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Data filtering for inverse dispersion emission calculations

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ABSTRACT

Inverse dispersion techniques are used to infer the emission rate of gas sources from concentration measurements and dispersion model calculations. Criteria for the selection of measurement intervals having wind conditions conducive to technique accuracy are examined on the basis of a short range tracer experiment. By introducing a supplementary condition that the measured vertical temperature gradient be quantitatively compatible with Monin–Obukhov similarity theory, it was possible to use a less stringent threshold for the friction velocity than has previous been used ($u_* \ge 0.05 \text{ m s}^{-1}$ instead of $\ge 0.15 \text{ m s}^{-1}$). Under the new criteria a larger proportion of measurement intervals are retained (76% versus 49%), while the ratio of inferred to actual emission rate Q_{LS}/Q exhibits negligible bias (average $Q_{LS}/Q = 1.00$) and an acceptably small level of random error (interval-to-interval standard deviation $\sigma_{0/0} = 0.25$).

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1. Introduction

"Inverse dispersion" refers to the practice of inferring the atmospheric emission rate (Q) of localized gas sources from the excess concentration (*C*) they cause, by modelling the *C*–*Q* relationship under the existing meteorological state. The technique has proven particularly successful for calculating emissions from discrete ground level sources using nearby concentration measurements (e.g., Ferrara et al., 2014). This micrometeorological scale problem requires only an upwind and downwind gas concentration, with substantial freedom to choose convenient measurement locations. The technique does have the disadvantage that, in its most practical form, it entails idealizations that may compromise accuracy in some circumstances. Chief among these is the assumption that a dispersion model predicated on horizontally-homogeneous winds will suffice for the inversion, obviating what is (otherwise) a burdensome computation. While strictly unobstructed wind fields are the exception, fortunately a number of studies in disturbed winds have indicated that the technique can be quite robust (e.g., Wilson et al., 2010).

Different types of dispersion models can be used for inverse calculations. A common implementation combines a Lagrangian

http://dx.doi.org/10.1016/j.agrformet.2014.07.010 0168-1923/© 2014 Elsevier B.V. All rights reserved. stochastic (LS) model with a Monin–Obukhov (MO) similarity theory description of the wind (Wilson et al., 2012), and to that end specialized "MO–LS" software has evolved¹. In an agricultural context MO–LS has been used to calculate emissions from barns (Harper et al., 2010), fields (Sanz et al., 2010), cattle feedlots (Todd et al., 2011), waste storage ponds (Flesch et al., 2013), grazing cattle (McGinn et al., 2011), and many other variations of source and environment.

An MO–LS emission calculation presumes MO accurately describes the vertical profiles of the average wind and turbulent statistics. The theory posits that these properties are characterized by the friction velocity u_* and Obukhov length L (in conjunction with the surface roughness length z_0). Light winds and extreme atmospheric stratification, associated with small magnitudes of u_* and L, limit the applicability of MO. Several studies show a deterioration in the accuracy of MO–LS emission calculations as u_* and |L| decrease (e.g., Flesch et al., 2004; Gao et al., 2009), which has led to the introduction of filtering criteria to remove periods when u_* and |L| fall below threshold values. For example, Flesch et al. (2005) used thresholds of u_* thres = 0.15 m s⁻¹ and |L|thres = 10 m, McBain







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¹ The MO–LS designation can include backward Lagrangian stochastic (bLS) calculations for area sources, or a corresponding forward calculation (fLS) for point sources.

Reflectors

and verified by weighing of gas cylinders. The gas was directed to a manifold and distributed to the release points. The combination of a large diameter manifold and long and equal length tubing was assumed to give equal emission rates from each release point. The total release rate was either 0.46 or 0.92 kg CH₄ h⁻¹ (equivalent to 50 to 150 cattle: a large release rate chosen to minimize concentration measurement errors). Releases took place intermittently from September 3 to 10, with a total of 215 15-min release periods. Of these, 144 occurred during the night (sunset to sunrise).

a mass flow controller (GFC47, AALBORG, Orangeburg, NY, USA)

2.2. Concentration and wind measurements

Open-path CH₄ lasers (GasFinder 2, Boreal Laser Inc., Edmonton, Canada) measured the average gas concentration along the four sides of the simulated paddock. There were four stand-alone lasers and one laser on a pan-tilt head that scanned between two retro-reflectors (DSM; PTU D300, FLIR Motion Control Systems, Burlingame, CA, USA). This setup gave measurement duplication on two of the four paddock sides. The average path heights of the four laser lines varied from 1.5 to 2.15 m due to gentle terrain undulations.

