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ESTIMATION OF MULTIPLE ROAD TRAFFIC SOURCE STRENGTHS IN A REAL URBAN AREA

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Abstract: This study evaluates an inverse dispersion modelling methodology that integrates source-receptor relationship calculated from CFD simulations with the Metropolis–Hastings MCMC algorithm to estimate the release rates from multiple traffic emissions at the street scale. This technique is based exclusively on observational data, supplemented by prior information on the emission rate range for each source, and is applied to the Augsburg city center using synthetic observations generated from a forward dispersion model with added Gaussian noise. Additionally, a sensitivity analysis investigates how sensor configuration and prior information influence the accuracy of the emission estimates. The results demonstrate that the estimated release rates are strongly dependent on both the number of sensors in the measurement network and the range of emission rates used as prior information. When the permitted emission rate range is narrow, high accuracy is achieved even with AQMN consisting of only 10 sensors. In contrast, expanding the allowable emission range reduces the performance, particularly for networks with fewer than 50 sensors. These findings underscore the importance of sensor density and informed prior knowledge in achieving reliable emission estimates.

Key words: inverse dispersion modelling, traffic emissions, sensor configuration analysis, computational fluid dynamics, Bayesian inference

INTRODUCTION

Inverse dispersion modelling techniques aim to estimate unknown parameters of air pollutant sources, such as location, emission rate, and intensity, by combining data from atmospheric transport and dispersion models (ATDMs) with observations from air quality monitoring networks (AQMNs) in the study area. In urban environments, where wind interacts with complex geometries and generates strong turbulence phenomena, Computational Fluid Dynamics (CFD) models are often applied as ATDMs. Most previous CFD-based research has focused on identifying source locations and emission rates for single or limited pollutant sources in urban areas. In contrast, relatively few studies have examined emissions from multiple sources or quantified their combined contribution to urban air quality. A

Different inverse modeling approaches exist depending on the type of ATDM employed. In CFD-based studies, the source-receptor relationship is typically derived by solving either the forward or the adjoint form of the advection-diffusion equation. Estimation of unknown source parameters is achieved by integrating concentration data from AQMNs with simulated concentrations from dispersion models. A range of algorithms have been employed for this purpose, including optimization methods, probabilistic approaches, and more recently, machine learning techniques. A detailed description of inverse modelling techniques is provided by Hutchinson et al. (2017). Despite the crucial impact of traffic emissions in urban air quality levels and concentration variability, inverse modelling methods have rarely been applied to traffic emission estimation. Current state-of-the-art tools, such as COPERT (Ntziachristos et al., 2009), rely primarily on vehicle fleet data (e.g., number, type, and emission control technologies) rather than inverse approaches.

This study aims is to estimate high-resolution release rates from multiple road traffic sources in an urban environment. To this end, the open-source CFD tool OpenFOAM is employed as an ATDM to simulate pollutant concentrations from individual sources and derive the source-receptor relationships. The case study focuses on the city center of Augsburg, Germany. The Bayesian inference-based algorithm, Metropolis–Hastings Markov Chain Monte Carlo (MCMC), is applied to estimate traffic emission rates. Synthetic measurements are generated using the forward model with added Gaussian noise, while prior information on expected emission ranges is incorporated. The algorithm is tested under varying sensor configurations, wind directions, and prior knowledge levels to assess how these factors influence the accuracy of estimated release rates.

METHODOLOGY

Consider a line source $r(l) = (x(l), y(l), x(l))$ in Cartesian coordinates (x, y, x), which continuously emits a passive pollutant a passive pollutant at a rate q_s. The parameter l represents the location of the source along the road. In this case, the dispersion of the pollutant within the spatial domain can be described by the advection–diffusion equation, assuming the pollutant behaves as a passive scalar, as given below:

$$\frac{\partial C}{\partial t} + u_j \frac{\partial C}{\partial x_j} - \frac{\partial}{\partial x_j}\left(D_m + \frac{v_t}{Sc_t}\right)\frac{\partial C}{\partial x_j} = q_s \delta\big(r(l)\big) \tag{1}$$

where C is the pollutant concentration, $u_j = (u, v, w)$ is the velocity vector in Cartesian coordinates $x_j = (x, y, z)$, $\delta(\cdot)$ is the Dirac delta function, representing the source, Sc_t is the turbulent Schmidt number, and v_t is the eddy viscosity. The source-receptor relationship, which represents the sensitivity of concentration C in each sensor, i, of the corresponding sensor of the AQMN is calculated from the equation:

$$C^c(r(l), q_s)_i = C(x_n, y_n, z_n)_i \tag{2}$$

Here ${C^c}_i$ is the source-receptor relationship, for sensor i, positioned at (x_n, y_n, z_n).

