Quantifying methane emissions using inverse dispersion modelling

Chief Scientist's Group research report

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Email: research@environment-agency.gov.uk

Author(s):
Christina Hood, Amy Stidworthy, Kate Johnson, David Carruthers, George McCosh, Victoria Hamilton (CERC), Adam Clegg (AQC)

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Research contractor:
Air Quality Consultants (AQC)
23 Coldharbour Road
Redland
Bristol BS6 7JT
0117 974 1086

Cambridge Environmental Research Consultants (CERC)
3 King's Parade
Cambridge CB2 1SJ
01223 357773

Environment Agency's Project Manager:
Mark Bourn

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Dr Robert Bradburne
Chief Scientist

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Executive summary

Methane is an important greenhouse gas, but methane emissions are currently uncertain and more information is needed about the emissions from ‘real world’ facilities. This study investigated the potential role of inverse dispersion modelling techniques in quantifying whole-site routine methane emissions from facilities regulated by the Environment Agency.

A literature review of inverse dispersion modelling techniques identified a range of methods which could be applied to estimate fugitive emissions based on ambient concentration measurements. The simplest method uses ground-level measurements along a cross-section of a fugitive plume and fits a Gaussian distribution to it, assuming ground-level source height. The most complex methods involve adjoint (reversed) computational fluid dynamics (CFD) modelling. Intermediate approaches can either consider emissions from a whole site as a single combined plume or differentiate between individual sources within a site.

The overall suitability of methods for source types, including landfill, biogas, onshore oil and gas, and wastewater sites depends on the source characteristics for each site type, especially horizontal extent and height. The surroundings of an individual source, such as the presence of other nearby sources, complex terrain or other flow obstructions, can restrict the range of suitable methods available. The selection of an inverse dispersion modelling method for a particular application should also balance uncertainty, complexity and cost.

The authors make the following recommendations regarding inverse dispersion modelling techniques and their selection for a particular application:

1. The selection of a suitable inverse dispersion modelling method for a particular source and application should consider:
    a. source characteristics such as horizontal length scale and likely emission height
    b. characteristics of the area surrounding the source such as open or complex terrain and/or nearby obstructions to flow, including buildings
    c. the presence of other nearby sources of the targeted pollutant, especially if upwind of the planned measurement locations
    d. the appropriate balance of required accuracy/uncertainty and cost
2. Inverse dispersion modelling methods are currently an area of active research and rapid development, driven by improvements in measurement technologies and increased availability of computational resources. The Environment Agency should continue to assess emerging inverse dispersion modelling methods as they become more mature.

3. Information about activities at a regulated site should be collected during any short-term measurement campaign that is to be used with inverse dispersion modelling methods, to assess how representative the inverse dispersion modelling results are of longer-term emissions.

4. Data quality thresholds for measurement data which is to be used with inverse modelling need to be developed with care, appropriate to each measurement technique and inverse dispersion modelling approach.

5. The main focus of this study was fugitive methane emissions. However, the recommendations above would apply similarly to other fugitive gaseous releases.

To test a selection of inverse dispersion modelling methods**,** an inverse dispersion modelling study was carried out using data obtained from repeated tracer gas dispersion method (TDM) surveys of 3 landfill sites (Rees-White and Beaven, 2020). During each survey a tracer gas was released from a ground-level location within the landfill site. Plume transect measurements of methane concentration and tracer concentration were collected at one second intervals by a vehicle driving along downwind roads which crossed the plume. Multiple plume transects at various downwind distances were measured during each survey. The number of available surveys varied between sites, from a minimum of 4 to a maximum of 7. Four inverse dispersion modelling methods were selected for the comparison study:

- **1D Gaussian profiles:** Landfill emissions were modelled as a single ground-level point source using the Atmospheric dispersion modelling system (ADMS) (Carruthers and others, 1994) and CERC (2023)), with a mean averaging time of one hour, and a simple Gaussian distribution was fitted to the downwind plume.
- **Standard Bayesian**: Landfill emissions were modelled in ADMS as separate volume sources representing different capping/activity areas, with a mean averaging time of one second. A Bayesian inverse dispersion modelling approach was implemented, including consideration of measurement uncertainty and covariances.
- **Modified Bayesian**: A modified application of the Standard Bayesian method was developed for this study, including measurement uncertainty and covariances. Short-term fluctuations in concentration were estimated by ADMS using a mean averaging time of one hour and a fluctuations averaging time of one second. The inverse dispersion model was applied to the measured peak concentration in each plume transect.
- **Backward Lagrangian Stochastic (WindTrax):** This statistical model was applied to trace large numbers of simulated flow particles backwards from the measurement locations to the landfill. This approach was only tested for the smallest of the 3 sites due to WindTrax limits on source-receptor distances.

These methods were applied to the TDM data to estimate the landfill methane emission rates during each survey. These estimates were then compared with those from the TDM survey report. There was considerable variation between the estimated landfill emissions using the different inverse dispersion modelling methods. The method with the closest estimates to the TDM method was the novel Modified Bayesian method, which takes

account of the short-term concentration fluctuations caused by the plume meandering that occurs due to fluctuations in wind speed, wind direction and turbulence. These fluctuations are significant on the one second timescale of TDM measurements. The 1D Gaussian and Standard Bayesian methods generally estimated much higher emissions, largely because they did not account for these effects. The Backward Lagrangian Stochastic (WindTrax) method was only used for the smallest site. For this site, WindTrax gave similar estimates to TDM for some surveys but also much larger estimates for other surveys.

If TDM survey data is to be routinely used with modelling and inverse dispersion modelling methods, then the authors make the following recommendations for TDM survey data collection:

6. TDM surveys should also collect high quality, high frequency (for example, one second) meteorological and turbulence measurements where possible, so that the model input can be optimally specified, thereby improving model performance.

7. TDM surveys should be conducted in atmospheric conditions where the models are best able to represent the atmospheric airflow and turbulence. These are conditions where both stability effects and wind direction changes are small, which is typically the case in near neutral conditions, with moderate wind speeds, consistent wind directions and not around sunrise or sunset.

8. TDM surveys should carry out repeated transects as close as possible to the site, while still capturing the whole plume.

The following recommendations relate to the inverse dispersion modelling approaches tested:

9. The study shows that the Modified Bayesian method performs well and is a viable approach to estimating emissions from transect measurements, supporting further testing and refinement, with additional TDM survey data sets, prior to routine application. The method combines the ADMS dispersion model, which is already widely used for regulatory purposes, with a Bayesian inversion approach, which is similar to those used by a number of different groups.

10. Another modification of the Standard Bayesian approach, not considered in this study but recommended for further examination, is to apply an inverse dispersion modelling method to the cross-wind plume-integrated concentration, reducing the complexities arising from short-term fluctuations.

11. The suitability of an inverse dispersion modelling method to the high measurement frequency (one second) and mobile nature of TDM survey data should be considered when selecting an inverse dispersion modelling method for use with TDM data.

12. A robust procedure is required for assessing each TDM survey transect in terms of its suitability for the chosen inverse dispersion modelling method. The procedure will depend on the inverse dispersion modelling method, but should take the limitations of the method into account. For example, the Standard Bayesian method requires the

modelled plume position to match the measured plume position, which may not be the case for all transects within a survey.

13. The inverse dispersion modelling study focused on emissions from one type of facility (landfill) using one type of measurement data (tracer gas plume transect measurements). Measurements made using a wider range of methods and around other types of facilities would be required to compare additional inverse dispersion modelling techniques.

14. The inverse dispersion modelling study found that the whole-site emissions calculated by the 1D Gaussian, Standard Bayesian and Modified Bayesian methods were unaffected by the choice of TDM survey used to provide the initial emission rate. This suggests that a method involving only one TDM survey combined with inverse dispersion modelling, and repeated or continuous methane and meteorological monitoring at other times of year, would be sufficient to provide a good estimate of annual landfill methane emissions. The recommended time to carry out the annual TDM survey would be when landfill emissions are expected to be relatively high, subject to the meteorological considerations set out in (7) above.

15. On the basis of (14) above, it is recommended that the Environment Agency considers further case studies and worked examples in order to develop a practical, ‘user-friendly’ protocol for site operators that sets out a typical annual sequence of measurements, inverse dispersion modelling and analysis for quantifying methane emissions at a regulated site.

1. Introduction

Methane is an important greenhouse gas, but methane emissions are currently uncertain and more information is needed about the emissions from ‘real world’ facilities. The Environment Agency commissioned an investigation into the potential role of inverse dispersion modelling techniques in quantifying whole-site routine methane emissions from nationally regulated facilities. This investigation aimed to:

- identify available inverse dispersion modelling techniques
- assess the suitability of inverse dispersion modelling techniques for different regulated source types
- test some inverse dispersion modelling techniques in comparison to existing landfill methane emissions measurement methods
- recommend possible inverse dispersion modelling techniques for long-term quantification and regulation of fugitive emissions

Fugitive emissions of methane are associated with a range of different source types, including landfill, biogas (anaerobic digestion), onshore oil and gas (OOG) and wastewater treatment. OOG methane emission sources and associated measurement techniques have been described in a previous Environment Agency study (SC210006/R, 2022). Where measurements are taken at sufficient distance downwind for individual releases to have merged into a single plume, the geometry of whole-site emissions is often simplified and treated as a point source for inverse dispersion modelling. However, in practice, fugitive emissions are likely to comprise a mixture of point (leak) and area (seepage/evaporation) emission geometries, for example, as described by Abichou and others (2010) for landfill sites:

> “Emissions from the landfill surface can be a combination of three distinct patterns. One emission pattern consists of a single high-emitting source, such as a hot spot associated with a crack and other defects in the soil cover. This pattern can also be due to leaking gas collection wells at the pipe intrusion or in the pipe fittings. A second pattern consists of multiple hot spots randomly located along the surface. A third emission pattern consists of uniform emissions from the entire landfill surface associated with concentration gradient and pressure difference across the landfill cover.”

Standard dispersion modelling calculates pollutant concentrations produced by a source with a known emission rate. Inverse dispersion modelling reverses these calculations to estimate unknown emission rates from measured downwind pollutant concentrations. Local measurements and inverse dispersion modelling approaches could, therefore, contribute to improved emission estimates for regulated facilities. However, the mathematical challenge of inverse dispersion modelling to find emissions locations and/or emission rates from concentration measurements can form an “ill-posed problem” when fewer measurements than parameters to find are available and multiple solutions may exist (Borowski and Borwein, 1989). It can also behave as an unstable or ‘ill-conditioned’

problem, where small changes in input parameters can cause big changes in outputs. Therefore, it is important for approaches to be tested for sensitivity to inputs and resulting output uncertainties. There are also challenges where measurements are taken during short-term campaigns but are used to quantify longer-term emissions, if the emissions are expected to vary with time.

This project began with a literature review of different inverse dispersion modelling approaches that have been used to quantify fugitive emissions of methane and other gases from point and area sources from concentration measurements. It then considered which of these methods are suitable to apply to source types regulated by the Environment Agency and tested a selection of these methods. Finally, some recommendations relating to inverse dispersion modelling approaches have been compiled.

Section 2 of this report lists available inverse dispersion modelling techniques identified through a literature review, presenting a method description for each technique, along with information about data requirements, constraints and uncertainties. Section 3 describes some common challenges which apply to many of the available inverse dispersion modelling techniques. The applicability of inverse dispersion modelling techniques to different source sectors is discussed in section 4. Section 5 describes the testing of selected inverse dispersion modelling techniques, using data supplied by the Environment Agency. Recommendations for further use of inverse dispersion modelling and the production of standard methods are proposed in section 6.

2. Inverse dispersion modelling techniques

2.1. Literature review scope and context

This section is derived from a literature review of available inverse dispersion modelling techniques. The review was carried out with an initial online search of journal articles, with relevant references followed up from leading papers. A small number of relevant reports and articles were recommended by the Environment Agency. The review is not intended to give an exhaustive list of studies, but to form a representative survey of reported techniques with examples of their development and application. More detailed information is included for techniques where a wider range of studies have been identified.

The literature review focused on emissions, dispersion and measurements in outdoor air, although examples of inverse dispersion modelling were also found relating to gas transport in soil (Jung and others, 2011) and within buildings (Sohn and others, 2002). This review considers techniques which are appropriate for identifying and quantifying individual or local sources (extending up to a few kilometres) rather than regional or global inventories, as considered by Hartley and Prinn (1993), Cui and others (2015), Henne and others (2016) and the IMPLiCIt project (O'Dowd and others, 2020). This study is primarily focused on deriving routine emissions, matching the Environment Agency's regulatory interests, although some techniques were originally developed in the context of emergency releases.

The rest of this section outlines some general principles of inverse dispersion modelling to give context to the information about specific techniques in sections 2.2 and 2.3. Section 2.1.1 describes the early history of inverse dispersion modelling and identifies some helpful reviews of multiple techniques. General data requirements for inverse dispersion modelling are discussed in section 2.1.2. Optimisation methods are generally used in combination with inverse dispersion modelling, in order to find the 'best' combination of emissions to fit the measured concentrations; a selection of common optimisation methods is described in section 2.1.3. Section 2.1.4 summarises the aims of inverse dispersion modelling in relation to total emissions from a site or identifying individual sources within a site.

2.1.1. Applications of inverse modelling

Early applications of inverse dispersion modelling and emissions estimation were developed in relation to emergency response modelling, as reviewed by Rao (2007). Volcanic emissions have also been a key driver for the development of emissions estimation methods, for example, as described by Boichu and others (2013). Trégourès and others (1999) and later Babillotte and others (2010) compared methods of estimating landfill emissions using measurement methods, including some simple inverse dispersion modelling. A review by Mønster and others (2019) gives a helpful overview of a wide range of different methods for measuring landfill methane emissions, including advantages and disadvantages, with some consideration of associated inverse dispersion modelling

techniques. Yeşiller and others (2022) also considered and compared multiple methods for assessing landfill methane emissions. There is considerable overlap between the measurement techniques used for landfill emissions and those suitable for onshore oil and gas (OOG) facilities identified in the Environment Agency's project report SC210006/R (EA, 2022). Fewer studies have been identified relating to biogas or wastewater emissions.

2.1.2. Inverse dispersion modelling requirements

All inverse dispersion modelling methods have aspects in common, such as the requirement for sufficient measurement data, generally at multiple locations. Near-field (<1 km from source) or far-field measurements are suited to different modelling techniques, as are short-term and long-term measurement campaigns. Different approaches also have varying requirements for the timescale and sensitivity of measurements, relative to turbulent fluctuations; travel speed of measurement equipment for mobile measurement approaches; and/or expected variation in source properties. For example, plume transect approaches, where measurements are taken moving through a plume approximately perpendicular to the wind direction, require measurements at a temporal resolution which can resolve the changing concentrations as the sensor moves through the plume. The faster travel speed for airborne sensors compared to ground vehicle-based sensors requires higher measurement frequencies for the sensors used in airborne applications, usually associated with higher costs. However, the temporal resolution on which emissions variations can be captured is often limited by the time taken to traverse the plume, while there is also a need for multiple measurements/transects to reduce uncertainties.

2.1.3. Optimisation methods

Many inverse dispersion modelling techniques require optimisation methods to find the best combination of source properties and dispersion for matching measured data. Optimisation procedures use a cost function, in the simplest case the difference between modelled and measured concentrations, and an iterative method for adjusting source parameters to reduce the value of this cost function. Cost function values may be allowed to increase between some iterations of the optimisation in order to allow the solution to move away from local minima towards an overall (global) minimum of cost function. Examples of optimisation algorithms which have been applied within inverse dispersion modelling include:

- non-negative least squares, which iterates through solutions fitting the non-negative criterion towards lower values of a quadratic cost function. This requires an assumption that all parameters have Gaussian probability distributions
- genetic algorithms, where an initial selection of possible input parameter values are tested, then 'successful' configurations are combined and modified to define properties for subsequent iterations. This approach was inspired by evolutionary processes of genetic variation, reproduction and natural selection
- simulated annealing, which by analogy with controlled metal cooling or heat treatment processes allows increases in cost function between some iterations, in order to be able to escape local minima in the set of possible

solutions and find a global minimum of the cost function. Increases in cost function are more likely to be accepted between earlier than later iterations

Markov Chain Monte Carlo algorithms are an approach to deriving the probability distribution for source parameters. Monte Carlo analysis refers to a process of modelling large numbers of possible solutions, then repeatedly taking random samples from the full set of solutions in order to derive probability distributions of the output relative to input parameters. The resulting probability distributions may take any form. The Markov chain approach makes the selection of the next sample for Monte Carlo analysis dependent on the current sample. This approach covers the full probability distribution more efficiently than standard Monte Carlo by reducing the number of samples (model configurations) required, especially for problems with large numbers of input variables. Markov Chain Monte Carlo techniques have also been applied as an optimisation approach for finding the most likely combination of source parameters to match an observed pattern of concentrations, with associated uncertainties.

2.1.4. Aims of inverse dispersion modelling

Existing inverse dispersion modelling techniques have been developed with varying aims, in relation to (a) total emissions across a combined source area, and/or (b) more detailed location and emission identification within a group of sources. While the current project is targeted at improving the representation of whole-site emissions, techniques which allow consideration of within-site variation may also help to improve understanding of onsite processes. Measurements suitable for determining within-site emissions are likely to be made closer to the source(s), before a composite plume has formed, leading to stronger but less homogeneous signals. For whole-site methods, a balance must be found between i) measurements made nearer to the source, with stronger signals but more heterogeneity, which may lead to a poorer estimate of the whole site emissions, or ii) measurements made further from the source, with more homogenous plumes but weaker signals, which may be harder to distinguish from background or other sources. The optimal balance would minimise the uncertainty in the resulting total emission.

The following discussion is divided into methods generally used for determining (a) total site emissions (section 2.2), and for (b) distinguishing individual emissions sources within a site (section 2.3). Within the sections, approaches are described in approximate order of increasing complexity. The data required, constraints on application and uncertainty of resulting emissions estimates have been summarised for each approach. Section 2.4 covers additional approaches for calculating emissions from concentration measurements without explicit dispersion modelling.

In general, the inverse dispersion modelling approaches for whole sites use less complex mathematical approaches than methods which attempt to identify sources within sites. In principle, approaches capable of within-site application could also be used to determine total emissions. Similarly, some whole-site methods could possibly be applied separately to individual well-spaced sources from a single large site. Within-site methods can be valuable for identifying a specific significant source among other more diffuse emissions, such as a leak from pipework at an OOG site.

2.2. Whole-site inverse dispersion modelling methods

Inverse dispersion modelling methods applied to measure and derive whole-site fugitive emissions include:

- horizontal plume transect measurements with 1D Gaussian profile fitting
- 2D vertical plane measurements with bi-Gaussian fitting
- airborne mass balance measurements
- single point measurements sampling a plume transect from varying wind directions
- Gaussian dispersion modelling using direct search with simulated annealing

Each of these approaches is described in the following sections.

2.2.1. Horizontal plume transects with 1D Gaussian profile fitting

Method description

Whole-site emissions are estimated by fitting a simple Gaussian profile to horizontal near-ground plume transect measurements, typically using least-squares fitting. This method was described by the US Environmental Protection Agency (EPA) OTM 33a methodology (Thoma and Squier, 2014). It was applied to Walleys Quarry Landfill in the SC210019 report (Rees-White and Beaven, 2022), with transects carried out at 3 downwind distances, comprising measurements of methane and hydrogen sulphide. Fredenslund and others (2019b) used it as a screening method for categorising methane emission rates from closed landfill sites in Denmark. It has also been applied to UK biogas plants, for example, by Bakkaloglu and others (2021).

Data required

Concentration measurements are made with vehicle-based equipment driven along roads approximately perpendicular to the wind direction and sufficiently downwind for a combined plume to have formed from all on-site sources. The measurements should capture the full horizontal extent of the plume from the targeted site, with a clear increase in concentrations above local background levels when measurements proceed across the plume from its edge to its centre.

