Gas emission tomography using open-path laser dispersion spectroscopy and Bayesian state estimation

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INTRODUCTION

Estimating greenhouse gas (GHG) emissions from various sources is a crucial part of applying effective mitigation. One important GHG contributing to global warming is methane (CH4), but its global atmospheric budget is still poorly understood due to lack of knowledge on its emission rates. We consider a continuous real-time monitoring system for CH4 emissions at facility scale.

Open-path laser dispersion spectroscopy (LDS) instrument utilizes both the absorption and dispersion spectra of target gases (e.g. CO2, CH4), to obtain sequential realizations of the path-averaged concentration. The instrument can be used to continuously monitor hectare-scale areas with good spatial (multiple paths with length of $\sim$10 m - 10^3 m) and temporal ($\sim$1 Hz / path) resolution.

Sequential laser dispersion data carry indirect information on the spatio-temporal distributions of gas concentration and emission rate. The focus of this work is on computational methods used for reconstructing the concentration and emission distributions from the measurements; the methods include approximating the dynamics of the gas concentration by a convection-diffusion model (the state evolution model), modelling the measurements (observation model), and combining these two with sequential laser dispersion data via Bayesian state estimation.

THE STATE ESTIMATION APPROACH

The computational LDS observation model consists of line integrals along each measurement path, resulting in linear model

$$y_t = H_t c_t + v_t, \tag{1}$$

where $c_t \in \mathcal{R}^n$ is the discretized concentration distribution at time t, $H_t \in \mathcal{R}^{m\times n}$ is a line integral operator corresponding to paths between the laser source and m retro-reflectors, and $v_t \sim \mathcal{N}(0, \Gamma_{v_t})$ is the observation noise process. Here n is the number of nodes in the finite element mesh.

We use a stochastic finite element approximation of the convection-diffusion (CD) equation to model the gas dispersion. The CD equation is of the form

$$\frac{\partial c}{\partial t} = -\bar{v}\cdot\nabla c + \nabla\cdot(\kappa\nabla c) + a, \tag{2}$$

where $c(x,t)$ is the concentration distribution, $a(x,t)$ is the source distribution, $\bar{v}(x,t)$ is wind field and κ is diffusion coefficient. Here, x denotes the spatial coordinate.

By applying initial and boundary conditions, and using the finite element approximation with Crank-Nicolson time integration, we obtain a linear evolution model of the form

$$c_{t+1} = F_t c_t + s_{t+1} + T_t a_t + e_{t+1}, \tag{3}$$

where F_t is the state evolution matrix, s_t is a source from input boundary, T_t is the time integration matrix for the gas source, and $e_t \sim \mathcal{N}(0, \Gamma_{e_t})$ is a model noise process.
Further, a dynamical model is written for the source variable a_t. We use a second order Markov model of the form

$$a_{t+1} = A_0 a_t + A_1 a_{t-1} + \nu_{t+1}, \tag{4}$$

where the coefficients of the matrices A_0 and A_1 are determined based on the expected temporal correlation, while the spatial correlation prior is included in the noise process covariance Γ_{ν_t}. In addition, we apply positivity constraints for the variables c_t and a_t by reparametrization. The resulting state-space model is of the non-linear form

$$y_t = h(\theta_t) + v_t \tag{5}$$

$$\theta_{t+1} = f(\theta_t) + w_{t+1}, \tag{6}$$

where θ_t is the compound state variable $\theta_t = [c_t^{\mathrm{T}}\ a_t^{\mathrm{T}}\ a_{t-1}^{\mathrm{T}}]^{\mathrm{T}}$. We use the extended fixed-lag Kalman smoother to estimate the posterior density of the state variable

$$\theta_t|\{y_1,\dots y_{t+p}\} \sim p(\theta_t|y_1,\dots y_{t+p}) \approx \mathcal{N}(E(\theta_t|y_1,\dots y_{t+p}), \Gamma_{\theta_t|y_1,\dots y_{t+p}}), \tag{7}$$

where p is the amount of lag.