Bayesian inference is a probabilistic framework based on Bayes' theorem for estimating the posterior probability of a hypothesis. It combines prior knowledge with both observed and simulated data. In the context of inverse dispersion modelling, let d denote the concentration values observed by an AQMN, and $s = (r(l), q_s)$ represent the set of source parameters. The posterior probability distribution $p(s|d)$, describing the likelihood of source parameters s given the observations d, can be expressed as:

$$p(s|d) \propto \frac{p(d|s)p(s)}{p(d)} \propto p(d|s)p(s) \tag{3}$$

Here, $p(d \mid s)$ denotes the likelihood, i.e., the probability of obtaining the observations d given the source parameters s, $p(s)$ represents the prior distribution, which encodes existing knowledge about s before the analysis, and $p(d)$ is the evidence, which is independent of s, that ensures the posterior distribution is properly normalized.

Let $q_{s_{min}}$ and $q_{s_{max}}$ represent the minimum and maximum accepted release rates of a source, which are defined before the inference. In that case the posterior probability distribution can be written as:

$$p(s|d) \propto \begin{cases} exp\left[-\frac{1}{2}\sum \frac{({C^o}_i - C^c(\theta)_i)^2}{\sigma_{o,i}^2 + \sigma_{c,i}^2}\right], \text{if } q_s > 0 \text{ and } q_{s_{min}} < q_s < q_{s_{max}} \\ 0, \text{else} \end{cases} \tag{4}$$

Here ${C^o}_i$ is the observed concentration in sensor i, while $\sigma_{o,i}^2$ and $\sigma_{c,i}^2$ are define the error of the instrument and model respectively.

In general, the maximum of the posterior probability corresponds to the most likely solution of the inverse problem. However, evaluating the posterior probability for all possible release rates within a predefined emission range requires substantial computational resources, making this approach impractical. To overcome this limitation, Bayesian inference employs sampling algorithms to generate posterior samples. Among these, the Metropolis-Hastings Markov Chain Monte Carlo (MCMC) method is one of the most widely applied in inverse dispersion modeling studies.

The methodology of the current work involves steady-state airflow simulations for 36 wind sectors (from 0° to 350° with 10° increments) to calculate wind and turbulence parameters, followed by derivation of source–receptor relationships using a forward dispersion model for each road traffic source. Synthetic observations are generated by adding Gaussian noise to concentrations calculated by the forward model. The Metropolis–Hastings MCMC algorithm is then applied to estimate source release rates by combining model concentrations, synthetic measurements, and prior knowledge of the emission rate range for each source. The algorithm is tested under varying sensor configurations and wind directions to assess the influence of sensor's number used by the AQMN. The algorithm's application is repeated with different prior release rate ranges to evaluate sensitivity to existing knowledge about each source emissions.

The case study investigated in the present work is the Augsburg city centre in Bavaria, Germany. Augsburg is a typical central European city with complexities in the city geometry and industrial activity in its surroundings. For the application of numerical simulation, a computational domain including the geometry of the city centre (2 × 1.6 km^2, with the maximum building height of 83.5 m) was structured. At the next step a tetrahedral computational mesh of more than 48 million cells was generated with very high resolution in the traffic emission sources (0.25 m), high refinement in the building and ground surfaces (1 m) and low resolution at the domain boundaries (30 m). A detailed description of the mesh is provided by Ioannidis et al., (2024). Within the computational domain 69 traffic sources were selected, from both major arterial roads and smaller but active streets, to release the passive pollutant. At the same time a network of 81 sensors was set up as the AQMN for the application of the current studies several scenarios. In Figure 1 are illustrated the geometry of the buildings of computational domain in $x - y$ level, the 69 traffic sources (red lines) and the 81 sensors (green dots) of the AQMN.