Simultaneous meteorological data are required to identify the wind direction and atmospheric stability for Gaussian profile fitting.

Data from multiple plume transects (at different distances from the site and/or repeated measurements from the same distance) are recommended for reducing uncertainties, for example, Fredenslund and others (2019b) used 4 transects for each site.

Constraints

Sources should be isolated from other emissions of the targeted pollutant (for example, methane), as in the simplest implementations no consideration is given to concentrations upwind of the site. It may not be possible to fit a Gaussian profile to measurements influenced by multiple distinct sources.

Emissions from the targeted site must generate concentrations which form a detectable plume at the transect road. Bakkaloglu and others (2021) were able to detect methane plumes from only 10 biogas sites out of 56 surveyed. The authors suggest that measurements could not be made close enough to 8 sites, 7 did not have suitable wind direction for plumes to be detected at public roads during the survey, and 9 were too close to other methane sources to have simple Gaussian plume shapes. 22 sites had suitable access and favourable atmospheric conditions (possibly only considering wind direction) during the surveys, but may not have been operating/emitting at the time of the survey. The lack of measured signals leading to sites being excluded from the study could also be due to plumes emitted at height not dispersing down to the near-ground measurement height.

Caulton and others (2018) suggest that measurements should be made within 300m of the site, partly in order to make sure that measured plumes could be associated with a specific visible (OOG) site, although this may be too close for a combined plume to have formed for larger sites. Fredenslund and others (2019b) made measurements at distances of 100 m to 2,200 m from closed landfill sites, with measurements required closer to lower-emitting sites due to detection limits.

Meteorological conditions should be broadly uniform for the duration of each transect, to ensure that measurements cover a full plume and are representative. Emissions are assumed to be constant on the timescale of a single transect (15 minutes or more). The precise limits for meteorological variability will depend on the details of the specific source and study, such as the source size and downwind distance to the transect measurement locations.

The simplified Gaussian plume expressions used to calculate emission rates tend to assume that the source, plume centreline and measurement heights are all identical. This assumption is reasonable for near-ground non-buoyant releases and near-ground measurements except in highly convective meteorological conditions. It is not suitable for buoyant releases (for example, flares) or releases with substantial initial vertical momentum (for example, tank depressurisation). USEPA OTM33 suggests that this method should not be used with source heights of more than 25 feet (7.6 m) due to the chance of the plume centreline passing over the measurement equipment. Some authors have extended the method to include the effect of source height, such as Bakkaloglu and others (2021).

The simplified Gaussian plume dispersion assumptions are best suited to sources located in flat, open terrain.

The Gaussian plume dispersion assumptions are not applicable in very low wind speed conditions, for example, < 0.75 ms^{-1} at 10 m above ground, where mean wind speed may be similar to turbulent fluctuation velocities in the along-wind direction, and mean wind directions have greater uncertainty.

The labour-intensive measurement method and restrictions on suitable meteorological conditions mean only intermittent short-term measurements tend to be available for this approach.

Uncertainty

Fredenslund and others (2019b) used this method for screening emission rates from Danish landfill sites, but found low accuracy compared to tracer dispersion methods (section 2.4.1). They estimated emissions by fitting a Gaussian plume to measurements made along a 1D transect, and found that the estimates from fitting were 72% of those derived from tracer dispersion. They found the estimated emission rates were sensitive to the assumed stability parameters; input wind speed and direction; land surface type ('urban' or open); and source-measurement distance. The relative uncertainty in source-measurement distance is greater for measurements made close to site boundaries than those made further downstream. The minimum detectable emission rate varies with measurement equipment, atmospheric conditions and downwind measurement distance, with an average value of 0.15 kg $hour^{-1}$ across all sites in this study.

Bakkaloglu and others (2021) attempted to calculate methane emission rates from all UK biogas plants based on their survey of 32 sites, with 10 detected plumes. They generated a lower bound estimate by assuming that the 22 sites with no detected plume had no emissions, and an upper bound estimate by assuming that all sites emit similarly to the 10 sites with detected plumes.

2.2.2. 2D vertical plane measurements with bi-Gaussian fitting

Method description

A similar approach to horizontal plume transects (section 2.2.1) but with measurements expanded to cover a 2D plane is sometimes referred to as 'vertical radial plume mapping' (VRPM). This approach is described in the US EPA OTM 10 methodology (Thoma and others, 2010). The approach aims to measure mass flux through a virtual vertical plane downwind of a site, approximately perpendicular to the plume centreline, with fitting of bi-Gaussian profiles to the planar profiles to estimate emissions. The use of vertical plane measurements may be more likely to capture plume centrelines in conditions where the plume centreline is above ground, provided that the vertical plane is sufficiently large to capture the full extent of the plume. However, the VRPM analysis assumes that the vertical peak concentration is located at ground level. Optical measurement techniques and smooth basis function minimisation fitting have been used with this method as described by Hashmonay and Yost (1999), Hashmonay and others (2001), and Wu and others (2014), all with open-path Fourier transform infrared spectrometer measurements. Shah and others (2019) and follow-up work in Shah and others (2020) describe a similar

approach but with measurements from an unmanned aerial vehicle (UAV) connected to a ground-based sensor and least squares Gaussian fitting.

Data requirements

Vertical plane measurements of concentration are required. Ideally, the measurement plane should cover the full 2D cross-section extent of the targeted plume. However, this can be challenging for large landfill sources. The US EPA methodology suggests that the area source length scale (for example, largest across-source distance) should be <75% of the horizontal extent of the measurement plane, with a distance from the source also <75% of the measurement plane horizontal extent. Simultaneous meteorological measurements are required for flux calculations, ideally including wind speeds at multiple heights.

Constraints

Similar to the 1D plume transect and Gaussian fitting method described in section 2.2.1, this method requires relatively consistent meteorological conditions throughout the measurement period, so that the measurement plane remains downwind for fixed optical measurements or during the time taken to traverse the measurement plane for UAV measurements.

Emissions are assumed to remain constant during each measurement period. Optical methods can scan the measurement plane in a few minutes, but measurements from several scans are generally combined to reduce uncertainties, giving an effective measurement period of around 15 minutes. Shah and others (2020) report UAV-based measurement survey periods of 8 to 9 minutes.

Optical measurement equipment could be left in place for long-term measurements, but would only provide useful data for wind directions and meteorological conditions where the plume is fully captured in the measurement plane, while UAV measurements are only available for short-term traverses.

Assumptions can be required to represent concentrations below the base of the measurement plane, which is likely to be higher above ground for UAV-based sensors than for optical approaches.

Sources should be isolated from other emissions of the targeted pollutant (for example, methane), as, by default, no consideration is given to concentrations upwind of the site.

It may not be possible to fit bi-Gaussian profiles to measurements influenced by multiple distinct sub-sources within the overall area of the target source.

The simplified Gaussian plume dispersion assumptions are best suited to sources located in flat, open terrain.

The Gaussian plume dispersion assumptions are not applicable in very low wind speed conditions, for example, <0.75 ms^{-1} at 10 m above ground, where mean wind speed may

be similar to turbulent fluctuation velocities in the along-wind direction, and mean wind directions have greater uncertainty.

In strongly convective atmospheric conditions, the increased vertical mixing may cause difficulty with capturing the full vertical extent of the plume in the measurement plane.

UAV safety considerations would prevent this method being used with UAV measurements in high wind speeds, for example, >6 to 10 ms^{-1} at the survey height.

Uncertainty

Abichou and others (2010) explore the uncertainties of this method in relation to simulated landfill sources, in particular describing challenges with:

- sources which are larger than the extent of the measurement plane
- sources located too close to or far from the measurement plane, such that plumes are not well formed or concentrations are close to sensor detection limits
- and/or plumes not fully covered by the measurement plane due to wind direction shift

There can be additional uncertainty in this approach where separate plume signatures are found in the plane, not well matched to the bi-Gaussian assumptions. Abichou and others (2010) estimated uncertainties as:

- -34% to 190% due to spatial heterogeneity of source emissions, estimated from data simulating dispersion from 2 small sources at increasing separation distances (the tendency to overestimate total emissions may relate to the fitting of a single-peaked bi-Gaussian profile to the twin-peaked ‘measurements’)
- ±20% due to change in wind direction during testing
- ±10-30% due to estimates of area contributing to flux, a function of atmospheric stability class

Hashmonay and others (2001) found a tendency for the vertical plane measurement method with optical measurements to underestimate emissions from controlled releases by 10 to 15%. Shah and others (2020) report uncertainties from -83% to +127% with UAV-based measurements, with again a small tendency to overestimate controlled release emissions.

Thoma and others (2010) excluded cases from a database of controlled releases where:

- the plume centreline was close to the edge of the measurement plane, defined as within 20% of the horizontal plane length from an edge, such that the plume was incompletely captured in the plane
- the wind direction led to a plume centreline approaching the measurement plane at an angle >60° from perpendicular, leading to increased uncertainty in the plume capture

2.2.3. Airborne mass balance

Method description

A further extension to the approach of planar plume cross-section measurements (described in section 2.2.2) has used aircraft-mounted sensors to calculate mass balance between flux through upwind and downwind sides of a cylindrical or spiral flight-path above and encircling the source. In the simplest form it is not strictly an inverse dispersion modelling technique, but it can be used in combination with plume fitting methods in order to form a more complete representation of downwind concentrations and a better estimate of emission rates. This approach has been described by Nathan and others (2015), Conley and others (2017) and Yeşiller and others (2022). The explicit measurement of upwind concentrations allows this method to be used for sites with other nearby sources, as long as the aircraft trajectory can distinguish the different plumes. It is also likely to be best suited to sources with larger length scales (for example, >1 km) and higher emission rates when using crewed full-scale aircraft.

Data requirements

Measurements are made with airborne concentration sensors with simultaneous flight data and wind speed measurements. The travel speed of aircraft requires high-frequency measurement equipment to resolve plumes. Conley and others (2017) determined that 20 to 25 measurement circuits around the plume are needed to produce a statistically stable estimate of emission rate.

Constraints

The minimum measurement height associated with aircraft, especially crewed aircraft, can make it difficult to capture pollutant transport near ground accurately. This makes this method best suited for sources and/or meteorological conditions where emissions rise above the ground.

The use of aircraft means that measurements are only available for short-term traverses. Nathan and others (2015) used a battery-powered UAV (model aircraft) for flights of around 6 minutes duration, making 4 to 8 circuits of the targeted source (OOG compressor station) in each flight. For crewed aircraft, the measurement time is likely to be determined by cost constraints. In both cases, it would not be possible to assess longer-term emissions variation with this approach.

Emissions are assumed to remain constant throughout the measurement period (approximately one hour in Conley and others (2017)).

Aircraft safety requirements could prevent this method being used in very strong winds. For UAV, this limit may be >6 to 10 ms^{-1} at the maximum measurement height.

Uncertainty

Cambaliza and others (2017) report emission rate ranges suggesting uncertainties of ±50%, while earlier work from the same group estimated uncertainties from this method at around ±30% (Cambaliza and others, 2014). Conley and others (2017) aimed to specify emission rates with this method to within ±20%. Nathan and others (2015) estimated uncertainties in emission rates of ±55% through statistical analysis. This is within the range reported by Shah and others (2020) for 2D plane measurements using UAV.

2.2.4. Stationary plume transect from single location measurements

Method description

An alternative approach to analysing a 1D plume transect has been developed using high-frequency single location measurements with simultaneous high-frequency wind direction measurements in order to measure a cross-plume profile as the wind direction varies across the sensor. This approach is also part of the USEPA OTM 33A methodology (Thoma and Squier, 2014), and has been applied by Brantley and others (2014), Lan and others (2015) and Foster-Wittig and others (2015).

Data requirements

High-frequency simultaneous concentration and wind measurements, including turbulent intensity and standard deviation of wind direction are required. Mobile measurement equipment allows a suitable location for stationary measurements to be selected by first driving along a downwind transect and stopping near the location of the peak concentration for a longer stationary measurement period. The analysis for calculating the emission rate is carried out on the stationary measurements rather than the initial mobile survey.

Constraints

The measurement location needs to be broadly downwind, but the wind direction needs to be sufficiently variable during the measurement period to allow sampling of a full crosswind plume profile.

Emissions are assumed to be constant during each measurement period (approximately 20 minutes).

Simplified Gaussian profile assumptions also limit the range of meteorological conditions for which this approach is applicable, for example, Gaussian plume assumptions are not valid in very low wind speed conditions (<0.75 ms^{-1} at 10 m above ground).

Similar to 1D transect measurements with moving sensors (section 2.2.1), there is an implicit assumption of identical source, plume centreline and receptor heights, which is not robust for all fugitive source types or in strongly convective atmospheric conditions.

This type of measurement could be carried out on a long-term basis, but might need multiple measurement locations surrounding a site in order to capture useful data in a wider range of wind directions.

Uncertainty

An uncertainty analysis for this approach in relation to known releases was carried out by Edie and others (2020). They found errors in estimated emissions of -75% to 50% for idealised releases in open terrain, but -60% to 170% for releases from simulated OOG equipment. Larger percentage errors were generally related to smaller emission rates (<0.5 kg hour^{-1}), with a tendency to overestimate smaller releases. More than 85% of the estimated emission rates were within ±50% of the known value.

Lan and others (2015) also explored uncertainties in emissions estimates from this approach using Monte Carlo sampling with varying input parameters, and comparisons of the derived emissions with controlled releases. Their calculated uncertainties in emission rates range from -28% to 81% for different OOG well pad sites, with uncertainties up to a factor of 3 for larger emitting OOG sites (compressor stations).

Brantley and others (2014) used a 3-part data quality filtering process, requiring peak concentration within ±30° of source direction; average in-plume concentration greater than 1 ppm; and a Gaussian fit with R^2 >0.80. 77% of their controlled release measurements and 71% of field study measurements met these criteria. Using this filtering, the authors found errors in emissions compared to controlled releases in the range -60% to 52%, with 72% of emission rates within 30% of the known rate.

Uncertainties found for controlled releases from point sources may be lower than those that would apply to real-world area sources, which are less likely to generate clean Gaussian concentration profiles.

2.2.5. Gaussian plume modelling with direct search

Method description

Thomson and others (2007) aimed to locate and estimate the emissions of a fugitive source in desert surroundings based on a small number of measurement locations. They used a simple Gaussian representation of dispersion from a grid of possible source locations with an iterative direct search algorithm to explore possible source distributions. The direct binary search method was developed in the context of hologram image processing (Seldowitz and others, 1987). It involves randomly perturbing one image component and evaluating the resulting cost function change to identify improvements. Thomson and others (2007) combined direct search with the simulated annealing optimisation approach to minimise the cost function of modelled concentrations compared to measurements.

Data requirements

A spatial array of concentration measurements within or around the source area are required. Thomson and others (2007) used the same measurement equipment for 15 minutes at each of 7 downwind locations in turn; this approach requires consistent meteorological conditions throughout the ~4hour overall measurement period.

Constraints

Care is required to define a suitable cost function which does not lead to spurious source locations related to noise in the measurement data set; these authors implemented cost functions which prioritise smooth distributions and minimise total emissions.

The use of simplified Gaussian dispersion expressions limits the meteorological conditions in which this approach could be applied. For example, Gaussian plume assumptions are not valid in very low wind speed conditions (<0.75 ms^{-1} at 10 m above ground).

It is likely to have higher computational expense than the simple 1D or 2D Gaussian fitting approaches. More than 4 million iterations of the search algorithm were required to reconstruct a source grid defined using 16 x 16 cells.

The approach of moving measurement equipment between different sites can require consistent meteorological conditions over long time periods.

Uncertainty

Thomson and others (2007) focused on the qualitative location of a controlled release and did not quantify the calculated emission or associated uncertainty.

2.3. Within-site inverse dispersion modelling methods

Methods used to distinguish emissions sources within a site with inverse dispersion modelling include:

- high-resolution spatial survey monitoring
- Backward Lagrangian stochastic approaches following backward trajectories of ‘parcels’ of air from sensors to likely source locations
- semi-analytical inverse Gaussian plume approaches
- Bayesian frameworks incorporating Gaussian plume or Lagrangian dispersion models
- Gaussian plume modelling with genetic algorithm optimisation
- adjoint modelling in complex flow fields
- machine learning

Each of these approaches is described in the following sections.

2.3.1. High-resolution spatial survey monitoring

Method description

Golston and others (2018) describe a conceptually simple approach to identifying and quantifying fugitive emissions based on high resolution spatial surveying with UAV-mounted sensors. The measurements are post-processed using simple identification of peak concentration locations. Emission flow rates are estimated by inverse correlation with wind speed. The approach of associating emission rates with wind speed includes an implicit modelling assumption of steady state dispersion. This is a relatively new approach with the emerging technology of UAV sampling, so has not yet been widely implemented.

Data requirements

High-resolution (<1 m) spatial survey(s) of concentrations above source of interest, with simultaneous meteorological data are required. The approach of measuring very close to sources, where concentrations are highest, has lower requirements for measurement equipment sensitivity than measurements further downstream.

Constraints

The small areas covered in each high-resolution survey flight, for example, 12 x 12 m, limited by UAV flight times, would suit small source areas and might not be easily extended to large landfill sites.

Improved spatial accuracy of leak detection was found by combining concentration measurements from multiple flights.

The use of UAVs limits this approach to short-term survey measurements.

UAV safety considerations would prevent this method being used in high wind speeds, for example, >6 to 10 ms^{-1} at the survey height.

Uncertainty

Golston and others (2018) identified strong sensitivities of the derived source location to errors in measurement positions and the quantity of measurement data available. The estimated emission rates showed different sensitivities to input bias and/or noise in development and validation test scenarios. Estimated flow rates were reported within 25% of controlled releases.

2.3.2. Backward Lagrangian stochastic approaches

Method description

Lagrangian flow models track ‘particles’ of air to generate flow trajectories, and can be used to calculate ‘backward’ trajectories from measurement locations to identify fluxes from likely source area(s). This backward Lagrangian stochastic approach is used in the

WindTrax2.0 software[1], with some simplified representations of atmospheric turbulence, as described by Flesch and others (1995, 2004), and further applications by Gao and others (2008), Riddick and others (2017) and You and others (2021). Bühler and others (2022) applied this method to biogas and wastewater sources, including testing assumptions about whole-site or within-site emissions. This approach can be applied to total site emissions or to distinguish within-site sources, although separating nearby sources can be challenging, whereas the total emissions may be more reliably estimated.

Data requirements

Concentration measurements from at least as many locations as sources with unknown emissions are required. For example, if there are 4 separate suspected leak sources within an industrial site, measurements from at least 4 monitoring locations would be required to calculate emissions from each leak. For whole-site applications, only one downwind measurement location is required. However, using measurements from multiple locations may increase confidence in the resulting emissions and/or allow calculations to proceed for a wider range of wind directions.

Meteorological conditions to define mean wind flow, atmospheric stability and surface roughness length. Averaging periods of 15 to 30 minutes are typical. This approach could be used with either short-term or long-term measurement data. It can use transect or optical linear measurements as well as individual point measurements. Bühler and others (2022) used linear optical measurement data both upwind and downwind of the targeted sites to help separate targeted emissions from other nearby sources.

Constraints

The flow calculations are likely to fail in low wind speed and/or very stable conditions. Riddick and others (2017) excluded periods from modelling when the measured wind speed (at 2 m above ground) was below 0.15 ms^{-1}. Flesch and others (2004) found reduced accuracy of emissions estimates with surface friction velocity (u_*) below 0.15 ms^{-1} and/or with magnitude of Monin-Obukhov length below 2 m.

If no concentration measurement locations are predicted to be influenced by a particular source, no emissions estimate can be made for that source.