EXPERIMENTAL SETUP AND RESULTS

The models were tested using numerical simulations and measurements collected from controlled CH4 releases by Rutherford Appleton Laboratory. In the experimental setup, the gas was released from 2 m $\times$ 2 m containers on ground level, at four different locations both within the measurement path-covered area and outside it. Measurements were collected with a seven-beam setup.

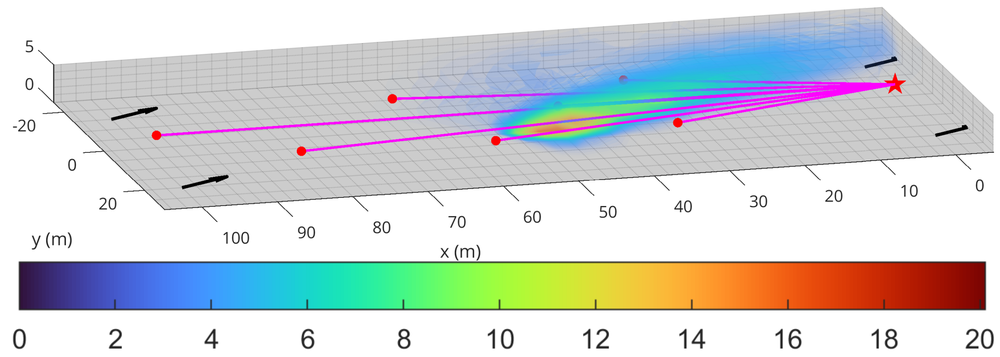

FIGURE 1: LDS MEASUREMENT PATHS (LINES) BETWEEN THE LASER SOURCE (STAR) AND RETRO-REFLECTORS (CIRCLES), MEAN WIND DIRECTION (ARROWS), AND THE RECONSTRUCTED CONCENTRATION DISTRIBUTION (ppm).

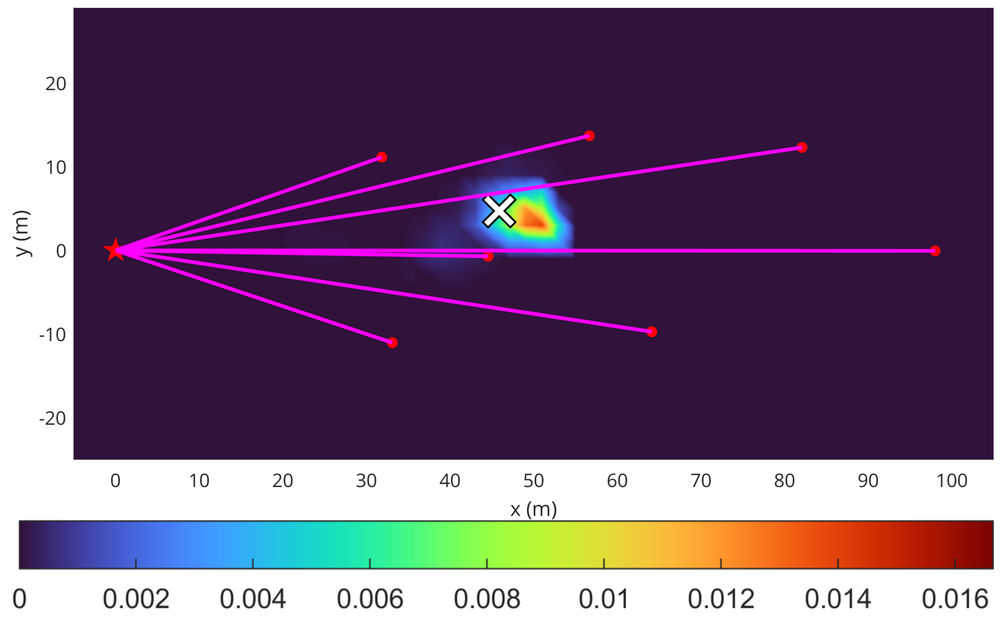

FIGURE 2: WEIGHTED TEMPORAL AVERAGE OF THE RECONSTRUCTED EMISSION RATE DISTRIBUTION (kg/m^{2}h). THE WHITE CROSS MARKS THE TRUE CENTER POINT OF THE GAS RELEASE.