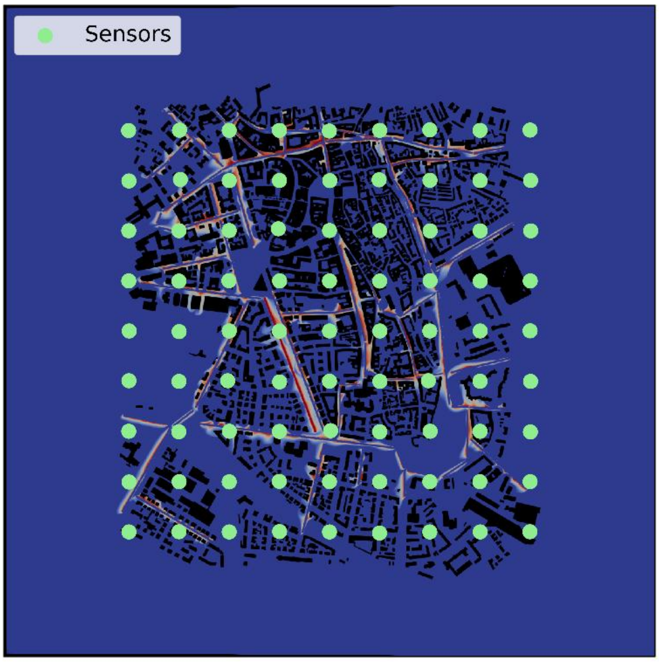

Figure 1. The geometry of the Augsburg city centre in $x - y$ plane the positions of the traffic emission sources illustrated in red lines and the sensors depicted in green dots.

For the CFD numerical simulations, the Reynolds-Averaged Navier–Stokes (RANS) approach was employed using the two-equation $k - \varepsilon$ turbulence model, implemented with the SIMPLE solver in OpenFOAM v2112 under steady-state conditions. Pollutant dispersion was modeled by modifying the solver to resolve the advection–diffusion equation for each emission source. In total, 69 pollutant plumes, corresponding to the number of sources, were obtained for each wind direction. For the probability density function (PDF) calculations, the Metropolis–Hastings MCMC algorithm was executed for 80,000 iterations, with the first 20,000 discarded as burn-in. The remaining 60,000 iterations were used to generate PDF samples. The synthetic measurement dataset was constructed by applying the forward dispersion model to compute concentrations and then adding Gaussian noise. To analyze sensor configurations, four wind direction scenarios were selected to represent different atmospheric conditions: 50°, 140°, 230°, and 320°.

RESULTS

To evaluate the influence of sensor number on release rate estimation, the Metropolis–Hastings MCMC algorithm was applied across different sensor configurations. These configurations were grouped according to the number of sensors: the first subgroup included 10 sensors randomly chosen from the total set of 81, and subsequent subgroups were formed by adding 10 additional sensors at each step until all sensors were included. For every wind direction and sensor subgroup, the algorithm was executed 20 times with different randomly selected sensor locations, yielding 80 PDF estimations per source for all 69 sources. The accuracy of the release rate estimations was assessed using the release rate ratio $\Delta q = max[(q_e/q_t), (q_t/q_e)]$. The ideal target is $\Delta q = 1$, indicating perfect agreement. Here, the estimated release rate is defined as the mean of the corresponding PDF.

Figure 2 illustrates the distributions of the estimated release rate ratios (Δq) for the 69 traffic sources across different sensor subgroups, comparing two cases: in the first (blue boxes), the release rate of each source ranges from 0.001 to 100 kg/s, while in the second (orange boxes), it ranges from 0.01 to 20 kg/s. The red dashed line indicates the target value for the release rate ratio ($\Delta q = 1$). It should be noted that Δq values are computed from the mean value of the PDF estimates for all 69 traffic sources, averaged across 80 randomly selected configurations (20 for each wind direction) within each sensor-count subgroup.