If there are flow obstructions such as buildings and/or fences between sources and measurement locations, a distance of at least 10 to 15 obstacle heights between sources and measurement locations is recommended.

[1] Freely available from http://www.thunderbeachscientific.com/, however the software licence conditions require permission from the developers for any commercial application.

WindTrax documentation recommends that the maximum distance between source(s) and sensor(s) should be approximately one kilometre.

Uncertainty

Uncertainties in estimated emission rates arise primarily due to inaccuracies in the input wind speed and stability class data used to characterise dispersion. WindTrax divides particles into 10 subgroups and calculates the model error from the standard deviation of mean values derived from each subgroup. Using more computational particles reduces the standard error reported by the model but increases computational time. For example, the study reported in section 5 used 1,000,000 particles for both forward (point source) and backward (area source) modelling within WindTrax, with average run times of almost 2 hours per model calculation. These run times were too long to allow repeated sensitivity runs.

Flesch and others (2004) report an uncertainty of ±36% in calculated emission rates compared to a controlled small area source release.

Bühler and others (2022) compared total emissions estimates calculated using either a single source to represent a wastewater site or more detailed modelling with multiple sources. They found differences of up to 43% in the total emissions between these 2 approaches, giving an indication of the level of uncertainty associated with simplifying site emissions to a single source.

2.3.3. Semi-analytical Gaussian plume inverse dispersion modelling

Method description

Semi-analytical approaches have been used to calculate inverse Gaussian plumes for multiple sources and receptors, for example, using a linear least squares solution as reported by Lushi and Stockie (2010) using deposition measurements. This approach uses known or assumed source locations (for near-ground and/or elevated sources) and aims to quantify emission rates. A similar approach was extended by Hosseini and Stockie (2016) to allow time-varying emissions with mixed receptor timescales, using Markov Chain Monte Carlo optimisation in a Bayesian framework to find the best set of emissions compatible with available measurements.

Data requirements

This approach can be used with either short-term or long-term measurement data. It has been used with deposition measurements as well as concentration data. It requires pollutant measurements from multiple locations, along with meteorological data.

Constraints

The use of somewhat simplified Gaussian dispersion, with discrete stability classes, may increase uncertainty in strongly convective or stable conditions. Hosseini and Stockie (2016) assumed constant neutral stability throughout their modelling period and showed substantial sensitivity of the derived emission rates to this assumption.

The simplified Gaussian plume dispersion assumptions are best suited to sources located in flat, open terrain.

The Gaussian plume dispersion assumptions are not applicable in very low wind speed conditions, for example <0.75 ms^{-1} at 10 m above ground, where mean wind speed is similar to turbulent fluctuation velocities in the along-wind direction, and mean wind directions have greater uncertainty.

Fugitive emissions from area sources are approximated by a single point source at the area centroid.

Uncertainty

When testing the method with synthetic data, Hosseini and Stockie (2016) found that the mean emission rate and time-variation of sources with larger emissions magnitudes were identified more accurately than sources with lower emission rates. They estimated an uncertainty range of ±15-18%. This is likely to be lower than would be found with more complex real data.

2.3.4. Bayesian inversion frameworks

Method description

A Bayesian inversion approach, solving a cost function between measured and modelled concentrations by non-negative least squares and matrix inversion techniques, has been described in relation to both regional and local-scale modelling by Boichu and others (2013), Thomson and others (2017), Carruthers and others (2019) and Pelley and others (2021). This technique is applied to known source location(s) with initial emission estimates to improve emission estimates, for example, for volcanic or road traffic emissions. Using more complex dispersion models (NAME – Jones and others (2007), ADMS – Carruthers and others (1994) and CERC (2023)) allows this technique to be applied in a broader range of meteorological conditions than those using simplified dispersion. It can also be used for both near-ground and elevated sources. The development of this method for operational use (especially in relation to volcanic emissions) has led to improved computational efficiency.

A further application of a Bayesian inference approach for inverse dispersion modelling, with dispersion from sources to receptors calculated using the ISCST3 model (US EPA 1995), was described by Goyal and others (2005). This approach used multiple non-linear (logarithmic) regression techniques to find unknown stack (elevated point source) and fugitive (near-ground area source) emission rates, with a Markov Chain Monte Carlo optimisation method. These authors also incorporated a ‘hierarchical’ framework with initial calculations for separate sites and subsequent assumptions about common factors in calculations across multiple sites. The approach was developed with small numbers of receptors per site and averaging daily measurements into monthly values, which reduces the temporal resolution of the derived emissions.

Data requirements

This technique requires an initial assumption of source location(s) and emission rates, along with modelled dispersion using meteorological data. The Bayesian framework requires estimates of the uncertainties in and co-variances between concentration measurements and source emissions. It can be applied with either short-term or long-term measurement data.

Constraints

When using discrete concentration measurement locations, emission rate adjustments will be most robust for sources which influence at least one of these locations.

Care is required in estimating the uncertainty and covariance values for concentration measurements and source emissions.

When using Gaussian plume dispersion models (ADMS, AERMOD, ISCST3) the underlying assumptions are not applicable in very low wind speed conditions, for example, <0.75 ms^{-1}, where mean wind speed may be similar to turbulent fluctuation velocities in the along-wind direction, and mean wind directions have greater uncertainty. However, alternative modelling approaches may be used in low wind speed conditions, such as radial dispersion in the ‘calms’ module in ADMS.

Uncertainty

Within the group of studies beginning from Boichu and others (2013), the uncertainty in transport and dispersion modelling has been neglected or treated as part of the measurement uncertainty. Therefore, part of the resulting adjustment of emissions from initial assumptions may compensate for inaccuracies in input meteorological data and/or dispersion calculations. The uncertainty in the derived emissions may be increased by other unknown sources nearby if not included in the modelling. Uncertainties are likely to be reduced by using measurement data from larger numbers of locations and longer periods. The uncertainties of this method are to some extent constrained by the initial emissions estimates and associated uncertainty and covariance values. However, they have not yet been quantified in relation to controlled releases.

2.3.5. Gaussian plume dispersion with genetic algorithms

Method description

An approach to establishing both source location and emissions, taking account of uncertainties in meteorological data, has been described by Allen and others (2007), with further development and/or applications by Kormi and others (2018), Bel Hadj Ali and others (2020) and Yeşiller and others (2022). This approach relies on repeated forward dispersion modelling with simplified Gaussian plume expressions, with potential source combinations developed according to ‘genetic algorithms’. These adjust properties towards an optimum solution based on combining and modifying successful solutions from a previous iteration. This approach was originally developed to use landfill surface

concentration measurements, but was extended by Bel Hadj Ali and others (2020) with UAV concentration surveys and downwind plume transect measurements, finding limitations with UAV-mounted sensor sensitivities and a tendency for underestimating total emissions when using downwind plume transect measurements compared to surface surveys.

Data requirements

Concentration measurements at multiple locations with associated meteorological data for mean wind and atmospheric stability are required. Bel Hadj Ali and others (2020) implemented this technique with downwind transects, surface and aerial surveys. Surface survey measurements require site access. This approach is most likely to suit short-term measurement techniques due to computational expense.

Constraints

The stochastic element in the genetic algorithm can require multiple runs to ensure that a robust solution has been found.

The combination of repeated forward dispersion modelling calculations within a single optimisation run and the need for multiple optimisation runs makes this approach computationally expensive for substantial measurement data sets and/or large source areas. Allen and others (2007) explained that the use of simplified Gaussian dispersion algorithms was required because a more complex dispersion model such as SCIPUFF would lead to prohibitive computational costs for running the full system.

The simplified Gaussian plume dispersion assumptions are best suited to sources located in flat, open terrain.

The Gaussian plume dispersion assumptions are not applicable in very low wind speed conditions, for example, <0.75 ms^{-1} at 10 m above ground, where mean wind speed is similar to turbulent fluctuation velocities in the along-wind direction, and mean wind directions have greater uncertainty.

Uncertainty

When this technique is used to identify within-site emissions the sources with higher emission rates tend to be located more accurately and reliably than sources with lower emission rates. This is also true for other within-source inversion modelling methods.

The Gaussian plume dispersion and genetic algorithms approach relies on an accurate estimate of the number of individual sources within the source area.

Bel Hadj Ali and others (2020) assessed sensitivity of the estimated total emission rates in relation to errors in meteorological data, with strong dependencies on the assumed atmospheric stability class and measured wind speed.

Kormi and others (2018) report emission rate errors of below 20% for the sources with highest emission rates in a case study using synthetic data. Uncertainties in emission rates are likely to be higher when using real-world data. These authors also identified strong sensitivities of the estimated emission rates to errors in input atmospheric stability, wind speed and direction. They estimated total emissions within 15% in comparison to tracer gas measurements on a real closed landfill site.

2.3.6. Adjoint modelling in complex flow fields

Method description

Adjoint modelling is a method for calculating advection and dispersion backwards in time from receptor locations to form a ‘conjugate concentration field’, which indicates areas where a source could have contributed to the concentration reading at the detector. This approach is suited to problems with unknown source location(s) and relatively few receptors. It has been applied with a variety of dispersion modelling approaches with differing levels of complexity, although primarily Eulerian grid-based models.

Brereton and others (2018) describe adjoint optimisation modelling, using multiple sensors within the area of expected emissions, along with a pre-computed 3D wind field, to locate and quantify unknown emission sources from broadly downstream measurements. The optimisation loop comprises forward dispersion modelling of assumed source parameters using the modelled wind field, assessment of predicted concentrations against observations, followed by inverse dispersion modelling to assess sources upstream of each receptor and adjust source rates. The use of both forward and inverse dispersion modelling makes this approach computationally expensive, although subsequent developments have improved efficiency by pre-computing inverse tracer transport (Brereton and others 2019). It could be useful for capturing complex local flow and dispersion patterns around industrial infrastructure.

Liu and others (2021) implemented a regional application of adjoint modelling, in a simplified 2D transport and dispersion model, with the aim of improving operational forecasting of hazardous pollution events. A limited memory quasi-Newton line search method was used for error minimisation between modelled and observed concentrations. The assumption of inert particulates on regional spatial and temporal scales, along with only 2-dimensional transport and dispersion, increases computational efficiency but is likely to limit the accuracy of this approach.

Keats and others (2007) applied an adjoint of computational fluid dynamic (CFD) modelling in a Bayesian inference framework, taking account of uncertainties in modelled and measured concentrations. They implemented Markov Chain Monte Carlo optimisation to identify the most likely location and magnitude of short-term releases in urban areas with complex geometries. With the adjoint modelling and Markov Chain Monte Carlo techniques, the computational effort for a fixed spatial extent scales linearly with the number of measurement locations and the number of source parameters.

Data requirements

These approaches all use a sparse spatial network of concentration measurements. They rely on detailed 3D flowfield modelling, which requires information about mean meteorological conditions and physical obstacles to the flow (buildings, terrain).

Constraints

This approach is likely to remain more computationally expensive than methods which assume simpler flow fields and dispersion properties, and limit its application to short-term measurement data.

CFD models are generally limited to neutral atmospheric stability conditions.

Where releases occur in a zone of rapid mixing, for example in the wake of a building, it may not be possible to identify a precise source location within this zone.

Uncertainty

Keats and others (2007) carried out a careful derivation of probabilistic uncertainties associated with the method. The mean emission rate from a controlled release in an array of obstacles was identified with an error of around +20%. Brereton and others (2018) found a tendency for the approach to overestimate total emissions, by up to 24% for a case study in a complex 3D geometry. Causes of error in total emissions include predicting spurious small sources, while also missing small sources. The uncertainty in results might be reduced by measurement data sets including a wider range of wind directions.

2.3.7. Machine learning

Method description

Standard machine learning techniques, such as neural networks and decision trees, have not yet been widely applied to pollutant emission estimation problems. These techniques generally need known data for model development (‘training data set’) before they can be applied to find unknown data. Kia and others (2022) tested several different machine learning algorithms with tracer gas dispersion modelling using the Weather Research and Forecasting (WRF) model at 510 m spatial resolution, forcing surface concentrations to match measurements and assessing the flux rates required to maintain these. This approach would not be suitable for smaller sites due to the relatively coarse resolution of the dispersion modelling used, while the modelling assumptions may need further development.

Machine learning approaches may become more useful in exploring emissions variation with other parameters when more robust emissions estimates are available from another technique. Positive Matrix Factorisation (PMF) is another mathematical approach which can be used to assess the significant influences of other measured parameters on concentrations, but it is unclear whether it can be used to quantify emissions. The US EPA

is no longer developing its PMF model[2], with which users had reported difficulties when working with large data sets.

Data requirements

Initial training data set with a wide range of known emissions, other input parameters such as meteorological data and associated resulting concentrations are required.

Constraints

The constraints of this approach will depend on the method used to compile the training data set.

Most machine learning approaches infer relationships between cause and effect without seeking to explain the underlying mechanisms such as dispersion. This brings novel challenges for both quality assurance and stakeholder communication.

Uncertainty

Emissions estimates for combinations of inputs which were not included in the training data set will have increased uncertainty. Robust estimates of uncertainty have not yet been reported for this approach.

2.4. Other methods for estimating fugitive emissions

Two methods for estimating whole-site fugitive emission rates from concentration measurements do not involve inverse dispersion modelling. However, they share many characteristics with inverse dispersion modelling techniques and are useful to consider in comparison with inverse dispersion modelling methods. The additional methods are:

- tracer dispersion methods, which assume analogous dispersion of tracer and target gases during a controlled tracer release
- eddy covariance methods which measure net vertical transport

These methods are described in the following sections.

2.4.1. Tracer dispersion method

Method description

Controlled releases of tracer gases have been used to estimate fugitive emissions by assuming analogous dispersion of tracer and target gases. This is not strictly an inverse dispersion modelling method, but it shares some characteristics with the other methods

[2] https://www.epa.gov/air-research/positive-matrix-factorization-model-environmental-data-analyses

assessed in this study, in using ambient concentration measurements to derive emissions data. This method was used by Fredenslund and others (2019a) and Matacchiera and others (2019). Delre and others (2017) applied it to 5 Scandinavian wastewater sites to assess emissions of both methane and nitrous oxide (N_2O). The tracer dispersion method (TDM) has also been used in previous landfill monitoring studies for the UK Department for Environment, Food and Rural Affairs (Defra), described in Rees-White and others (2019) and Rees-White and Beaven (2020).

Data requirements

This method is centred on the controlled release of a tracer gas, with current practice favouring acetylene (C_2H_2). Downwind transect measurements are made of both the tracer and target gases, typically using vehicle-mounted sensors. Meteorological data are used to identify suitable downwind transect routes. Matacchiera and others (2019) used forward dispersion modelling to identify suitable locations for tracer release and transect measurements in differing meteorological conditions.

Constraints

When a point source tracer release is used to represent a larger scale target gas source (for example, landfill methane), there can be a mismatch of initial release properties including:

- release location
- release horizontal scale (point or area)
- release height (surface or above ground)
- plume rise (depends on release buoyancy)
- relative magnitude of background and in-plume concentrations

These discrepancies can become less important at larger distances downwind, but measurements further downwind require sensor equipment able to detect lower concentration increments of both tracer and target gases.

The tracer dispersion method may require the source of interest to be isolated from other sources of the target gas.

As with 1D transect measurement methods and Gaussian fitting (section 2.1.1), this method may fail to detect the plume if emissions and/or atmospheric mixing lift the plume substantially above the near-ground measurement height. Rees-White and Beaven (2020) had to abandon one survey as weather conditions changed from overcast to sunny. This meant that the tracer gas plume was no longer detectable in the transect measurements due to increased vertical mixing.

When measurements are made along crosswind trajectories, Fredenslund and others (2019a) found the best match of controlled release emissions with calculations when emissions estimates were based on simple arithmetic integration of raw tracer and target gas concentration measurements along the plume transect trajectory rather than fitting

Gaussian profiles. They also noted that real landfill plume measurements may not have clean Gaussian profiles due to heterogeneous spatial distributions of emissions within the landfill.

As with simpler plume transect measurements, the time required to make multiple transect measurements (4 to 5 minutes per transect, 10 to 15 transects recommended), in order to reduce uncertainties, limits the resolution with which emissions variations can be identified. However, it may be possible to make measurements in a wider range of meteorological and topographical conditions, subject to sensor detection limits, than for single pollutant plume transect methods as Gaussian profile dispersion assumptions are not used.

The use of controlled tracer gas release, which is likely to require site access, limits the duration for which this method can be applied.

Uncertainty

Fredenslund and others (2019a) report errors of ±10% for higher rate controlled releases but ±18% for lower releases. This increase in the magnitude of uncertainties with reducing tracer release rate may be associated with a reduced signal-to-noise ratio in the downstream measurements. This study also estimated overall errors as likely to be within ±20% when following best practice for measurements.

2.4.2. Eddy covariance

Method description

Eddy covariance measures net vertical transport of a pollutant through a horizontal plane and equates this to the surface emissions flux. This method has been described by Trégourès and others (1999), Lohila and others (2007), L. Zhang and others (2019) and You and others (2021). EddyPro software has been developed to process measurement data into flux values. Eddy covariance is a vertical net mass balance approach, and so does not fit strict definitions of an inverse dispersion modelling approach. However, assumptions or modelling are required to estimate the area of emissions source which may be contributing to the measured flux values.

Data requirements

Eddy covariance analysis is based on high-frequency simultaneous concentration and meteorological measurements, focused on vertical fluctuations. More general meteorological data is also needed to define atmospheric stability. Roughness length values for the ground surface are also required to give context to the meteorological data.

Constraints

This approach may not be suitable for heterogeneous area sources, as it assumes that the surface properties at the single measurement location and contributing emissions area are representative of the full source.

The eddy covariance method does not explicitly consider background concentrations around the target source. If background concentrations are spatially homogeneous and temporally slowly varying relative to a typical eddy covariance averaging time of 30 minutes, then they will not contribute to the net turbulent flux used to calculate emission rates.

This method fails in calm and/or strongly stable conditions with no vertical mixing, and may fail in conditions of heavy rain (Lohila and others, 2007).

Eddy covariance can estimate negative emissions values, which may not be physical.

Within each averaging period (typically 30 minutes), mean meteorological conditions are assumed to remain steady.

Eddy covariance measurements can be carried out on a long-term basis. As eddy covariance only captures emissions from a footprint area upwind of the measurement site, multiple measurement locations might be required around a site boundary in order to capture useful data in a range of wind directions.

Uncertainty

The calculation of the 'footprint' area contributing to the measured fluxes is dependent on measurement height, wind speed and assumed stability conditions and is a significant source of uncertainty. Kljun and others (2004) and Kljun and others (2015) present parameterisations of footprint area based on meteorological data, receptor height and surface properties, derived from Lagrangian dispersion modelling. Lohila and others (2007) report estimates of 90% of flux measured at a height of 2.5 m originating within 150 m of the measurement location. Trégourès and others (1999) found methane flux rates from eddy covariance techniques an order of magnitude lower than tracer gas or surface chamber measurements. This may have been due to a low measurement height for the eddy covariance data (1 m) capturing only a small area of the heterogeneous surface.

2.5. Summary

Some important criteria with simple categorisations have been developed to allow a consistent assessment of the characteristics of each inverse dispersion modelling method. This assessment is useful for considering which techniques are suitable for different source types and applications. There can be a balance between the uncertainty and cost associated with particular methods, so it may be appropriate to consider a low cost, high uncertainty method for an initial 'reconnaissance' survey, followed up with a higher cost, lower uncertainty method where high emissions are detected.

Table 1 gives a summary of the main aspects of each of the inverse dispersion modelling techniques considered in this section. Machine learning has been excluded as insufficient information was available. The row criteria are as follows:

- Widely used? Whether the method has been used by multiple groups and/or is well established for regulatory purposes (**L**ow/**M**edium/**H**igh).

