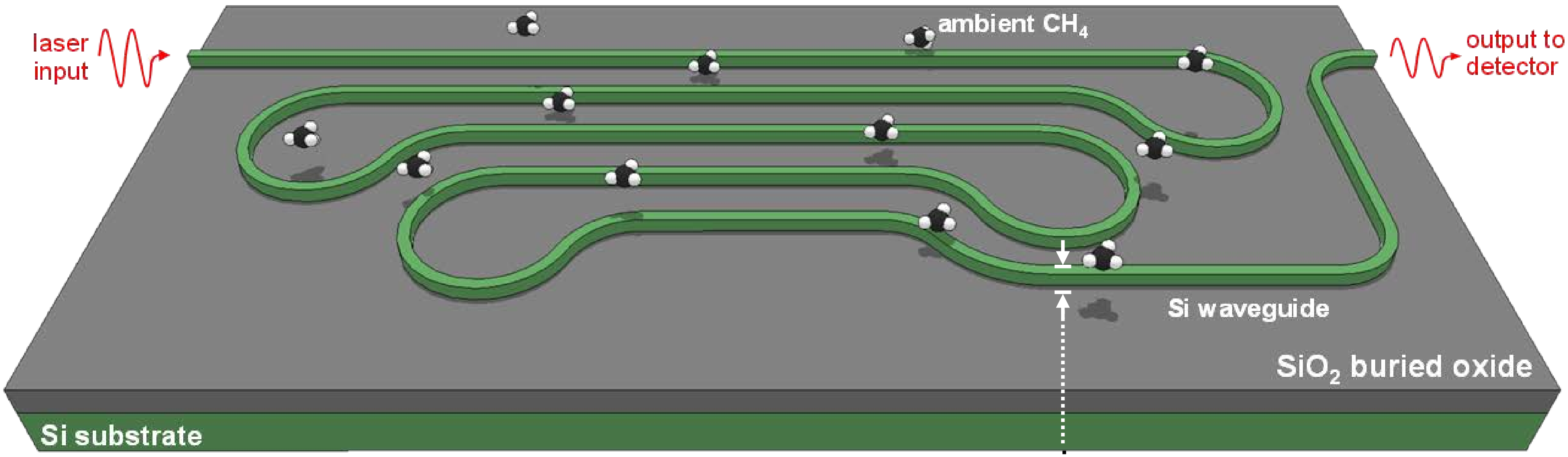
Flow rate: $$Q_c \propto [CH_4](\mathbf{r}_s) \cdot \langle |\vec{\mathbf{v}}_w| \rangle \cdot d^2$$

RF-based supervised learning:

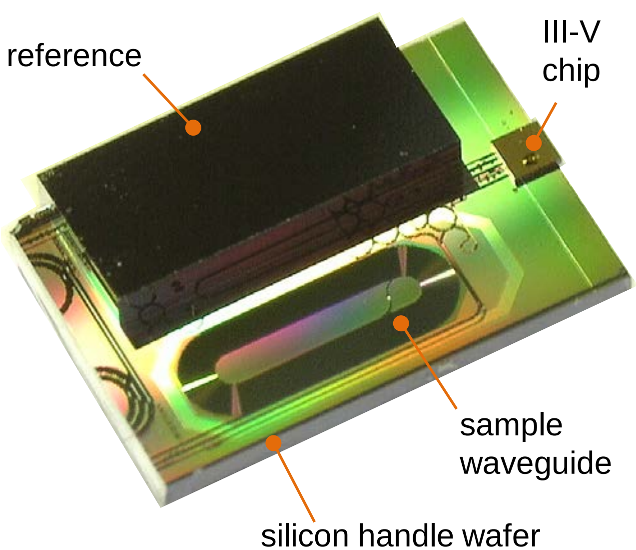
- Random-forest (RF) regressor model, 75/25 training-to-test split ratio
- Supervised training (20 s CH_4 data input bins), 3-fold CV w/ randomized HP optimization

Feature	Relative Significance [%]
Source distance	56.0 ± 6.6
CH_4 amplitude	20.9 ± 11.1
Wind speed (max.)	10.9 ± 10.2
Wind angle (rel.)	5.0 ± 1.1
Wind speed (avg.)	3.9 ± 5.8
Wind angle (abs.)	1.8 ± 0.8
Wind speed (dev.)	1.6 ± 0.6

Silicon photonic chip sensor design



Integrated photonic chip sensor

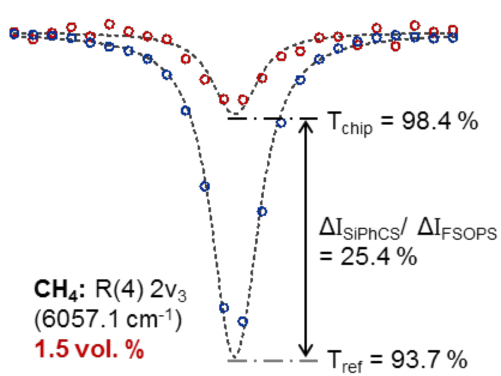


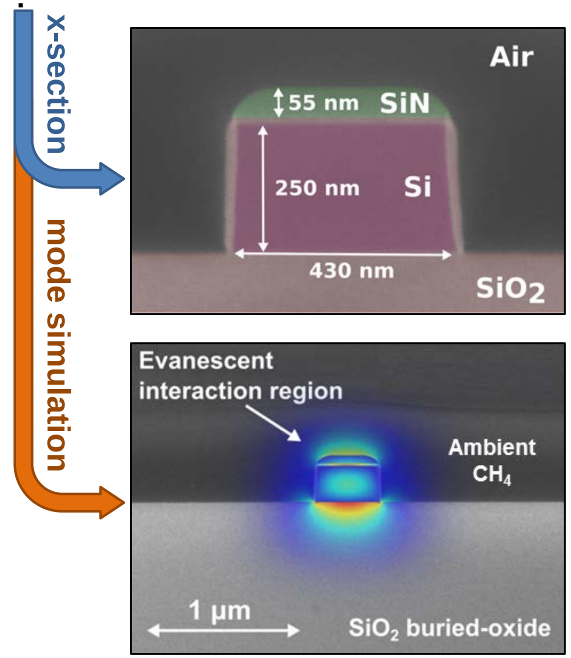
Detection sensitivity:

σ_{adv} = 6.3 ppmv · $Hz^{-1/2}$

Noise-equivalent absorp:

$(\alpha L)_{min}$ = 3.3×10^{-5} $Hz^{-1/2}$





Conclusions

Fugitive emissions monitoring of CH_4:

- CH_4 as a clean fuel → reduce GHG loading via leak monitoring
- Requirements: spatial + temporal resolution (real-time, large-area SN)

Demonstration of a field-deployable portable TDLAS sensor:

- Fiber coupled open-path (5 cm) absorption sensor ($\alpha_{min} = 6.5\times10^{-7}$ $cm^{-1}\cdot Hz^{-1/2}$)
- Benchmark performance for next generation integrated photonic chip sensors
- 5-day field deployment at METEC facility (5 Control, 2 Blind, 6.3 hours data)
- Demonstrate correspondence vs. custom MOX sensors (TDLAS → specificity)

Physical analytics for source localization/quantification:

- AOA calculation via CH_4 weighted mean wind-angle
- Single-sensor source estimation via Gaussian plume + ML models
- Generalizable to alternative sensing modalities (or multiple sensors in WSN)

Next generation: integrated photonic chip sensor nodes for significant SWaP-C benefits → facilitate large-scale deployment of real-time WSNs

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