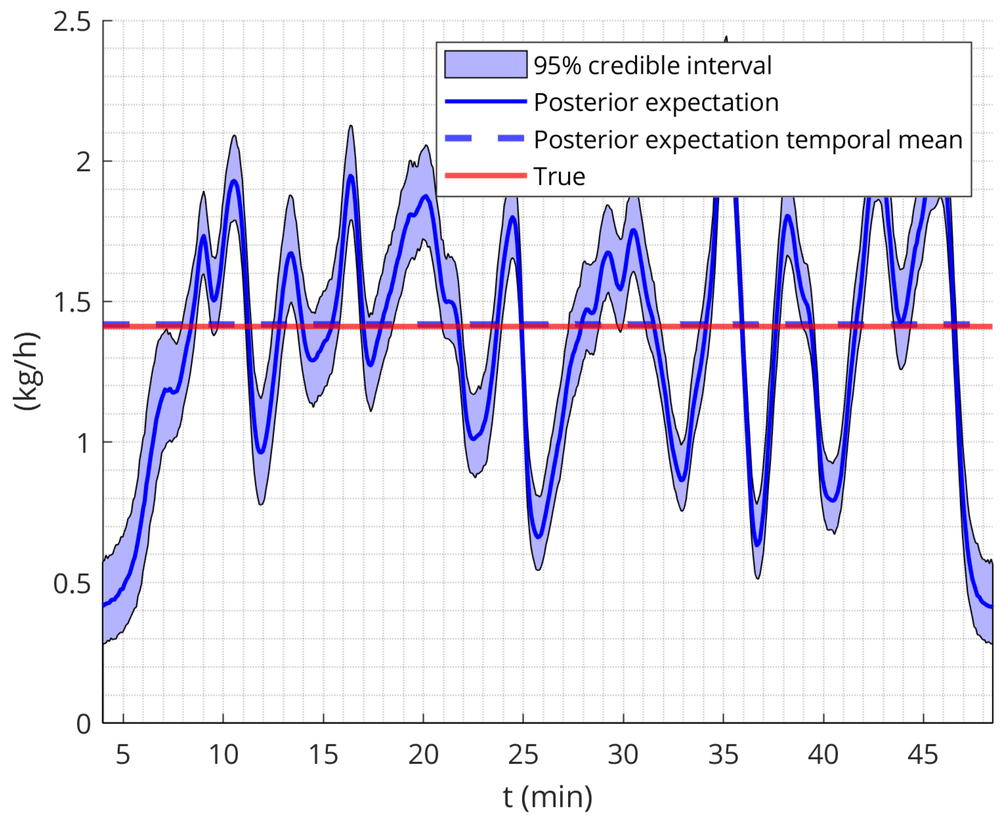

FIGURE 3: THE TRUE AND ESTIMATED TOTAL EMISSION RATE.

CONCLUSIONS AND FUTURE WORK

In this work, we developed a 3D framework for estimating spatio-temporal distributions of GHG sources. The feasibility of the method was tested with a data set collected from a controlled CH4 release experiment. Both the location of the CH4 source and its temporal average emission rate were reliably inferred (Figs. 2 and 3).

Our future work involves developing the computational models to estimate GHG sources in more versatile situations. The current emphasis is studying diffuse GHG sources and sinks in agriculture. Reliable estimation methods are needed to verify the effects of agricultural practises—such as fertilization, water table manipulation, and species selection—on the gas exchange.

FIGURE 4: MIRICO ORION DUAL GAS (CO2, CH4) ANALYZER IN AGRICULTURAL FIELD.

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