- Site access? Whether the method requires site access (**Y**es/**N**o/**U**nclear or depends on implementation). Some methods can be applied with measurements/equipment either within or outside a site.
- Long-term? Whether the method can be used for long-term monitoring purposes (**Y**es/**N**o/**U**nclear or depends on implementation), compatibility with short-term monitoring data only is assumed by default.
- Complex terrain? Whether the method can be applied to sites in complex terrain or with other flow obstructions (**Y**es/**N**o/**U**nclear or depends on implementation).
- Elevated sources? Whether the method can be applied to sites with elevated sources (**Y**es/**N**o/**U**nclear or depends on implementation).
- Nearby sources? Whether the method can be applied to sites with other nearby sources of the same target pollutant (**Y**es/**N**o/**U**nclear).
- Uncertainty? Uncertainty in derived emission rates (**L**ow/**M**edium/**H**igh/**U**nclear).
- Cost? Estimated costs of method (**L**ow/**M**edium/**H**igh), considering both measurement and computational costs. Methods requiring greater specialist expertise are also assumed to have higher associated costs.

As an example of how the table contents can be used to select an inversion modelling method, consider a biogas site. These generally have a relatively small horizontal extent but can include tall tank structures, with potential leak locations up to 19 m above ground. An important requirement, therefore, is that methods are suitable for elevated sources. Within the whole-site methods, possibilities include 2D plane measurements (if the plane has sufficient vertical extent) or airborne mass balance. However, airborne mass balance is likely to have a disproportionate cost for this type of small site. Therefore, one of the moderate cost within-site options, such as Backward Lagrangian Stochastic or Bayesian inversion, may be more appropriate.

Table 1 – Summary of available inverse dispersion modelling methods

	Whole-site inverse modelling methods					Within-site inverse modelling methods						Other	
	1D horizontal plume transect (2.2.1)	2D vertical plane measurements (2.2.2)	Airborne mass balance (2.2.3)	Stationary plume transect (2.2.4)	Gaussian plume direct search (2.2.5	High-resolution spatial survey (2.3.1)	Backward Lagrangian Stochastic (2.3.2)	Semi-analytical Gaussian (2.3.3)	Bayesian inversion (2.3.4)	Gaussian, genetic algorithms (2.3.5)	Adjoint modelling (2.3.6)	Tracer dispersion method (2.4.1)	Eddy covariance (2.4.2)
Widely used?	H	H	M	H	L	L	M	L	M	L	M	H	M
Site access?	N	U	N	N	U	Y	U	N	N	U	U	Y	U
Long-term?	N	U	N	Y	U	N	Y	Y	Y	N	N	N	Y
Complex terrain?	N	N	Y	N	N	Y	N	N	Y	N	Y	U	U
Elevated sources?	N	U	Y	N	N	Y	Y	Y	Y	Y	Y	N	U
Nearby sources?	N	N	Y	N	Y	Y	Y	Y	Y	U	Y	N	N
Uncertainty?	H	M	M	H	U	M	M	M	U	L	M	L	H
Cost?	L	M	H	M	L	H	M	M	M	H	H	M	M

3. Challenges of inverse dispersion modelling

This section describes the challenges of inverse dispersion modelling which are common to multiple techniques. It is related to the ‘Constraints’ subsections within the descriptions of each inverse dispersion modelling technique in sections 2.2 and 2.3.

The challenges of inverse dispersion modelling methods include obtaining sufficient input data, at multiple locations and/or for multiple time periods, as well as taking into account uncertainties in measured concentrations and meteorological parameters. The requirements for input measured data become more extensive as the underlying source and dispersion conditions become more complex.

Many of the approaches listed in this review only apply in limited atmospheric stability conditions, as well as in particular ranges of wind speed and/or direction. For example, methods using Gaussian plume assumptions are unsuitable in very low wind speeds, while unmanned aerial vehicle (UAV) measurements may not be possible in high wind speeds.

For reliable measurements of a Gaussian-type plume, measurement locations need to be far enough downwind of the source to avoid additional uncertainties from initial plume formation, but close enough to the source to identify plume concentrations above background and/or sensor noise. Also, the local area upwind of the source should have relatively few other sources so that background concentrations are low and homogeneous.

Quality thresholds applied to measurement data can lead to substantial data losses, for example, Bühler and others (2022) report losses of 50% and above for optical linear measurements, with greater losses during night-time periods. Foster-Wittig and others (2015) found only 41 out of 106 virtual plume transects measurements passed their 4 data quality thresholds for further calculations. Data quality thresholds may need to be set with care, possibly for individual cases, in order to optimise the reliability of calculated emissions from available measurement data.

It is particularly difficult for inverse dispersion modelling approaches to find both unknown source location and source emissions simultaneously, as the increased number of unknown variables has increased requirements for measurement data. Low-emitting sources located close to a higher-emitting source are especially likely to be missed by inverse dispersion modelling.

For techniques using airborne measurements, there are constraints on the measurement locations for safety reasons, with minimum measurement heights which can restrict the accuracy of concentration and/or flux estimates near the ground. High precision methane sensors are only just being developed with weights within typical UAV payload limits, while tethered UAV, which pass sampled air to ground-based sensors through a fixed length of tubing, have limited spatial range. Airborne measurements are usually only available for short periods due to cost constraints.

Comparisons of different inverse dispersion modelling and emissions estimation methods show substantial differences in the resulting emissions from each method, for example, Babillotte and others (2010) report flux estimates from 12 to 163 gs^{-1} from 5 methods, while Yeşiller and others (2022) found emissions estimates covering 2 orders of magnitude. Mønster and others (2019) provide a summary of intercomparisons between different methods applied to real landfills and controlled releases; larger variations are usually found for real sources, with increased complexity of source and terrain conditions compared to controlled releases.

When considering the cost and applicability of inverse dispersion modelling methods, the cost and complexity of measurement approaches should be considered alongside the computational cost of associated modelling. Mobile measurement approaches are generally only available for short surveys, whereas fixed measurements at a small number of locations could be available for longer-term analysis.

Forward dispersion modelling can be used to inform planning of measurements for inverse dispersion modelling, as described by Matacchiera and others (2019). However, this requires an initial assumption of emission rates and locations. It may also require care to identify the conditions in which there is greater uncertainty in forward modelling results, for example, low wind speeds, which may also lead to greater uncertainty in inverse dispersion modelling.

4. Applicability of inverse dispersion modelling methods

The applicability of inverse dispersion modelling methods to different source sectors depends on the characteristics of each sector type. The following sections (4.1 to 4.5) summarise the characteristics of methane-emitting sources currently regulated by the Environment Agency and discuss suitable inverse dispersion modelling methods for each type. Applicability to other source types, for example, methane emissions due to land use change in the creation of new wetlands, could be derived by considering the source properties in conjunction with the summary of inverse dispersion modelling methods.

Methods classified as 'medium' or 'high' in the category of 'Widely used?' (Table 1) have primarily been considered in this section, along with methods included in the recommendations of the onshore oil and gas (OOG) study (EA, 2022). The remaining methods are more recently developed, generally within a single academic group, and would require substantial further development to become more widely applicable and available to other users.

Methane emissions for 2019 reported by the UK under the Pollutant Release and Transfer Register (UK-PRTR[3]) are summarised by source activity types in Table 2. The latest reporting year available from the UK-PRTR is 2020. However, activity levels, and resultant emissions, are likely to have been impacted by the Covid-19 pandemic, so the 2019 data may be more generally representative. The table shows that landfill sites are both the largest contributor (74.1% of total methane emissions reported under UK-PRTR) and the most numerous site category (210 regulated sites) in this data. This reporting only includes sites which have estimated emissions exceeding the reporting threshold of 0.1 kt $year^{-1}$. It excludes some smaller-scale emissions such as urban wastewater treatment plants with capacity below 100,000 population equivalent. There is uncertainty about the cumulative impacts from small-scale sources such as biogas, where individual sites do not exceed the emission threshold, but there are substantial and rapidly increasing numbers of small sites (660 operating sites in the UK in 2019 with an additional 390 planned, Bakkaloglu and others, 2021). Methane emissions reported under UK-PRTR for 2019 represent 11% of total methane emissions in the UK in 2019 (UK Greenhouse Gas Inventory, 1990 to 2021).

[3] Available as a searchable online database via https://www.gov.uk/guidance/uk-pollutant-release-and-transfer-register-prtr-data-sets

Table 2 – Summary of UK methane emissions in 2019 reported under UK-PRTR. The 'Reported sites' column is the number of installations which report emission rates above the reporting threshold. '% reported methane' is the contribution of this sub-sector activity to total reported methane emissions.

Annex I activity description	Sub-sector activity	Reported sites	Annual methane emissions (kt)	% reported methane	Release type
1 Energy sector	Thermal power plants and other combustion installations with a thermal input greater than 50MW	97	43.02	18.0%	Point
	Mineral oil and gas refineries (includes terminals and refineries)	13	5.29	2.2%	Point, fugitive
2 Production and processing of metals	Metal ore roasting or sintering	1	0.24	0.1%	Point, fugitive
3 Mineral industry	Ceramic products manufacture	1	0.21	0.1%	Point
4 Chemical industry	Manufacture of simple hydrocarbons	1	0.17	0.1%	Point
	Manufacture of oxygen containing hydrocarbons	1	0.11	<0.1%	Point
	Manufacture of fertilisers	1	2.15	0.9%	Point, fugitive

Annex I activity description	Sub-sector activity	Reported sites	Annual methane emissions (kt)	% reported methane	Release type
5 Waste and wastewater management	Incineration of non-hazardous waste	11	0.18	0.1%	Point
	Landfill	210	174.96	74.1%	Point, fugitive
	Other treatment of non-hazardous waste (including anaerobic digestion/biogas)	12	9.34	4.0%	Point, fugitive
	Waste water treatment	3	0.43	0.2%	Fugitive
7 Intensive livestock production and aquaculture	Intensive livestock production	1	0.16	0.1%	Fugitive
8 Animal and vegetable products from the food and beverage sector	Food and beverage production	1	0.21	0.1%	Point, fugitive

4.1. Landfill

Landfill sites may be small (length scales ~500 m) or large (several km), and may be closed or still active. For active sites, there may be different forms of surface covering for older and newer deposits, with variable emission properties. Active landfill sites accepting biodegradable waste will have equipment to capture and process gas, with pipework and pumping stations. Some closed landfill sites also have gas capture and processing equipment. In general, fugitive emissions are expected to occur near ground level and with minimal buoyancy. However, there may also be some point source emissions due to incomplete combustion (methane slippage) in landfill gas engines and possibly flares. The magnitude and spatial distribution of landfill emissions can vary with time due to both changes in activity patterns and environmental conditions. This has been investigated in a parallel study (Environment Agency, 2023).

Most of the available inverse dispersion modelling methods identified in this study have been applied to landfill sites. Smaller landfill sites are likely to suit the simpler whole-site methods, while larger sites may require more detailed within-site approaches. Closed sites with permanent coverings are likely to have lower emissions than active sites with temporary coverings and may require more sensitive measurement techniques to detect emissions.

Applicable inverse dispersion methods for small landfill sites in open terrain and without other nearby sources could include 1D plume transects; 2D vertical plane measurements; tracer dispersion methods; Backward Lagrangian Stochastic and Bayesian inversion techniques. The first 3 methods use short-term survey measurements, whereas the last 2 can be used with either short-term surveys or longer-term measurements at a small number of monitoring locations.

Applicable methods for larger active landfill sites with complex terrain and/or other nearby sources might include airborne mass balance, and Bayesian inversion techniques.

4.2. Anaerobic digestion plant (biogas)

Anaerobic digestion is a technique for processing organic waste materials, which captures gases from decomposition for use as energy (biogas). A rapidly increasing proportion of organic waste is diverted from landfill into alternative processes such as biogas plants. Methane makes up 50 to 70% of biogas, so there is potential for fugitive emissions from the processing equipment. Where biogas is used in onsite combined heat and power (CHP) engines, ‘methane slip’ (where unburnt methane gas passes to exhaust gases) is also likely to be a significant contributor.

Waste materials typically used as input to anaerobic digestion include livestock manure, food waste, crop wastes and sewage sludge. When biogas plants are located on livestock farms it may be difficult to distinguish fugitive emissions from biogas equipment and from livestock housing. Similarly, the emissions from biogas plants used for sewage sludge and located within wastewater plants may be difficult to differentiate from other methane emissions within the wastewater processing site. Optimum temperatures for biogas

production are 35 to 37°C (Cioabla and others, 2012), which is likely to make fugitive releases weakly buoyant.

Bakkaloglu and others (2021) carried out 1D plume transect surveys of biogas plants in southern England. However, they were only able to derive emissions estimates from 10 out of 56 sites, due to difficulties with road access, proximity to other methane sources leading to non-Gaussian plume shapes, or a lack of detectable plumes. For the sites where they were able to make emissions estimates, the maximum facility heights, for example, tank roofs are reported as 6 to 19 m where known.

Applicable methods for biogas plants in open terrain include 2D vertical plane measurements (if no other nearby sources of the target gas); high-resolution spatial survey; Backward Lagrangian Stochastic; and Bayesian inversion techniques. Airborne mass balance measurements and adjoint modelling techniques are likely to be excessively costly for these relatively small sites, due to specialist personnel, equipment and/or computational requirements.

4.3. Onshore oil and gas (OOG)

The project report ‘Onshore oil and gas: quantifying whole-site methane emissions and associated uncertainties’ (EA, 2022) classifies UK OOG sites into 4 categories, based on size, site type and surrounding location characteristics:

- small production site, simple topography, limited potential emission sources, likely to be near-ground
- small production site, complex topography (woodland), more complex potential emission sources
- large production site, complex topography (woodland), multiple within-site areas and activities forming potential emission sources, including some more elevated locations
- large processing site, complex topography (terrain), with a large number of potential emission sources, including elevated locations

The ‘Onshore oil and gas: quantifying whole-site methane emissions and associated uncertainties’ project (EA, 2022) considered a wide range of methods for quantifying emissions, not restricted to inverse dispersion modelling methods. Tracer gas methods and OTM33a (1D plume transect) methods are recommended by the OOG methane quantification report within the first 3 quantification approaches for all site types, as having moderate cost. The tracer gas method is assessed as having substantially lower uncertainty than plume transect methods. The suitability of other methods varies between site types, with component-level measurements considered prohibitively uncertain for large complex sites and airborne mass balance measurements excessively costly for small simple sites.

In addition to the methods recommended by the Environment Agency (2022) report, the following could be applied to small production sites in open terrain: vertical plane

measurements; high-resolution spatial survey (similar to component-level measurement); Backward Lagrangian Stochastic; and Bayesian inversion.

For the remaining site types, with larger extents, more complex sources and/or complex terrain, Bayesian inversion or adjoint modelling methods could be applicable.

4.4. Wastewater treatment plant

Wastewater treatment plants vary in size and complexity, but generally include a range of storage tanks and processing equipment. Methane emissions are likely to be dominated by near-ground releases from open storage tanks and open flow channels, which will have higher emission rates than covered tanks with gas recovery. Emission rates from different types of storage or processing tanks can vary. For example, Bühler and others (2022) report that emissions per unit area from sludge storage tanks are expected to be substantially higher than those from secondary settlers. There may also be emissions from onsite anaerobic digestion, as described in section 4.2.

Applicable methods for inverse dispersion modelling of wastewater treatment plant emissions will depend on the size of the site; the maximum emission height from onsite equipment; and the complexity of the surrounding terrain. Large, open sites dominated by near-ground sources could be assessed using 1D plume transects; stationary plume transects; tracer dispersion methods; Backward Lagrangian Stochastic techniques; or Bayesian inversion techniques. Large complex sites including elevated sources could be assessed using airborne mass balance; Backward Lagrangian Stochastic techniques or Bayesian inversion techniques.

4.5. Other source types

There are minor methane emissions from a range of industrial processes, including metal ore roasting, manufacture of ceramics, and manufacture of fertilisers. Part of these emissions originate from ‘methane slip’ (unburnt gas) or from process releases containing methane, both of which are discharged through chimney stacks and can be represented as point sources. Other industrial methane emissions are fugitive, for example, pipe leaks or storage tank venting. Emissions from leaks could be represented as point, line, area or volume sources, depending on any other knowledge about likely release locations.

Industrial sources are likely to be associated with complex structures. Stack-based emissions can be monitored using in-stack measurement equipment. Fugitive emissions could be assessed using high-resolution spatial surveys, Bayesian inversion or adjoint modelling approaches.

The conversion of large areas of land to create wetland environments as a flood prevention measure may lead to new methane emission sources. These are likely to be ground-based emissions over large open areas. Suitable inverse dispersion modelling approaches would include 1D horizontal plume transect, stationary plume transect and/or Bayesian inversion.

4.6. Summary

Table 3 summarises the applicable inverse dispersion modelling methods for each source sector and type as discussed in the previous sections. Note that large landfill sites are expected to have larger spatial extents than either large OOG or wastewater sources. The suggestions for OOG sites are influenced by the recommendations of the ‘Onshore oil and gas: quantifying whole-site methane emissions and associated uncertainties’ report (EA, 2022). This placed 1D plume transect methods (OTM33a) lower down the listed quantification approaches for larger and/or more complex sites due to high uncertainty. Biogas sources are expected to be small in horizontal extent but include above-ground releases and built structures.

Table 3 – Summary of applicable inverse dispersion modelling techniques by source type

Source sector	Source characteristics	Inverse dispersion modelling methods								
		1D horizontal plume transect	2D vertical plane	Airborne mass balance	Stationary plume transect	High-resolution spatial survey	Backward Lagrangian Stochastic	Bayesian inversion	Adjoint modelling	Tracer dispersion
Landfill	Small, open terrain	Y	Y				Y	Y		Y
	Large, complex			Y				Y		
Biogas	Open terrain		Y			Y	Y	Y		
OOG	Small, simple	Y	Y			Y	Y	Y		
	Large and/or complex	Y		Y				Y	Y	Y
Wastewater	Open, near-ground	Y			Y		Y	Y		Y
	Complex			Y			Y	Y		
Other industrial	Fugitive					Y		Y	Y	
Wetlands	Large, open	Y			Y			Y		

5. Inverse dispersion modelling study

An inverse dispersion modelling study has been carried out using data obtained from repeated tracer gas dispersion method (TDM) surveys of 3 landfill sites, as reported in Rees-White and Beaven (2020). A selection of inverse dispersion modelling approaches have been applied to this data to estimate whole-site methane emissions. The objectives of this study were to:

- compare the emission rates estimated by the selected inverse dispersion modelling approaches with the emission rates previously calculated using the TDM approach
- investigate the potential for a methane quantification approach that involves:
- a single detailed annual TDM survey
- some other methane concentration monitoring through the rest of the year, either at intervals or continuously
- inverse dispersion modelling

Section 5.1 summarises the available data and section 5.2 describes the initial data processing required to use this data in inverse dispersion modelling. The selected inverse dispersion modelling approaches are described in section 5.3 and the forward model refinement based on the tracer gas measurements is described in section 5.4. The inverse dispersion modelling results for the selected approaches are presented in section 5.5, the potential for a methane quantification approach involving one annual TDM survey is discussed in section 5.6, and section 5.7 presents a more general discussion of the inverse dispersion modelling study.