Laser calibration was completed after the study. Recently, Gas-Finder lasers were found to have a previously unaccounted for temperature and pressure dependence (discussed by Laubach et al., 2013). This has been addressed by Boreal Laser Inc. in a new calibration procedure that gives temperature and pressure correction factors, and our lasers were re-calibrated after the study and these corrections were applied retroactively. Laser calibrations were also adjusted to match on-site measurements from a gas chromatograph (GC). Air samples were collected during a single 15-min interval between release periods, and laser-specific ratiometric correction factors were applied to force agreement between the lasers and the GC measured concentration (1.77 ppm_v).

Laser measurements were processed to give 15-min average concentrations. Concentrations were converted from the reported ppm_v to g m⁻³ using measured air pressure and temperature. Laser observations were not used if a 15-min period did not include more than 25% good data (i.e., light levels > 2000 units and R2 > 96: quality parameters reported by the laser).

A 3-D sonic anemometer (CSAT-3, Campbell Scientific, Logan, UT, USA) provided the wind information for our calculations: friction velocity u_* , Obukhov length L, surface roughness length z_0 , and wind direction β (calculated as described in Flesch et al., 2004). The anemometer was positioned just north of the release site at a height of 2.0 m above ground. Wind statistics were calculated for 15-min intervals matching the CH₄ concentration record.

2.3. MO-LS emission calculations

Emission rates were calculated using the freely available Wind-Trax software. The software combines the MO–LS model described by Flesch et al. (2004) with mapping capabilities. Dispersion from each release point was simulated with a forward LS model using 10,000 trajectories. Identical emission rates were assigned to the eight release points in the calculation. From each set of 15-min laser concentrations, WindTrax calculated the total emission rate Q_{LS} (kg CH₄ h⁻¹) and the corresponding background concentration C_b . This problem is mathematically over-determined (e.g., six concentrations used to solve for two unknowns) and a best-fit procedure was used in the WindTrax calculation.

In the following analysis 19 out of the 214 release periods (15min each) are not used. Fifteen had a calculated z_0 greater than the source height of 0.5 m; one period violated the Cauchy–Schwarz inequality (error in calculated wind statistics that can occur in light winds); in one extremely stable nighttime period the calculated

Fig. 1. Field site (top) and equipment and gas release configuration (bottom).

100 m

and Desjardins (2005) suggested $u_{\text{thres}} = 0.19 \text{ m s}^{-1}$, while Laubach et al. (2008) used 0.12 m s⁻¹.

A consequence of filtering is the loss of potentially valuable data. With $u_{\rm *thres} = 0.15 \,{\rm m\,s^{-1}}$ our experience has been of data loss rates of 40 to 50%, and sometimes more than 75% in long term rural studies (clearly this loss depends on the regional climate and the weather encountered during a campaign). The loss of low wind speed data hinders efforts to characterize sources having an emission rate that correlates with wind speed (e.g., ammonia from waste ponds), since emissions during light winds are unresolved. And because filtering preferentially removes light wind nighttime data, a daytime-biased dataset is created. This complicates the calculation of average emissions from diurnally varying sources, such as animals or industrial sites having a daily activity pattern.

The focus of this study is the filtering criteria used in MO–LS calculations. Our motivation comes from the perspective of animal studies, where the loss of nighttime data is a significant problem for characterizing emissions. We will examine the potential of u_* , L, wind speed and air temperature as filtering criteria, and consider how these affect MO–LS accuracy and the rate of data retention (particularly at night). A tracer release study, designed to mimic the configuration of a small herd of cattle, provides a large dataset for this evaluation.

2. Methods

2.1. Tracer release experiment

Lasers

A tracer release experiment was conducted in September 2012 at Onefour, Alberta, Canada (49°06′N; 110°30′W; elevation 925 m). This semi-arid grassland site was selected because of its extensive short grass terrain and the absence of nearby gas sources (Fig. 1). The study was designed to mimic the configuration of a small herd of cattle. Eight release points were clustered near the centre of an imaginary 100×100 m square paddock (Fig. 1), at a height of 0.5 m above ground. Methane was released at a known rate using



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