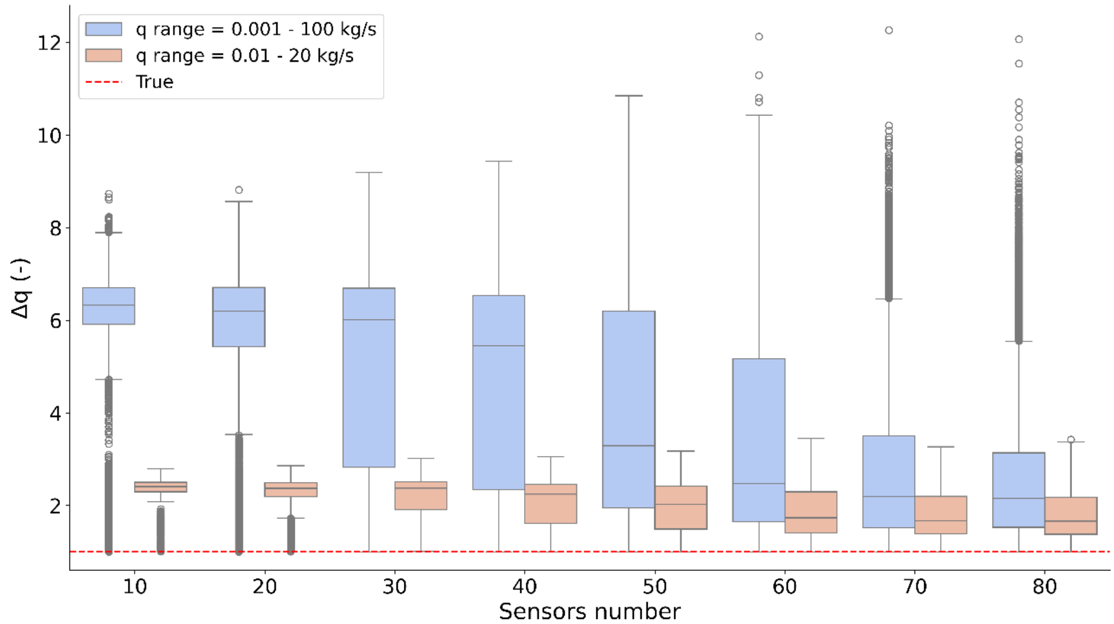

Figure 2. The release rate ratios (Δq) represent the comparison between the mean estimated and true source emission rates across all traffic sources within each sensor group. Each box shows the results from 80 random configurations. The blue boxes correspond to the scenario where release rates range from 0.001 to 100 kg/s, while the orange boxes represent the range from 0.001 to 20 kg/s. The red dashed line indicates the target value of Δq.

Overall, for both scenarios investigated, it is evident that increasing the number of sensors in the AQMN leads to substantially higher accuracy in release rate estimation. Specifically, for configurations that include more than 60 sensors, the majority of the estimated release rates approach the ideal target value, demonstrating the strong influence of sensor density on estimation performance. This trend is particularly noticeable in the scenario where a wider prior release rate range is allowed in the Metropolis–Hastings

MCMC application (with q ranging from 0.001 to 100 kg/s), as the larger uncertainty in the prior makes accurate estimation more challenging. To evaluate the quality of the estimations, a criterion previously adopted in the study by Kovalets et al. (2011) is applied. According to this criterion, a solution is considered to be of "good" quality when the release rate ratio Δq is less than 4. In the present study, this condition is satisfied for all sources when the allowed range of release rates is relatively narrow, indicating reliable performance even with fewer sensors.

In the first scenario, which permits a wider release rate range, the median Δq calculated from the estimations initially exceeds 6, reflecting the increased difficulty of accurately estimating sources under such conditions. However, as the number of sensors in the AQMN increases, estimation accuracy improves. Once the network consists of more than 50 sensors, the median Δq converging to 2, showing that the algorithm can effectively handle the wider range by adding sensors in the AQMN. In the second scenario, where q ranges from 0.01 to 20 kg/s, the results are more accurate even with a relatively small number of sensor sub-group. For example, an AQMN with just 10 sensors already produces satisfactory estimations, with most release rate ratios around 2.5. As in the first scenario, adding more sensors continues to improve performance. With higher sensor counts, the median Δq converges toward the ideal value, demonstrating that a denser AQMN consistently enhances the reliability and accuracy of release rate estimations.

CONCLUSIONS

The findings of this work indicate that the proposed methodology is capable of providing accurate release rate estimates for multiple traffic sources in an urban area by integrating CFD modelling with the Metropolis–Hastings MCMC algorithm. The implementation relies solely on data from the measurement network, supplemented with basic prior knowledge of the approximate emission range for each source. As demonstrated, reducing the uncertainty in the prior information and increasing the number of sensors in the network both contribute to higher-quality estimations. The effectiveness of the approach is further highlighted by the observation that the vast majority of estimated emission rates fall within an order of magnitude of the true release rates in both test scenarios. The main limitation of the current study is that the methodology has been evaluated only on noisy synthetic datasets and assumes the pollutant behaves as a passive, non-reactive contaminant. Therefore, further research is required to assess the performance of this approach for real-world air quality applications using real observational data.

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