5.1. Data available

The 3 landfill sites with available data are referred to as sites A, B and C, all located in southern England. Site A is a medium-sized closed site, whereas sites B and C are larger and active sites. Appendix A in the report document (Rees-White and Beaven, 2020) gives the following information relating to each site and the measurement surveys:

- brief description of site characteristics, including activity status, gas collection equipment, and surface covering materials
- outcome of background screening measurements to identify any nearby sources of methane (only found for site B)
- schematic map – this shows the tracer release locations (often the centre of the landfill site but sometimes offset for operational reasons) and the site outline, with indications of active/covered areas where relevant, but does not show any gas collection equipment, gas engine or flare locations
- overview tables for each survey day, with summary data for each transect, including which transects were included or excluded from further analysis

In addition to the TDM report document, the authors were supplied with spreadsheets for each site survey which contained:

- summary sheet: date of survey; description of meteorological conditions; coordinates, release rate and start/end times of acetylene tracer gas release; distance to monitoring road with estimate of tracer gas arrival time
- met data sheet: The content of this sheet varied between survey days. In the majority of cases, it contained meteorological data at 5-minute resolution from a portable weather station: wind speed and direction; ambient temperature; humidity; and pressure. The measurement height was uncertain, so was assumed to be a typical hand-held height, 1.5 m. In some cases (only sites A and B) it contained onsite 30-minute resolution meteorological data: peak and 10-minute average wind speed; wind direction; ambient temperature; rainfall; and pressure. For site C, it sometimes contained 3-hourly data from a national network weather station
- TDM data: one second average methane and acetylene concentration measurements with associated times and latitude-longitude coordinates for each transect measurement

The one second averaging time for concentration measurements leads to transects which represent the instantaneous plume from the site. This contrasts with longer-term measurements and modelling approaches, which represent an ensemble average plume. One second average concentrations are strongly influenced by short-term fluctuations in wind direction and turbulent intensity; this is discussed further in section 5.3.

5.2. Initial data processing

The following initial data processing tasks were carried out for all inverse dispersion modelling approaches:

- reformatted meteorological data as required by models
- digitised maps of landfill sites with reference to satellite imagery as required, using tracer gas release latitude-longitude coordinates to identify sites
- identified typical surface conditions (for example, roughness length) for landfill sites and surrounding area
- cross-referenced spreadsheet transect data, with report appendix tables that label transects as included/excluded
- reformatted transect measurement locations to receptor co-ordinates as required by models
- identified periods where the vehicle was stationary and assigned the median measured value to these receptors
- assessed quality of transect data – this step excluded transects where the apparent wind direction was different to the other transects in a survey

Landfill site activity data was not used in this study, since the primary objective was to compare the emission rates estimated by the selected inverse dispersion modelling approaches for the selected surveys. This is discussed further in section 5.3.

5.3. Selected approaches

The inverse dispersion modelling approaches tested were initially selected based on the measurement data available, the characteristics of each site in relation to applicability considerations as discussed in section 4.1, and methods available to the project team. During this study the authors developed an additional inversion modelling method, which is a modified version of the 'Standard' Bayesian method. This new 'Modified Bayesian' method takes account of the short-term concentration fluctuations present in the TDM survey data due to the very high time frequency of the measurements (one second). Simulating high time frequency measurements using forward or inverse Gaussian plume models is challenging, because these models are generally designed to model hourly mean plumes. Short-term fluctuations in wind direction, wind speed and turbulence can be considerable on a one-second timescale, and a Gaussian plume model would not be expected to capture this behaviour. However, the ADMS fluctuations module estimates the effects of these fluctuations on concentration at a given location, and this has been used in the 'Modified Bayesian' method.

The 4 selected inverse dispersion modelling approaches were:

- **Modified Bayesian inversion**: A modified application of ADMS and CERC's Bayesian inversion scheme (Carruthers and others (2019), section 2.3.4), developed by the authors for this study. This method uses ADMS to estimate the short-term fluctuations in concentration caused by short-term fluctuations in wind direction and turbulent intensity, and applies the inversion scheme to only the measured peak concentration in each transect. The modelling used a mean averaging time of one hour and a fluctuations averaging time of one second. Measurement uncertainty, measurement covariance and emissions covariance were set appropriately based on the available information. This approach was applied to all 3 sites. It was applied to methane using the same landfill volume source definitions as the Standard Bayesian method (described below), and to the tracer, which was modelled as a point source at the tracer release location with height one metre. The method is described in the Appendix (section 7.1).
- **Standard Bayesian inversion** (section 2.3.4): ADMS and CERC's Bayesian inversion scheme were used to simulate the landfill surface methane emissions as separate, ground-based, one metre deep, volume sources representing different capping/activity areas, with a mean averaging time of one second. The one metre volume source depth helps to represent the undulations in the landfill surface and the resulting small variations in release height over the site. Measurement uncertainty, measurement covariance and emissions covariance were set appropriately based on the available information. This approach was applied to all 3 sites. The method is described in the Appendix (section 7.2).
- **1D Gaussian profiles** (section 2.2.1): ADMS and CERC's inversion scheme were used to simulate the landfill methane emissions as a single ground-level point source located at the landfill centroid, with a mean averaging time of one hour. The measurements were assigned zero uncertainty and zero error covariance. This approach reduces the inversion scheme to a 1D least-squares Gaussian solver. This method is generally only recommended for small landfills in open terrain (Table 3). Sites B and C are slightly larger than

recommended for this method. However, since it is commonly used for landfills of this size it was applied to all 3 sites in this study. The method is described in the Appendix (section 7.3).

- **Backward Lagrangian Stochastic** (section 2.3.2) (WindTrax): WindTrax is recommended for horizontal distances of up to approximately 1km, for both source size (= 'site length scale') and distance between source and measurement location. Sites B and C both have site length scales bigger than 1 km, therefore, this approach was only tested for methane emissions from site A, the smallest of the 3 sites. The method is described in the Appendix (section 7.4).

5.4. Forward model refinement using tracer gas data

For each landfill site and for each TDM survey, tracer gas measurements from selected transects were used to refine our understanding of the site characteristics and meteorological conditions during the surveys. Forward ADMS modelling of the tracer gas release was used to calculate tracer concentrations at the transect measurement locations. This modelling used the known tracer gas flow rate. Details of the ADMS forward modelling configurations for each site are given in the Appendix (section 7).

Gaussian plume models such as ADMS are designed to model an hourly mean plume. They do not generally account for the plume meandering caused by fluctuations in wind speed, wind direction and turbulence that occur at timescales of less than one hour. This makes comparing ADMS modelled concentrations with one-second measurements very challenging. However, short-term concentration fluctuations caused by short-term meteorological variability can be estimated using the ADMS 'fluctuations' module. This has been used in this study to predict the maximum likely concentration at each transect measurement location and time, given the meteorological variations that occur on a one-second timescale. This quantity is hereafter referred to as the 'fluctuations local maximum concentration'.

Hourly mean modelled and one-second fluctuations local maximum tracer concentrations were compared with measured tracer concentrations for each site for each survey, with the aim of obtaining reasonable agreement between the peak measured value in each transect and the modelled fluctuations local maximum concentration at the same location and time. Model refinements to improve the model agreement were made as follows:

- For a given survey, the wind direction value was aligned with the direction from the source to whichever location had the highest monitored concentration out of all the transect locations measured in the survey.
- Wind speed data was taken from nearby meteorological observation sites if the observed site data resulted in a poor correlation with observed concentrations.
- Boundary layer height data were calculated using full day observations from nearby meteorological observation sites if modelling with the individual hour of observed site data resulted in poor agreement with observed concentrations.
- Transects were excluded from inverse dispersion modelling if the measured tracer plume location was different to the modelled plume location using the

refined modelled wind direction for that hour, suggesting greater wind direction variability within the survey than can be treated by any of the inversion methods.

Example modelled and measured tracer concentrations for 2 transects (one at site B, one at site C) are shown in Figure 1. This demonstrates that the refinement of the modelling configuration leads to good agreement for some transects (for example, site B example). In other cases (for example, site C), there may be variations of wind direction between transects for the same survey which are not captured by the current approach, leading to poorer model performance. This effect has been minimised by selecting only transects where the measured plume location agrees with the modelled plume location (a list of transects included for each site is given in section 7.1). The chosen settings were further validated by running the modified Bayesian inversion method on the tracer. No change in the tracer gas emission rate means that the model agreement for the tracer gas is good enough to give confidence in using the refined model configuration for estimating CH_4 emissions. Section 7.1 gives details of the tracer gas inversion results.

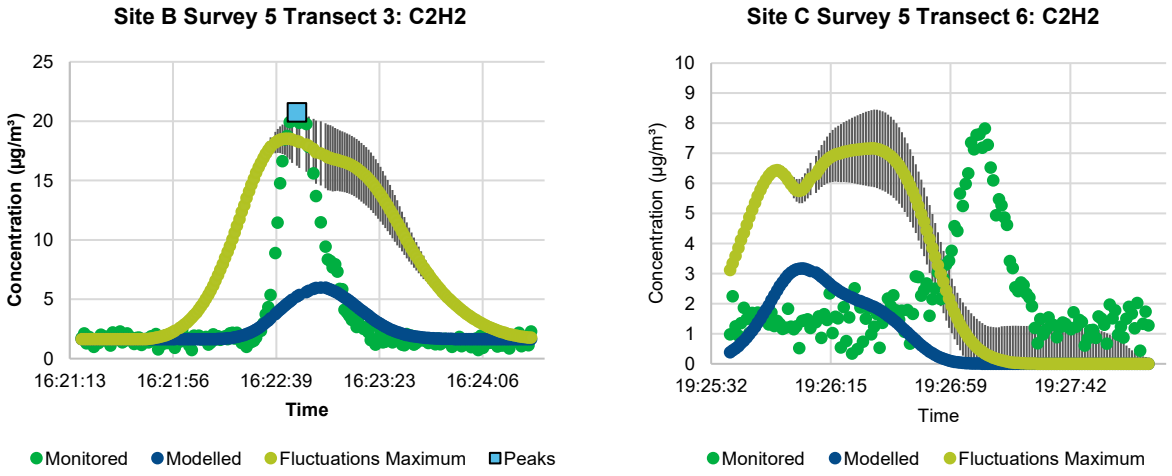

Figure 1 – Example transect evaluation results with hourly mean modelled tracer concentration in dark blue, modelled fluctuations local maximum tracer in lime green and monitoring data in bright green, showing variation in model performance. The error bars around the fluctuations local maximum value represent the standard deviation of the concentration due to short-term meteorological fluctuations. The pale blue square on the left-hand plot shows the peak measurement location and value used in the modified Bayesian approach.

The refined ADMS forward modelling configuration was also used as a basis for the WindTrax model configuration for site A. Additional information about the input data processing, configuration and post-processing used for WindTrax is given in the Appendix (section 7.4). WindTrax generated separate values of landfill emissions corresponding to multiple model calculations for each transect, with (i) values for standard deviation/mean emissions ratio, and (ii) the fraction of the landfill area calculated to influence the relevant measurement point(s) on the transect. These values were combined into overall average emissions estimates by (i) excluding negative emission rates, (ii) applying a minimum

threshold to the fraction of landfill area calculated to influence the measurements, and (iii) applying a maximum threshold to the standard deviation/mean ratio.

5.5. Inverse dispersion modelling methane emissions results

Following refinement of the forward ADMS modelling based on the tracer measurements, inverse dispersion modelling was carried out using the selected approaches to calculate whole-site methane emission rates, for comparison with the methane emission rates calculated by the TDM survey approach.

Estimates of total methane emissions calculated by the 4 inverse dispersion modelling methods were compared with the emission rates calculated from the original TDM survey. The resulting emission rates are shown in scatter plots in Figure 2. Numerical results from each inverse dispersion modelling method are given in Tables 4 to 6. The inverse dispersion modelling methods capture the general variation in the magnitude of emissions between the sites, with the lowest emission rates for site A and higher rates for sites B and C. However, the inverse dispersion modelling results tend to predict higher emission rates than TDM for sites B and C.

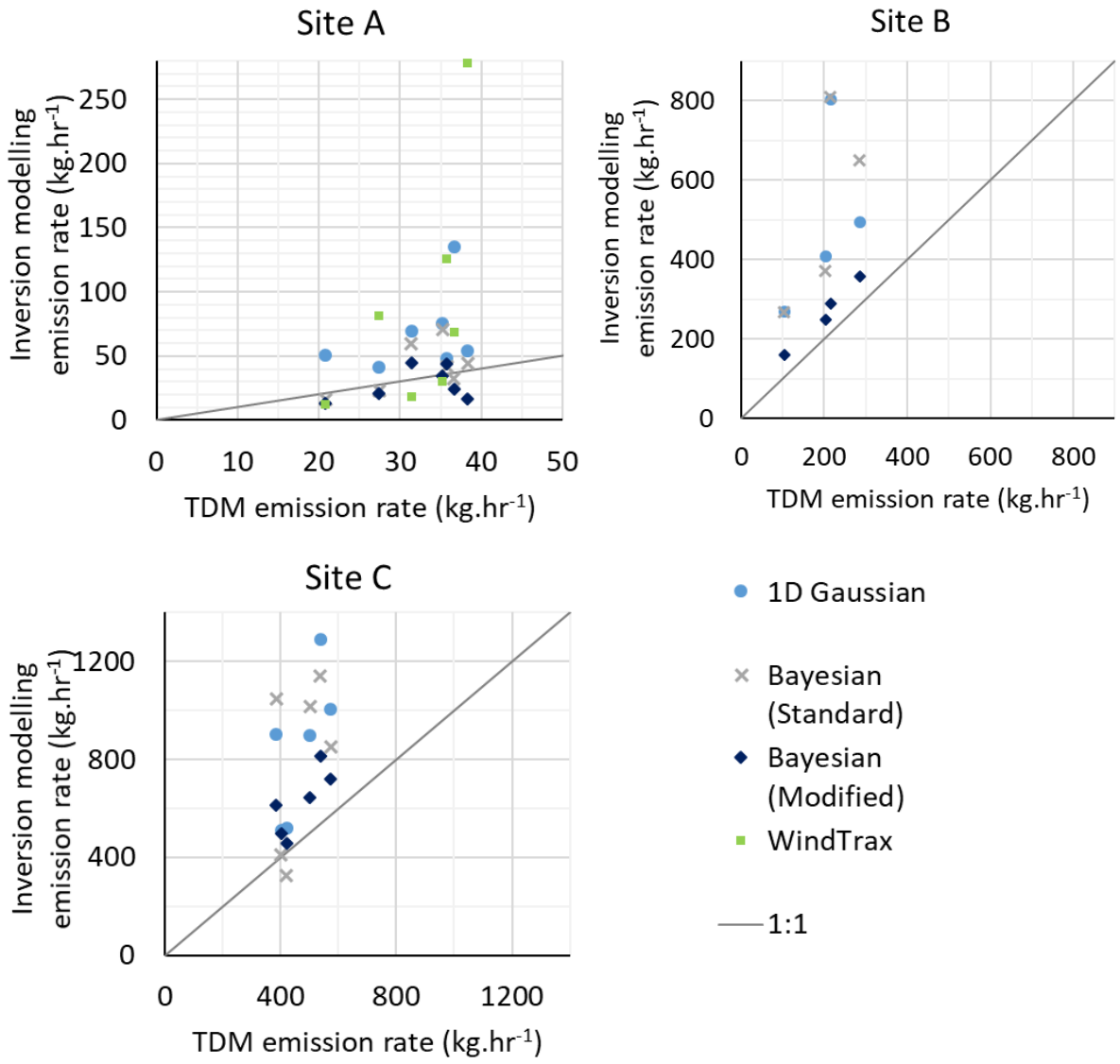

Figure 2 – Scatter plots comparing total site methane emission rates derived from TDM with inverse dispersion modelling results. Each point represents a single survey, comprising multiple transects measured on the same day (survey).

The modified Bayesian method generally agrees more closely with the TDM method than the other 3 methods. The 1D Gaussian method generally predicts higher emissions than the modified Bayesian method. This is likely to be because the 1D Gaussian method predicts a wider and more dispersed plume with lower peak concentrations, leading to the measured plume being associated with a higher emission rate. Also, the 1D Gaussian method does not account for measurement uncertainty, so requires closer agreement between modelled and measured values.

There is considerable variation between surveys in the spread of emission predictions from TDM and the inverse dispersion modelling methods. Possible causes for this variation have been explored by plotting the predicted emission rates against 2 important dispersion modelling parameters: input wind speed (Figure 3) and stability parameter H/LMO (Figure 4). H/LMO represents the relative importance of thermal and mechanical

mixing in the atmosphere. Large negative values are associated with unstable, convective conditions with vigorous vertical mixing. In contrast, positive values correspond to stable conditions with reduced vertical mixing. Boundary layer height (H) and Monin-Obukhov length (LMO) are both calculated by the ADMS meteorological pre-processor.

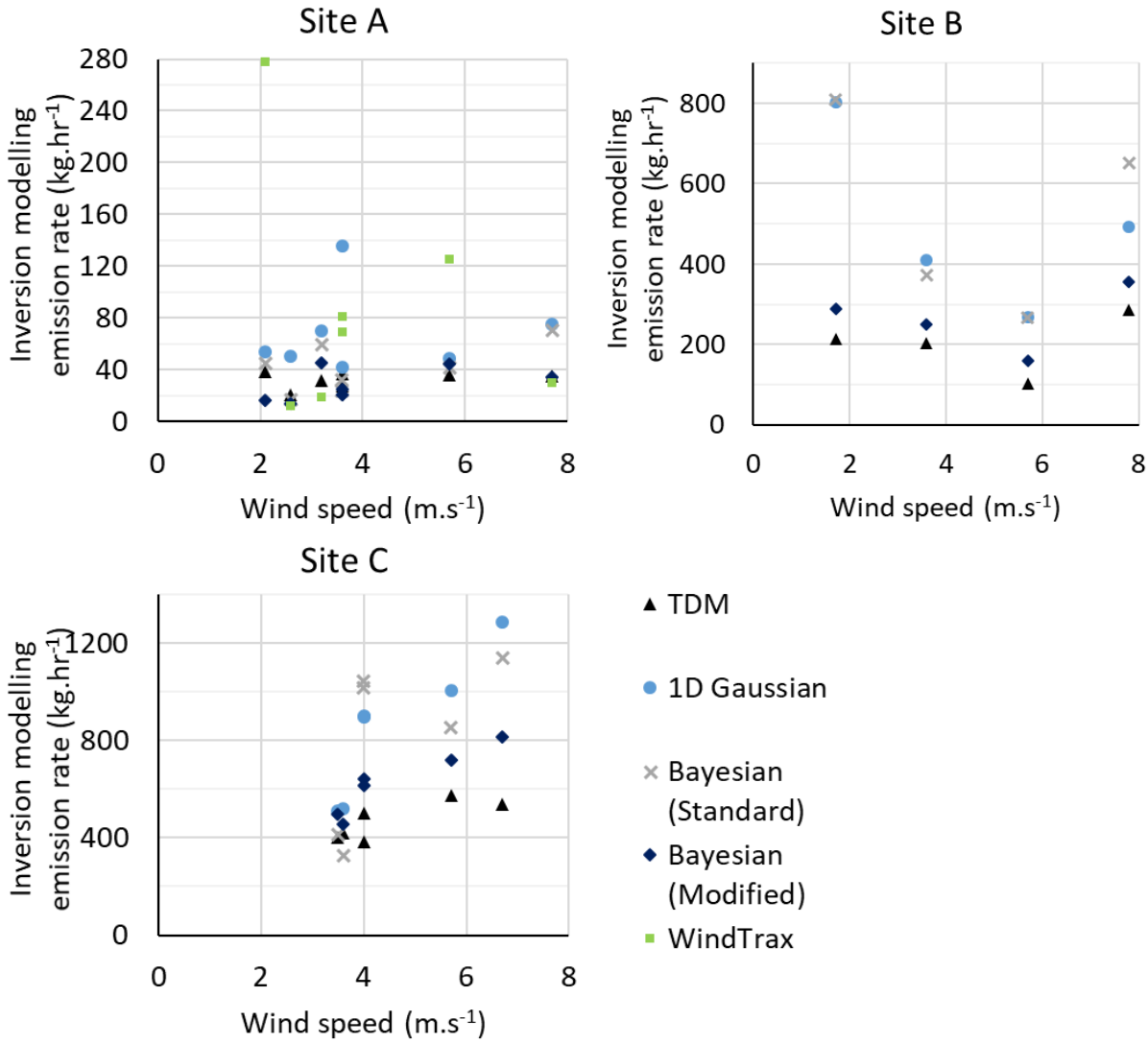

Figure 3 – Variation of predicted methane emission rates for each site from TDM and inversion modelling methods, plotted against local wind speed in m.s^{-1}.

