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Gas Source State Estimation with Reynolds-Averaged Dispersion Model and Time-Averaged Measurements

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Summary: In this work, the Gas Source State Estimation (GSSE) problem in non-trivial geometries is approached by combining a non-stationary gas dispersion Partial Differential Equation (PDE) with in-situ gas measurements under the assumption of known flow. The GSSE problem is formulated as an optimization problem with PDE constraints and solved efficiently using the adjoint method. The approach is simulatively validated on a 2D problem with laminar flow around a circular obstacle and data from gas dispersion simulations. Thereby, a single Gaussian gas source could be localized accurately for most trials with randomly placed sensor.

Keywords: gas source state estimation, sensor network, PDE-constraint optimization, Reynolds averaging

Background and Motivation

The early detection, localization and quantification of unwanted gas sources in industrial plants helps to increase their resource efficiency and at the same time reduces their environmental impact. However, estimating the state, i.e., the spatial distribution, of a gas source poses significant challenges due to the complex processes that govern atmospheric gas dispersion. For in-situ measurements, further difficulties arise since they can only be made at sparse locations. To address these challenges, this work uses a model-based GSSE approach that combines measurements with a dispersion model. Similarly, Wiedemann et al. modeled dispersion in a 2D domain with the non-stationary Advection-Diffusion (AD) PDE [1]. The required flow field was estimated from anemometer measurements. Though, an open domain without obstacles was assumed which is rarely the case in industrial plants. Khodayi-mehr et al. studied GSSE in geometrically more complex domains with stationary gas transport and fully known flow [2]. The problem was formulated as an optimization problem with PDE constraints. However, the stationary assumption is often violated in outdoor environments. This motivates to investigate GSSE in non-trivial geometries with non-stationary models and fully known flow.

Gas Dispersion Model

The proposed GSSE approach is studied on an exemplary 2D problem "flow around a cylinder". The modeling domain $\mathbf{\Omega}$ is a rectangular channel of and height H and length $L \gg H$ with a circular obstacle of radius r at position $\mathbf{x}_c$, see Fig. 1. In an industrial plant, the obstacle may correspond to a gas tank. The flow $\mathbf{v}(\mathbf{x}, t)$ and pressure $p(\mathbf{x}, t)$ at location $\mathbf{x} \in \mathbf{\Omega}$ and time t is modeled by the incompressible Navier-Stokes PDE

$$\rho\left(\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v}\cdot\nabla)\mathbf{v}\right) = \mu\nabla^2\mathbf{v} - \nabla p\,, \tag{1a}$$

$$\nabla\cdot\mathbf{v} = 0\,. \tag{1b}$$

A parabolic inflow velocity (left wall), no-slip conditions at the top/bottom wall and obstacle and a zero initial condition are assumed [3]. The gas concentration $c(\mathbf{x}, t)$ is described by the AD PDE

$$\frac{\partial c}{\partial t} = D\nabla^2 c - \mathbf{v}\cdot\nabla c + S\,, \tag{2}$$

with the positive source term $S(\mathbf{x}) \geq 0$. A zero initial condition and no-flux boundary conditions are assumed. For realistic gas dispersion with Reynolds Re and Péclet Pe numbers $> 10^5$, problem-specific Finite-Element (FE) solvers with small time/space discretization are required for numerical stability [3]. To avoid these difficulties, GSSE is studied in the laminar flow regime with $Re = 100$ and advection-dominated transport with $Pe = 10$. In this case, a triangular mesh with $n_e = 1038$ elements and a time step $\Delta t_s = 0.01\,\mathrm{s}$ can be used.

Gas Source State Estimation Method

GSSE aims to estimate the field $S(\mathbf{x})$ in eq. (2) from n_s gas measurements $y(\mathbf{x}_m^j)$ at locations $\mathbf{x}_m^j$ given the flow $\mathbf{v}$. The required data is artificially generated from simulations of eq. (1) and eq. (2). To cope with turbulence, only time-averaged flow $\bar{\mathbf{v}}$, concentration $\bar{c}$ and measurements $\bar{y}$ are used. The averaged quantities in the period $\Delta\bar{t}$ are computed using each $\Delta t_m \gg \Delta t_s$ time step to emulate sensors with sampling times Δt_m larger than turbulent effects. Time-averaging of eq. (2), using the Reynolds decomposition, leads to the Reynolds-averaged (RA) AD PDE [4]

$$\frac{\partial \bar{c}}{\partial \bar{t}} = \bar{D}\nabla^2\bar{c} - \bar{\mathbf{v}}\cdot\nabla\bar{c} + \bar{S}\,, \tag{3}$$