There is no clear trend in the spread in the emission rates from the different inversion modelling methods with wind speed for all sites. The emission rates calculated for site C show an increase in emission rates with increasing wind speed for all methods, whereas there is no clear relationship between emission rates and wind speed at the other sites.

For sites B and C, there is a weak trend towards increasing spread in the emission rates as atmospheric conditions become more unstable, particularly for the Gaussian and standard Bayesian results. There is no consistent observable trend at site A. For site A, the Backward Lagrangian Stochastic (WindTrax) method tends to predict higher emission rates as atmospheric conditions become more unstable.

TDM studies are usually carried out in conditions with low wind speed and limited vertical mixing in order to measure clear tracer plumes. This may help inverse dispersion

modelling if it improves the data quality of the tracer and methane measurements, with greater contrast between in-plume and background concentrations. However, the changes in wind direction and, therefore, different transect paths relative to the site locations for each survey may also contribute to the different behaviour of each method.

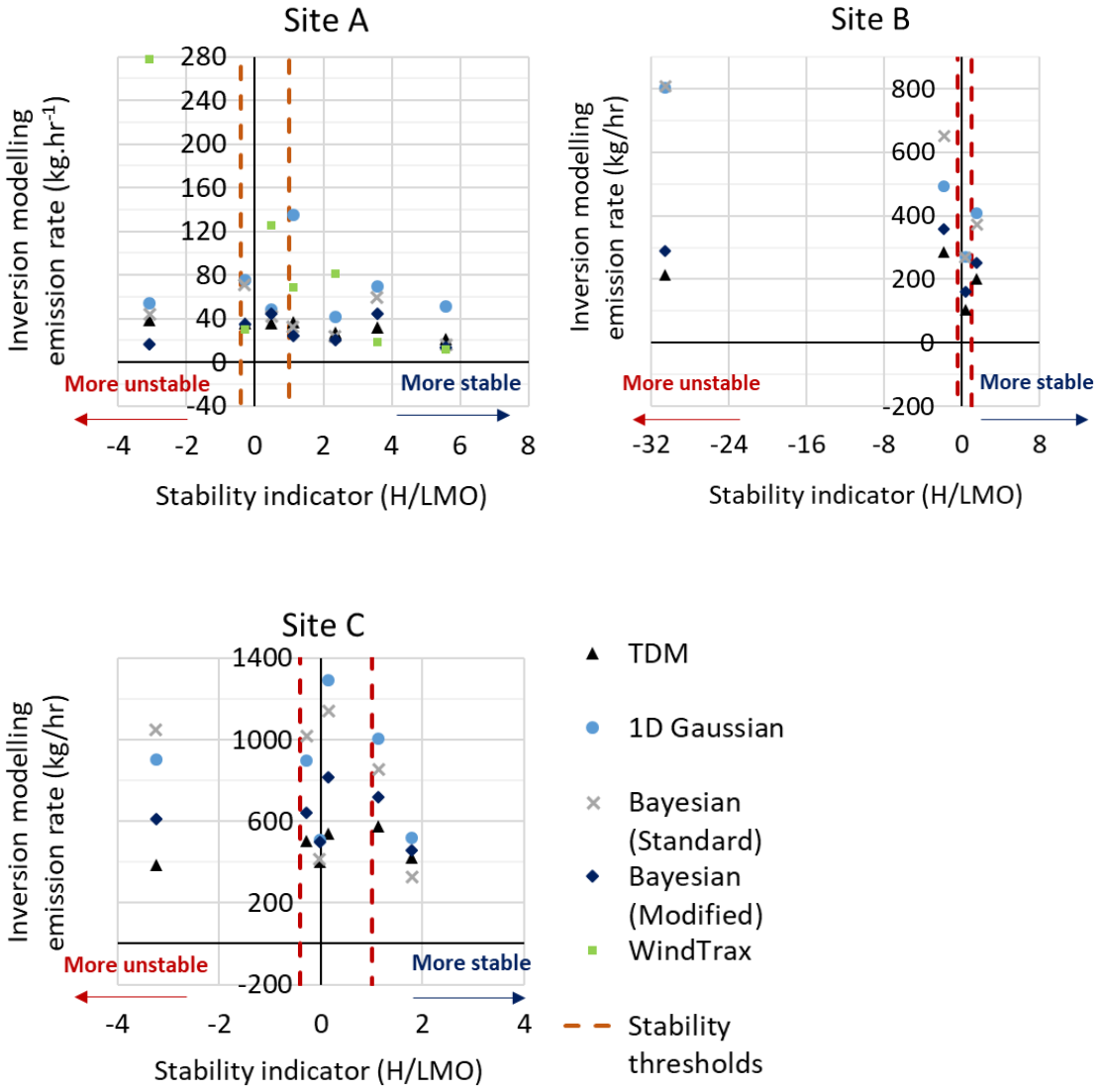

Figure 4 – Variation of predicted methane emission rates for each site from TDM and inversion modelling methods, plotted against H/LMO stability parameter. Red dashed lines show the thresholds between atmospheric stability categories: H/LMO < -0.4 indicates convective or unstable conditions with vigorous vertical mixing; H/LMO > 1.0 indicates stable conditions with suppressed vertical mixing; while H/LMO close to 0 indicates neutral stability conditions with moderate vertical mixing.

Table 4 - Comparison of total site methane emission rates derived from TDM and inverse dispersion modelling methods for site A.

Survey	Methane emission rate (kg hour^{-1})				
	TDM	1D Gaussian	Standard Bayesian	Modified Bayesian	Backward Lagrangian Stochastic (WindTrax)
1	35.26	75.33	70.52	34.36	30.12
2	27.41	41.69	23.36	20.62	81.08
3	38.30	53.86	44.35	16.61	278.15
4	20.84	50.71	16.24	13.50	12.06
5	35.75	48.46	41.71	44.20	125.52
6	36.63	135.12	32.26	24.39	68.99
7	31.42	69.49	59.42	44.86	18.59
Mean	32.23	67.81	41.12	28.36	87.79
Median	35.26	53.86	41.71	24.39	68.99

Table 5 – Comparison of total site methane emission rates derived from TDM and inverse dispersion modelling methods for site B.

Survey	Methane emission rate (kg hour^{-1})			
	TDM	1D Gaussian	Standard Bayesian	Modified Bayesian
3	214.78	803.12	808.60	288.93
4	103.56	269.30	267.86	159.51
5	202.89	408.96	371.91	250.20
6	286.05	493.79	651.07	357.06
Mean	201.82	493.79	524.86	263.93
Median	208.84	451.37	511.49	269.56

Table 6 – Comparison of total site methane emission rates derived from TDM and inverse dispersion modelling methods for site C.

Survey	Methane emission rate (kg hour^{-1})			
	TDM	1D Gaussian	Standard Bayesian	Modified Bayesian
2a	573.36	1,005.95	852.93	720.01
2b	537.87	1,288.99	1,141.49	813.15
5	420.02	521.00	327.58	456.71
6	402.24	509.10	412.34	498.91
7a	385.09	903.27	1,046.19	613.20
7b	502.18	898.60	1015.20	642.84
Mean	464.46	854.48	799.29	624.14
Median	430.49	900.94	934.06	628.02

5.6. Additional uncertainty using a single TDM survey

The Environment Agency is interested in exploring the potential for an alternative methane quantification approach that requires only one annual TDM survey, together with inverse dispersion modelling and downwind methane concentration monitoring to provide estimates of annual methane emissions. Such an approach would reduce the amount of tracer gas concentration monitoring activity needed, reducing the need for site access and supervision of the tracer gas release. In this section, we discuss the feasibility of such an approach and any additional uncertainty that may arise due to the timing of the TDM survey.

Section 5.4 described how the forward modelling was refined based on the tracer gas results. Tracer gas measurements from a singular survey would be sufficient to refine the ADMS forward modelling in a general sense. Although ADMS model input parameters such as wind direction, surface roughness and wind direction variability were refined to give the best tracer agreement on a survey-by-survey basis, methane measurements could be used for this refinement stage, in the absence of tracer gas measurements, and would likely yield a similar result.

Nominal unit emission rates were used as the initial methane emission rates for the inverse dispersion modelling described in the previous section. The TDM methane emission rates were only used for comparison purposes, which maintained the independence of the methods for the comparison. However, in the scenario where a singular TDM survey and subsequent modelling are different stages of the same quantification approach, the TDM survey could provide the initial methane emission rate estimate used to initialise the inverse dispersion modelling.

Different TDM surveys produced different methane emissions estimates, so the sensitivity of the inverse dispersion modelling methane emission results to which TDM survey was used for the initial methane emission rates has been investigated. The 1D Gaussian, Standard Bayesian and Modified Bayesian inverse dispersion modelling methods were all run for all 3 sites for all surveys using the modelling setup described in the previous section. Each survey was repeated using the TDM calculated methane emission rate for each of the other surveys as the initial emission rate. Separate WindTrax modelling was not carried out for this analysis due to excessively long run times.

For each of the 3 sites, for each survey, and for each of the 3 inverse dispersion modelling methods, the methane emissions results were found to be exactly the same regardless of which TDM survey was used for the initial methane emission rates; these are the values given in Tables 4, 5 and 6. This suggests that it would be feasible to have a methane quantification approach that requires one annual TDM survey together with inversion dispersion modelling and downwind methane concentration surveys. Subsequent annual TDM surveys could be used to validate and refine the inverse dispersion modelling.

5.7. Discussion

The literature review and applicability phases of this project considered a wide range of inversion modelling approaches and source types. However, the active modelling phase only had access to measurement data for landfill sources, modelled as large near-ground volume sources. This means that approaches more appropriate to sources with smaller horizontal but larger vertical extents, such as 2D Gaussian fitting or adjoint modelling, have not been tested.

There is considerable variation between the estimated landfill emissions using the different inversion methods. The method with the closest estimates to the TDM method is the Modified Bayesian method discussed above. The 1D Gaussian and Standard Bayesian methods generally estimate much higher emissions, due to the recognised mismatch between the one second measurements and the hourly mean plume modelling. The Backward Lagrangian Stochastic (WindTrax) method was only used for site A, because it is only suitable for domains up to 1 to 2 km. WindTrax gave similar estimates to TDM for some surveys, but also much larger estimates in other cases.

An alternative inversion approach, not investigated in the current study, would be to apply an inversion method to the crosswind plume-integrated concentration, therefore reducing the complexities arising from fluctuations. This could be done with standard ADMS model output by adding receptors across the plume, for individual transects, manually integrating modelled concentrations, and applying the inversion method to the integrated totals. Alternatively, the ADMS model code could be modified to add this type of output.

6. Recommendations

Following the project literature review and applicability assessment (sections 2, 3 and 4), the authors make the following recommendations:

1. We recommend that the selection of a suitable inverse dispersion modelling method for a particular source and application should consider:
    a. source characteristics such as horizontal length scale and likely emission height
    b. characteristics of the area surrounding the source such as open or complex terrain and/or nearby obstructions to flow including buildings
    c. the presence of other nearby sources of the targeted pollutant, especially if upwind of the planned measurement locations
    d. the appropriate balance of required accuracy/uncertainty and cost

2. Inverse dispersion modelling methods are currently an area of active research and rapid development, driven by improvements in measurement technologies (for example, UAV-borne sensors) and increased availability of computational resources. We recommend that the Environment Agency continues to assess emerging inverse dispersion modelling methods as they become more mature.

3. It is important to collect information about activities at a regulated site during any short-term measurement campaign that is to be used with inverse dispersion modelling methods, in order to estimate how representative the inverse dispersion modelling emissions results are of longer-term emissions.

4. Data quality thresholds for measurement data which is to be used with inverse modelling need to be developed with care, appropriate to each measurement technique and inverse dispersion modelling approach.

5. The main focus of this study was fugitive methane emissions. However, the recommendations above would apply similarly to other fugitive gaseous releases, for example, when estimating nitrous oxide emissions from wastewater treatment facilities. Different measurement techniques might affect which inverse dispersion modelling methods are most suitable, but the same broad principles apply.

The remainder of the project recommendations relate to the active modelling phase of the project (section 5).

If TDM survey data is to be routinely used with modelling and inversion methods, then the authors make the following recommendations for TDM survey data collection:

6. We recommend that TDM surveys also collect high quality, high frequency (for example, one second) meteorological and turbulence measurements where possible so that the model input can be optimally specified, thereby improving model performance. During the forward ADMS modelling stage of this project, in many cases the available

wind speed and direction data was found to be inconsistent with the location of the peak tracer gas and methane concentrations in survey transects, so the wind direction had to be adjusted.

7. We recommend that TDM surveys for use with modelling and inverse dispersion methods are carried out in atmospheric conditions where the models are best able to represent the atmospheric airflow and turbulence. These are conditions where both stability effects and wind direction changes are small, which is typically the case in near neutral conditions, moderate wind speeds, consistent wind directions and not around sunrise or sunset.

8. We recommend that TDM surveys for use with modelling and inverse dispersion modelling methods carry out repeated transects as close as possible to the site while still capturing the whole plume, instead of undertaking transects at different distances from the site (this is more difficult for elevated sources). In the modelling study, transects closest to the site with the strongest landfill signal were the most useful. Fewer transects with a stronger landfill signal in general are more useful than more transects with a lower signal. Many TDM survey transects were excluded from the inverse dispersion modelling because the tracer signal was too faint. However, measurements made too close to a source may include uncertainties from initial plume formation, as discussed by Matacchiera and others (2019).

The following recommendations relate to the selected inverse dispersion modelling approaches:

9. The study shows that the Modified Bayesian method performs well and is a viable approach to estimating emissions from transects which would warrant further testing and refinement, with additional TDM survey data sets, prior to routine application. The method combines the ADMS dispersion model, which is already widely used for regulatory purposes, with a Bayesian inversion approach, which is similar to those used by a number of different groups.

10. Another modification of the Standard Bayesian approach, not considered in this study but recommended for further examination, is to apply an inverse dispersion modelling method to the crosswind plume-integrated concentration, reducing the complexities arising from short-term fluctuations.

11. The suitability of an inverse dispersion modelling method to the high measurement frequency (one second) and mobile nature of TDM survey data should be considered when selecting an inverse dispersion modelling method for use with TDM data.

12. A robust procedure is required for assessing each TDM survey transect in terms of its suitability for the chosen inverse dispersion modelling method. The procedure will depend on the inverse dispersion modelling method, but should take the limitations of the method into account. For example, the Standard Bayesian method requires the modelled plume position to match the measured plume position, which may not be the case for all transects within a survey.

13. The inverse dispersion modelling study focused on emissions from one type of facility (landfill) using one type of measurement data (tracer gas plume transect measurements). Measurements made using a wider range of methods and around other types of facilities would be required to compare additional inverse dispersion modelling techniques.

14. The inverse dispersion modelling study found (section 5.6) that the whole-site emissions calculated by the 1D Gaussian, Standard Bayesian and Modified Bayesian methods were unaffected by the choice of TDM survey used to provide the initial emission rate. This suggests that a method involving only one TDM survey combined with inverse dispersion modelling, and repeated or continuous methane and meteorological monitoring at other times of year, would be sufficient to provide a good estimate of annual landfill methane emissions. The recommended time to undertake the annual TDM survey would be when landfill emissions are expected to be relatively high, subject to the meteorological considerations set out in (7) above.

15. On the basis of (14) above, we recommend that the Environment Agency considers further case studies and worked examples in order to develop a practical, ‘user-friendly’ protocol for site operators that sets out a typical annual sequence of measurements, inverse dispersion modelling and analysis for quantifying methane emissions at a regulated site.

7. Appendix: Inverse dispersion modelling methods and results

This section describes the inverse dispersion modelling methods that have been applied to estimate landfill CH_4 emissions using the TDM survey data available for the 3 landfill sites in southern England known as sites A, B and C.

Four inverse dispersion modelling methods have been applied:

- Modified Bayesian inversion (section 7.1): A modified application of ADMS and CERC's inversion scheme (Carruthers and others (2019)), using ADMS to estimate the short-term fluctuations in concentration caused by short-term fluctuations in wind direction and turbulent intensity. The inverse dispersion modelling scheme was applied only to the measured peak concentration in each transect. This approach was applied to all 3 sites.
- Standard Bayesian inversion (section 7.2): ADMS and CERC's inversion scheme used to simulate the landfill emissions as separate volume source(s) representing different capping/activity areas. Measurement uncertainty, measurement covariance and emissions covariance were set appropriately based on the available information. This approach was applied to all 3 sites.
- 1D Gaussian profiles (section 7.3): ADMS and CERC's inversion scheme used to simulate the landfill emissions as a single ground-level point source, with the measurements assigned zero uncertainty and zero error covariance. This approach reduces the inverse dispersion modelling scheme to a 1D least-squares Gaussian solver. It was applied to all 3 sites.
- Backward Lagrangian Stochastic (section 7.4) (WindTrax): WindTrax is recommended for horizontal distances of up to around 1 km, either within a source or between source(s) and measurement locations. Sites B and C both have site length scales bigger than 1 km, therefore, this approach has only been tested for site A, the smallest of the 3 sites.

Three of the methods (1D Gaussian, Standard Bayesian and Modified Bayesian) used the ADMS dispersion model for the forward modelling stage. A summary of the ADMS configuration differences between the 3 methods is given in Table 7. CH_4 concentration results from these 3 methods are given in section 7.5.

Table 7 – Differences in ADMS configuration between the 3 inverse dispersion modelling methods where ADMS was used for the forward modelling.

	Mean averaging time (s)	Wind direction variability	Fluctuations averaging time (s)	Sources
Modified Bayesian	3,600	Calculated from wind direction data	1	Multiple volume sources
Standard Bayesian	1	n/a	n/a	Multiple volume sources
1D Gaussian	3,600	n/a	n/a	Single point source in the centre of the landfill

7.1. Modified Bayesian inversion method

Gaussian plume models such as ADMS are designed to model an hourly mean plume; they do not generally account for the plume meandering caused by fluctuations in wind speed, wind direction and turbulence that occur at timescales of less than one hour. This makes comparing ADMS modelled concentrations with one-second measurements very challenging. However, short-term concentration fluctuations caused by short term meteorological variability can be estimated using the ADMS 'fluctuations' module. A 'Modified Bayesian' inversion method has been developed to account for this.

The ADMS fluctuations module has been used to predict the maximum likely modelled concentration and standard deviation of the mean modelled concentration at the location of the peak measurement in each transect for each survey. This modelling used a mean averaging time of one hour (approximately equal to the duration of each survey), wind direction variability calculated as the standard deviation of the measured wind direction during each survey, and a fluctuations averaging time of one second. The maximum likely modelled concentration accounts for both horizontal and vertical fluctuations, while the measurements are recorded at a single height and, therefore, only capture the horizontal plume position. The maximum likely modelled concentration captures vertical fluctuations not captured by the measurements and, therefore, should be expected to exceed the measured concentration at a given transect measurement location.

The CERC Bayesian inversion scheme (Carruthers and others (2019)) has been applied to this reduced set of measurement locations (one location per transect per survey). The modelled concentration used was the maximum likely modelled concentration. The combined model and measurement uncertainty was taken to be the standard deviation of the mean modelled concentration.

This method was first applied to estimate tracer gas emission rates and the modelling, then refined to yield the minimum possible change in C_2H_2 emission rates, since the tracer emission rates are known. This was done to increase confidence that differences between modelled and measured CH_4 levels were mainly due to CH_4 emission errors.

Using this method results in whole-site CH_4 emission values because the ADMS fluctuations output relates to total concentrations. The initial CH_4 emission rate used in the inverse dispersion modelling was 1×10^{-5} g m^{-3} s^{-1}. The uncertainty and covariance values that were used in the CH_4 inverse dispersion modelling with this method are given, with justifications, in Table 8.

Table 8 – Uncertainty and covariance values used in the Modified Bayesian inversion scheme for all sites for CH_4.

Parameter	Value	Unit	Comment
Measurement uncertainty	Variable	µg m^{-3}	Set equal to the sum of the fluctuations standard deviation of the concentration at the location of the peak measurement and the instrument accuracy (1.3 µg m^{-3}).
Measurement uncertainty covariance	0		Set to zero to allow the error to vary between the different transect peaks.
Emissions uncertainty	0.01	g m^{-3} s^{-1}	Set to a high value to allow the initial nominal unit emission rate ($1x10^{-5}$ g m^{-3} s^{-1}) to be changed as much as necessary to obtain good model agreement

Adjusted modelled methane concentrations using this method are compared with results for the Standard Bayesian method and the 1D Gaussian method in section 7.5.

The following sections give information about the input configuration of the ADMS forward runs for the Modified Bayesian inversion method for each site. A pre-release version of ADMS 6 (version 5.9.0.1) was used for the forward modelling. Tracer gas evaluation results are also provided for each site.

7.1.1. Site A inputs

Site A was represented by 14 volume sources representing the landfill cells, as shown in Figure 5. The total source area was 150,390.5 m^2. Each volume source had a depth of 1m. It was found that some of the measurement locations provided needed adjusting in order to achieve alignment with the roads. This is likely to be due to GPS errors. The adjustment applied was -115 m in the X direction and +42 m in the Y direction.

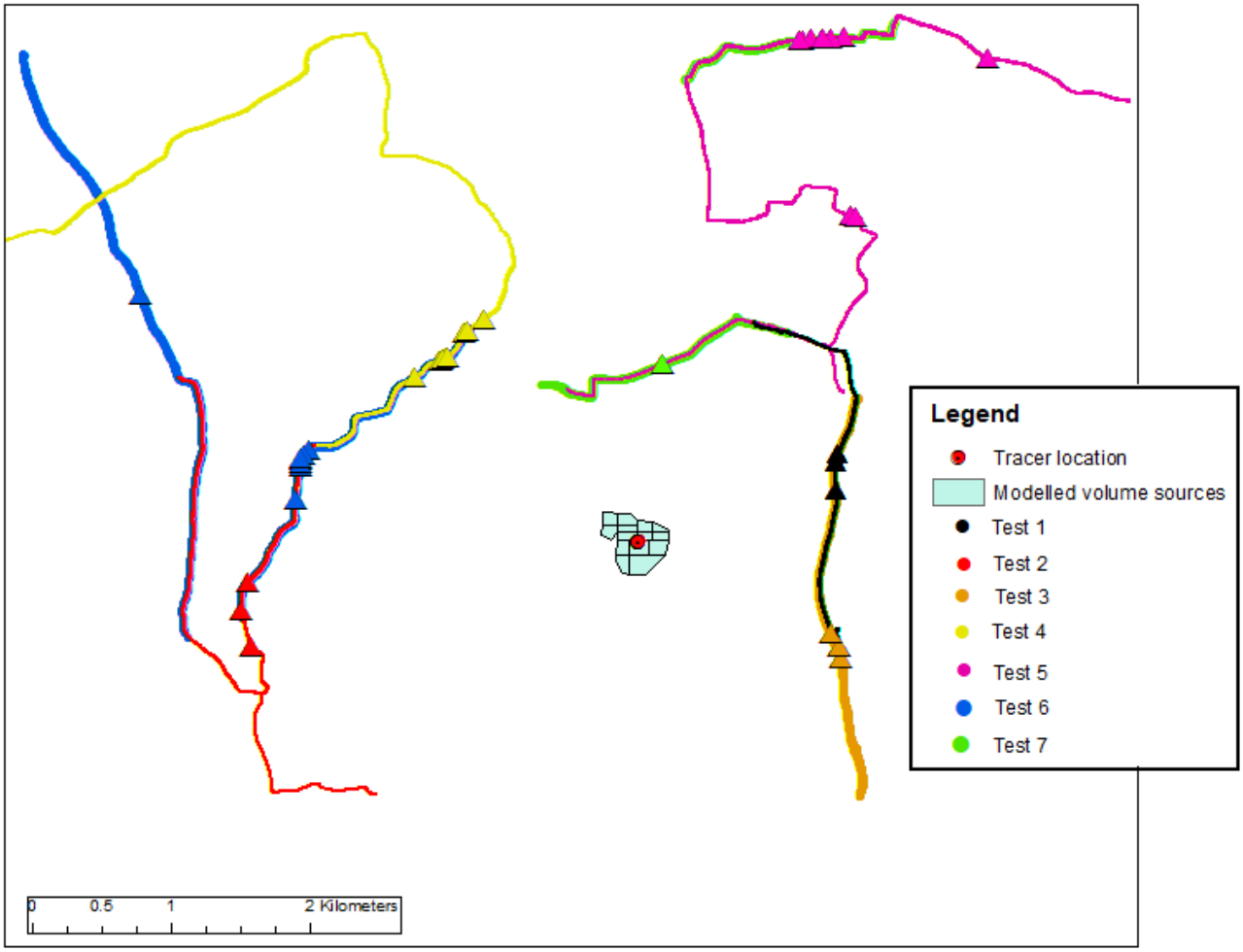

Figure 5 – Site A showing transect locations relative to tracer release site and modelled volume sources used to represent the landfill site. Receptor locations highlighted using a triangle symbol locate the position of the maximum values used for the inverse dispersion modelling.

The modelling used a latitude of 51.92°. All other site options, such as minimum Monin-Obukhov length were left as the model default values.

The tracer release was modelled as a point source with a height of 1 m, a diameter of 0.02 m and a volume flow rate calculated using the release mass of pollutant with the ambient temperature and pressure recorded on site for each survey. The supplied tracer emission rates were input for each survey. The input values are shown in Table 9.

Table 9 – Site A tracer gas emission parameters for each survey.

Survey	Tracer emission rate of C_2H_2 (gs^{-1})	Tracer volume flow rate (m^3s^{-1})
1	0.73	6.67E-04
2	0.76	6.60E-04
3	0.37	3.30E-04
4	0.90	7.90E-04
5	0.88	7.83E-04
6	0.83	7.41E-04
7	0.87	7.91E-04

Initial modelling used the provided onsite meteorological data. Inspection of the results and comparison of the provided meteorological data with data available for a nearby Met Office site at Mildenhall suggested that the wind direction data was not accurate enough for precise modelling.

Sensitivity testing was carried out to find the meteorological parameters that gave the best agreement between modelled and measured tracer gas concentrations, leading to the minimum change in tracer gas emission rate using this inverse dispersion modelling method. Surface roughness values were selected separately for each survey as part of this process. The final set of input meteorological parameters are shown in Table 10.

Table 10 – Site A meteorological parameters for each survey.

Survey	Surface roughness (m)	10 m height wind speed (ms^{-1})	Wind direction (degrees)	Cloud cover (Oktas)	Temperature (ºC)	Wind direction variability (degrees)
1	1.00	7.7	245	0	12.7	12.1
2	0.08	3.6	80	0	2.8	1.0
3	2.00	2.1	300	0	3.8	1.0
4	0.15	2.6	130	0	5.4	5.0
5	0.10	5.7	210	8	8.4	3.0
6	0.01	3.6	105	0	8.6	3.4
7	2.00	3.2	195	8	8.8	7.5

Initial estimates of background concentrations of CH_4 were taken from monitoring data at the UK government BEIS network measurement site at Tacolneston. These values were largely in agreement with the background concentrations suggested from the monitored data at site A. The initial background concentrations of C_2H_2 were assumed to be zero, however the monitored data baseline was above zero for some surveys, suggesting that a low background concentration should be applied in these cases. The final background concentrations used are shown in Table 11.

Table 11 – Site A background concentrations.

Survey	CH_4 (mg m^{-3})	C_2H_2 (mg m^{-3})
1	1.277	0
2	1.323	0.00108
3	1.396	0.00162
4	1.423	0.00216
5	1.323	0
6	1.370	0.00216
7	1.330	0.00216

A subset of the TDM survey transects were used for each survey, to choose transects where the landfill signal was strong and the modelled wind direction was consistent with the measured values. Transects used for each survey are given in Table 12.

Table 12 – Transects used for Site A.

Survey	Total number of transects available	Number of transects used	Transects used
1	9	3	9,10,11
2	8	3	1,2,3
3	6	4	4,5,6,7
4	16	10	5,6,7,8,9,10,15,16,17,18
5	12	10	4,5,6,7,8,9,10,11,12,14
6	9	7	2,3,4,5,6,7,8
7	16	2	1,3

7.1.2. Site A evaluation

The Modified Bayesian inversion approach was applied to estimate tracer gas emission rates for site A, to evaluate the model configuration. A perfect model configuration would lead to the inverse dispersion modelling input and output emission rates being equal.

The inverse dispersion modelling input and output tracer gas emission rates are compared in Figure 6 and Table 13. In general, the differences are small, only surveys 4 and 5 give a change of more than 0.1 g s^{-1}. The mean change is 0.001 g s^{-1}.

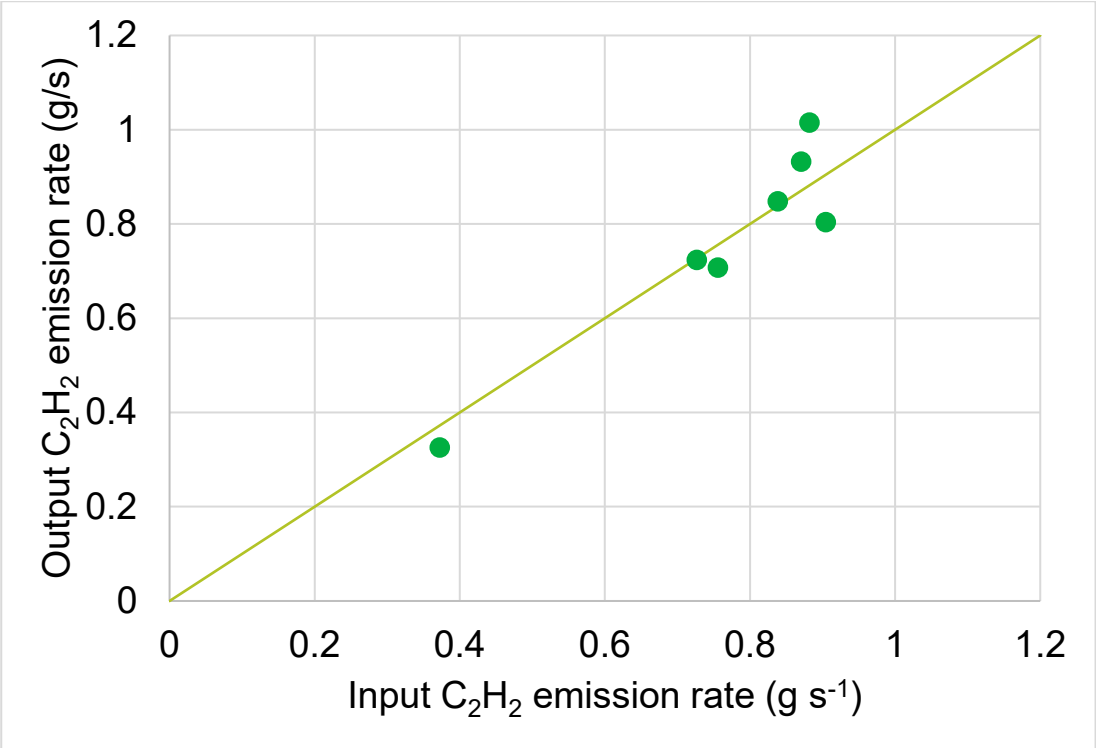

Figure 6 – Inverse dispersion modelling output C_2H_2 emission rate versus input C_2H_2 emission rate for the 7 surveys for site A.

Table 13 – Inverse dispersion modelling input and output C_2H_2 emission rate for the 7 surveys for site A.

Survey	Input C_2H_2 emission rate (g s^{-1})	Output C_2H_2 emission rate (g s^{-1})	Difference (g s^{-1})
1	0.73	0.72	-0.002
2	0.76	0.71	-0.047
3	0.37	0.33	-0.046
4	0.90	0.80	-0.100
5	0.88	1.02	0.134
6	0.84	0.85	0.008
7	0.87	0.93	0.063
Mean	0.76	0.77	0.001

Modelled and measured C_2H_2 concentrations for site A for each survey are compared in Figures 7 to 13. Transects used in the inverse dispersion modelling are identified by the blue squares marked ‘Peaks’ – these represent the measured peak values in the included transects. In general, the mean modelled concentration (dark blue) is considerably lower than the measurements (bright green), while the fluctuations local maximum concentration (lime green) is higher at most locations, but gives a reasonable match to measurements at the measured peaks used. This is the expected behaviour, because the mean modelled concentration has an averaging time of one hour, and the fluctuations local maximum represents the maximum likely one-second concentration at all locations during a one-hour period, so at any given time should only be expected to match the measurement at the measured peak location, not everywhere.

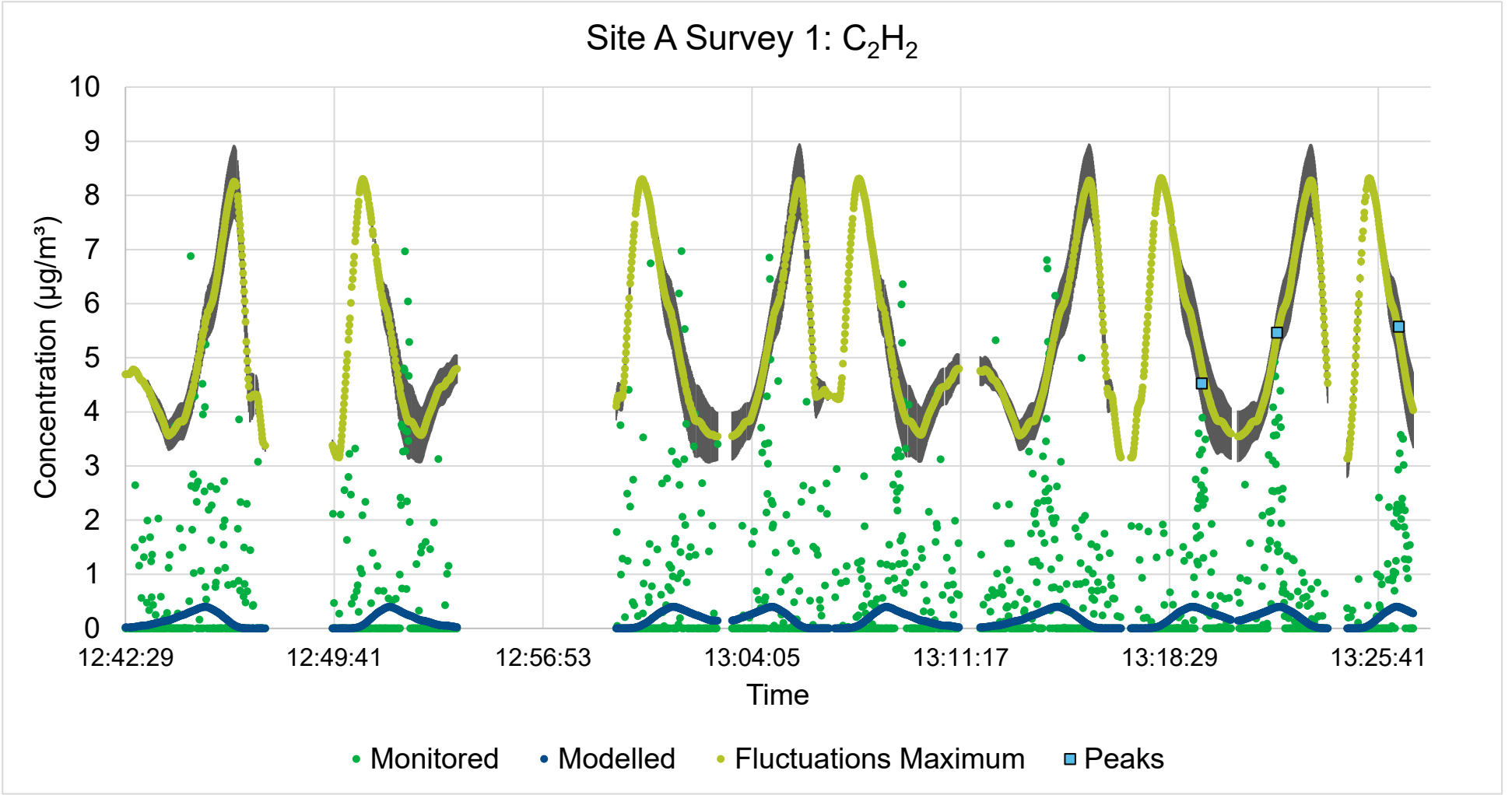

Figure 7 – Time series graph of hourly mean modelled (dark blue), modelled one-second fluctuations local maximum (lime green) and monitored (bright green) C_2H_2 concentrations for site A survey 1. The error bars represent the one-second fluctuations standard deviation of the modelled mean concentration. The 'Peaks' (blue squares) highlight the measured one-second peak C_2H_2 concentrations in the used transects (3 out of 9). The monitoring data is noisy with clearer peaks towards the end of the survey. The measurement noise could have been caused by the relatively strong wind speed during this survey (7.7 ms^{-1}).