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where $\bar{D} = D + K$ is the sum of molecular D and turbulent $K \gg D$ diffusivity. Thus, turbulent mixing is modeled as diffusion. The GSSE problem is formulated as an optimization problem

$$\bar{S}^* = \arg\min_{\bar{S}} \sum_{i=1}^{n_T} \sum_{j=1}^{n_s} \left(\bar{c}_i^j - \bar{y}_i^j \right)^2 , \tag{4a}$$

$$\text{s. t. eq. (3) and } \bar{S}(\mathbf{x}) \geq 0 , \tag{4b}$$

with the RA AD PDE as constraint. Here, the Crank-Nicolson scheme with time step $\Delta\bar{t}$ is used for temporal discretization [3]. The objective is to minimize the error between the average concentration measurements $\bar{y}_i^j = \bar{y}(\mathbf{x}_m^j, i\Delta\bar{t})$ of sensor j and the corresponding concentrations $\bar{c}_i^j = \bar{c}(\mathbf{x}_m^j, i\Delta\bar{t})$ at time step i. Note that Reynolds-averaging reduces the computational cost of solving eq. (4) since a larger time step $\Delta\bar{t} \gg \Delta t_m$ and thus less steps $n_T = T/\Delta\bar{t}$, can be used. The problem is minimized iteratively with the Conjugate-Gradient Method [3]. The required gradient w.r.t. S is computed with the adjoint method using the Firedrake package [5].

Results

The GSSE approach was tested with $n_s = 20$ spatially fixed gas sensors, fully known flow field $\bar{\mathbf{v}}$ and a single 2D Gaussian-shaped source

$$S(\mathbf{x}) = \frac{q}{2\pi\sigma^2} \exp\left(\frac{-1}{2\sigma^2} \left\| \mathbf{x} - \mathbf{x_s} \right\|_2^2 \right) , \tag{5}$$

at location $\mathbf{x_s}$, width σ and constant emission rate density q. The total emission rate Q is obtained by integrating $S(\mathbf{x})$ over the domain $\mathbf{\Omega}$. The center $\mathbf{x_s}$ and area A_σ, containing $\approx 0.68Q$ of the total emission rate is depicted in Fig. 1. From FE simulations for $T = 10\,\text{s}$, the average fields and measurements are generated by averaging simulation data with a sampling time $\Delta t_m = 50\Delta t_s$. In eq. (4), time averaging over period $\Delta\bar{t} = T$ is performed and a diffusivity $\bar{D} = 0.8$ is used. The estimated source location $\mathbf{x}_s^*$ is obtained by searching for the midpoint of a circular area that includes the most emissions. The performance of the GSSE approach is statistically evaluated with histograms obtained from 80 trials of random sensor locations. The sensor locations $\mathbf{x}_m^j$ are sampled from a Sobol sequence to avoid sensor-clustering. The estimated field $\bar{S}^*(\mathbf{x})$ for a specific sample is shown in Fig. 1. The source was localized with a median error of $0.061L$ of the channel length L. In $71\,\%$ of the trials, the location error was below $0.1L$. The emission rate was overestimated in median to $1.842Q$, with $80\,\%$ of the trials in the range $[1.11Q, 2.54Q]$.

Conclusion

The proposed GSSE approach allows to estimate the spatial distribution of a gas source from in-situ gas measurements in geometrically non-trivial domains under the assumption of known

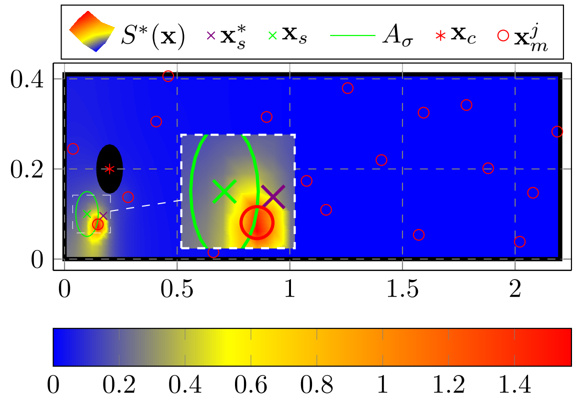

Fig. 1: Estimated source field $\bar{S}^*(\mathbf{x})$ from eq. (4) and location $\mathbf{x}_s^*$ for one trial. Ground truth $S(\mathbf{x})$ from eq. (5) indicated in green. Obstacle and channel boundaries shown in black. Sensor locations $\mathbf{x}_m^j$ shown as red circles.

flow. Thereby, measurements are combined with a non-stationary dispersion model with known initial and boundary conditions. Time-averaging of the model and measurements is performed to reduce the computational cost of the GSSE problem. From the estimated source field, the source-location could be determined accurately for most trials with different sensor placements. However, the emission rate was overestimated in all trials. It was observed that the source estimate improves when sensors are near the source. This indicates the importance of proper sensor placement for reliable GSSE. From an optimization perspective, it may also be beneficial to reduce the dimension of the problem by using a mesh-size-independent parametrization of the source field, e.g., a Neural Network with fewer parameters than the number of elements n_e [5]. Moreover, an approach to estimate the flow field from measurements is required to relax the restrictive assumption of known flow.

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