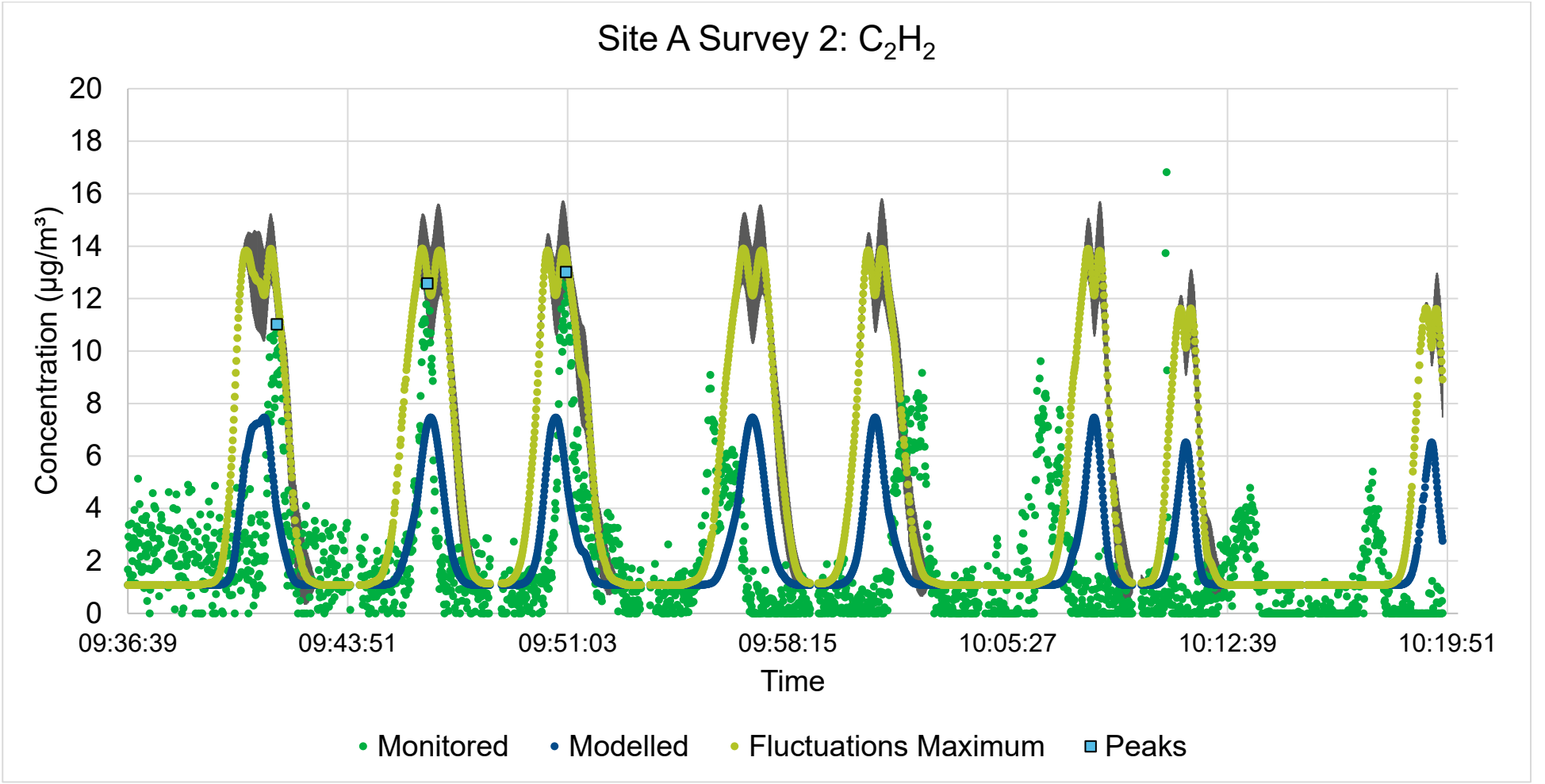

Figure 8 – Time series graph of hourly mean modelled (dark blue), modelled one-second fluctuations local maximum (lime green) and monitored (bright green) C_2H_2 concentrations for site A survey 2. The error bars represent the one-second fluctuations standard deviation of the modelled mean concentration. The 'Peaks' (blue squares) highlight the measured one-second peak C_2H_2 concentrations in the used transects (3 out of 8). This was a morning survey (9.30am) in cold, clear conditions. The modelled wind direction was in line with measured peaks for the first 3 transects, then the wind direction changed, because the measured peaks moved round gradually by 10 degrees over transects 4 to 8.

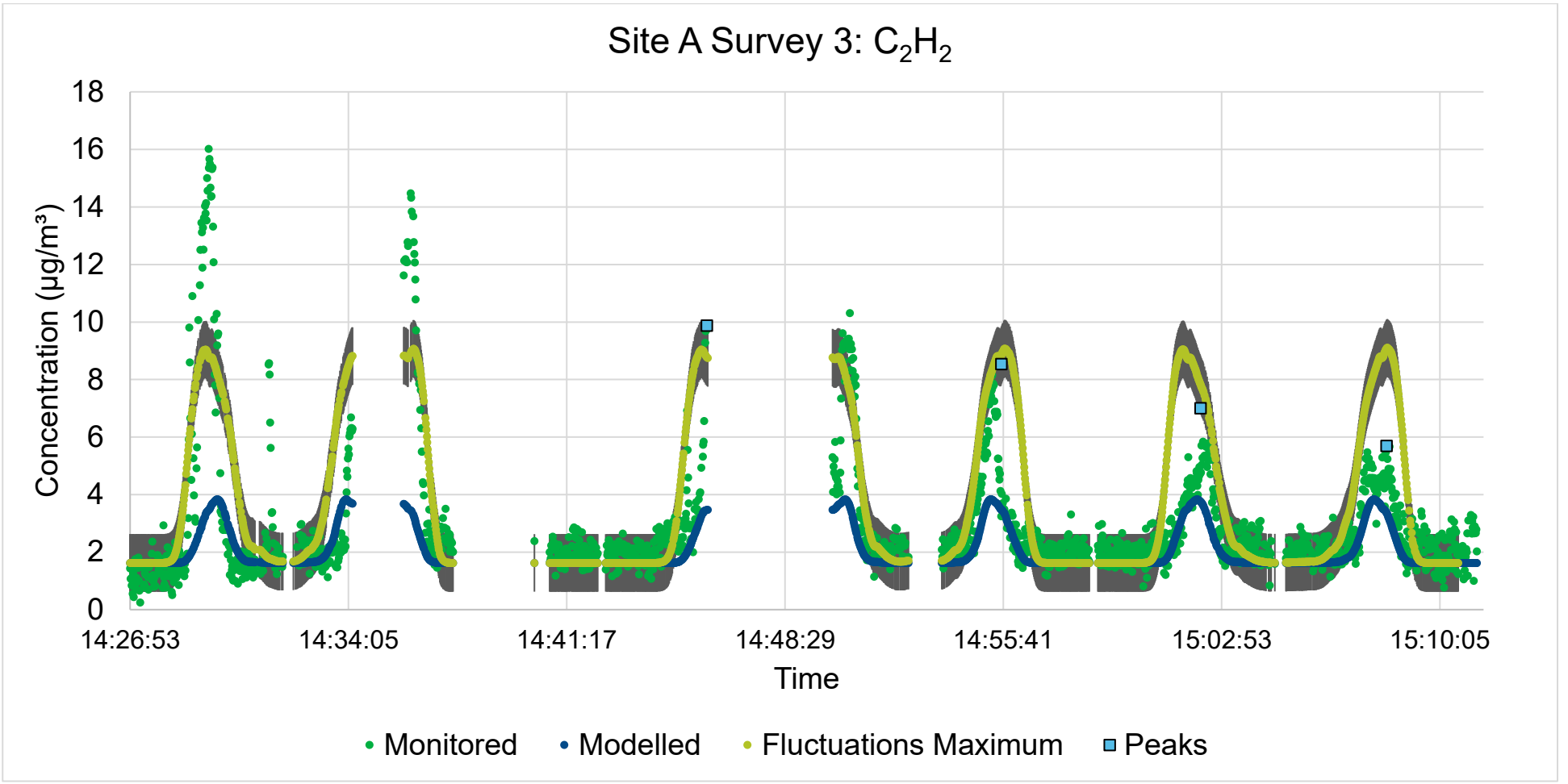

Figure 9 – Time series graph of hourly mean modelled (dark blue), modelled one-second fluctuations local maximum (lime green) and monitored (bright green) C_2H_2 concentrations for site A survey 3. The error bars represent the one-second fluctuations standard deviation of the modelled mean concentration. The 'Peaks' (blue squares) highlight the measured one-second peak C_2H_2 concentrations in the used transects (4 out of 6). All measured peaks were in line with the modelled wind direction, but the measurements show a significant reduction in the peak from the start to the end of the survey, which was not present in the modelled values.

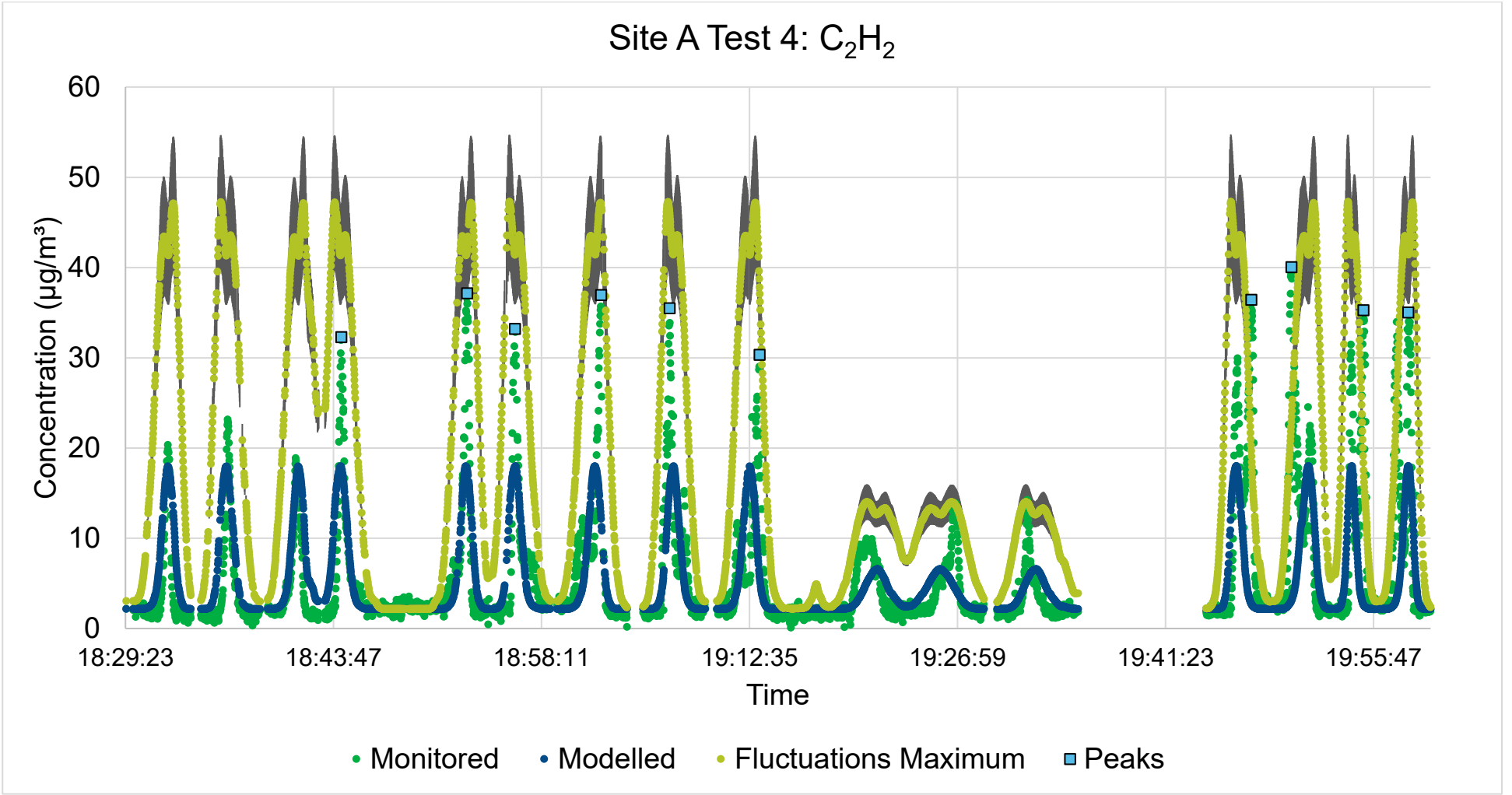

Figure 10 – Time series graph of hourly mean modelled (dark blue), modelled one-second fluctuations local maximum (lime green) and monitored (bright green) C_2H_2 concentrations for site A survey 4. The error bars represent the one-second fluctuations standard deviation of the modelled mean concentration. The 'Peaks' (blue squares) highlight the measured one-second peak C_2H_2 concentrations in the used transects (10 out of 16). The measured peaks aligned well with the modelled wind direction. The initial and final transects were 2 km from the site; the 3 transects at 19:20, 19:26 and 19:31 were 4 km away.

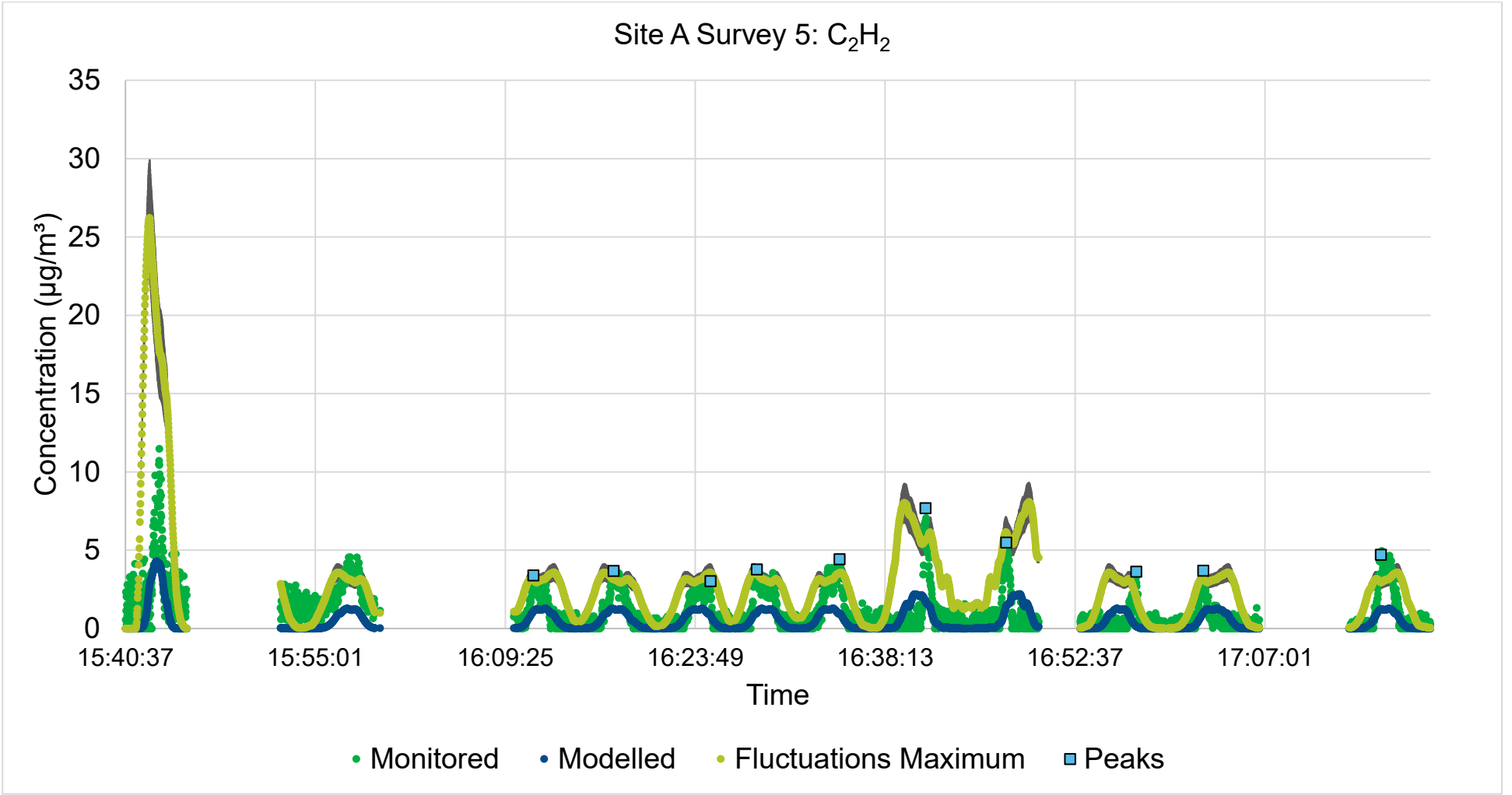

Figure 11 – Time series graph of hourly mean modelled (dark blue), modelled one-second fluctuations local maximum (lime green) and monitored (bright green) C_2H_2 concentrations for site A survey 5. The error bars represent the one-second fluctuations standard deviation of the modelled mean concentration. The 'Peaks' (blue squares) highlight the measured one-second peak C_2H_2 concentrations in the used transects (10 out of 12). The survey was carried out at dusk. Transects were measured at distances of 2, 3 and 4 km. The beginning and end transects were in line with the modelled wind direction; the middle transects were offset.

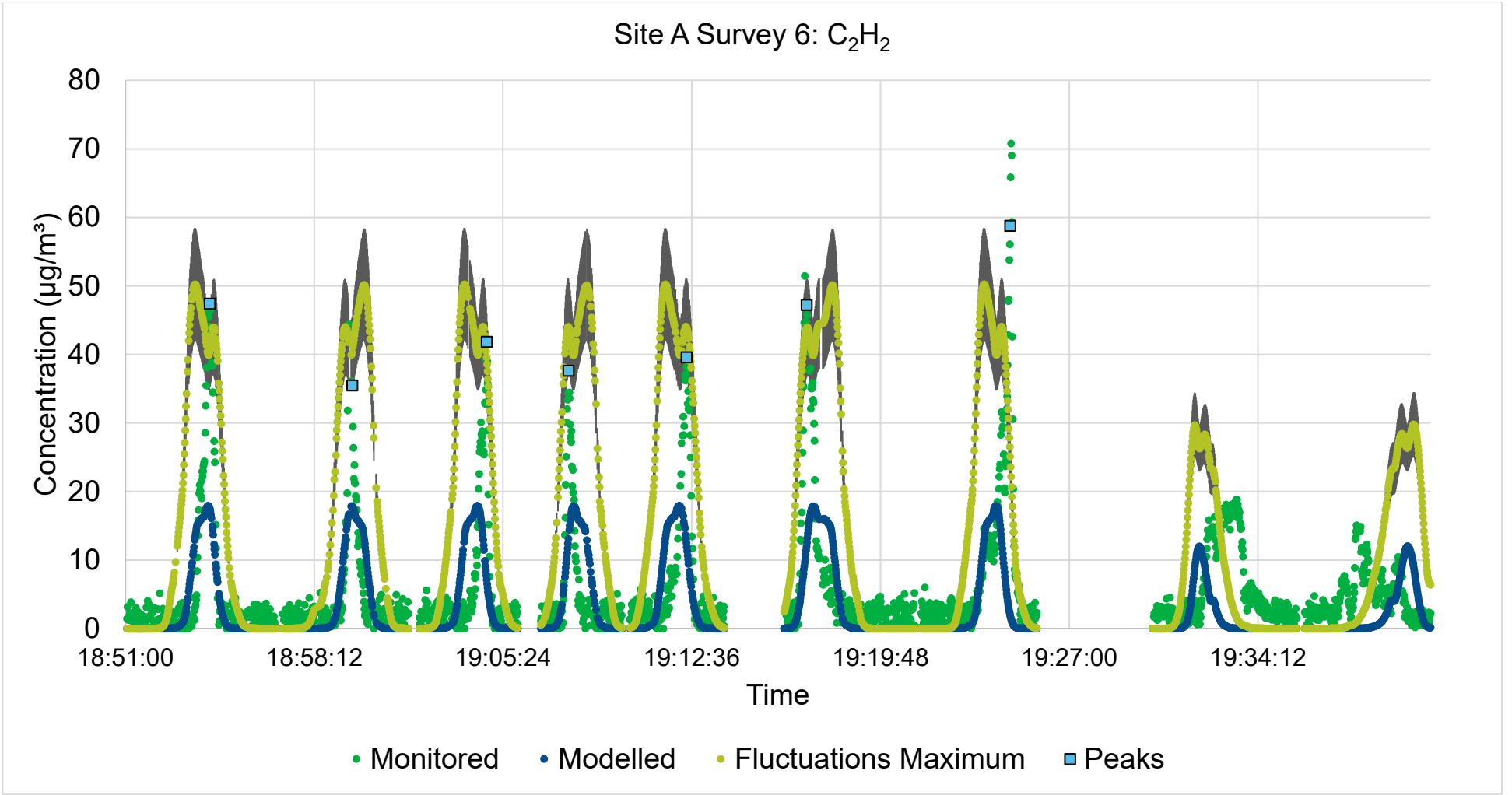

Figure 12 – Time series graph of hourly mean modelled (dark blue), modelled one-second fluctuations local maximum (lime green) and monitored (bright green) C_2H_2 concentrations for site A survey 6. The error bars represent the one-second fluctuations standard deviation of the modelled mean concentration. The 'Peaks' (blue squares) highlight the measured one-second peak C_2H_2 concentrations in the used transects (7 out of 9). The survey was carried out at dusk. The initial transects had monitored peaks in line with the modelled wind direction, but then the wind direction changed.

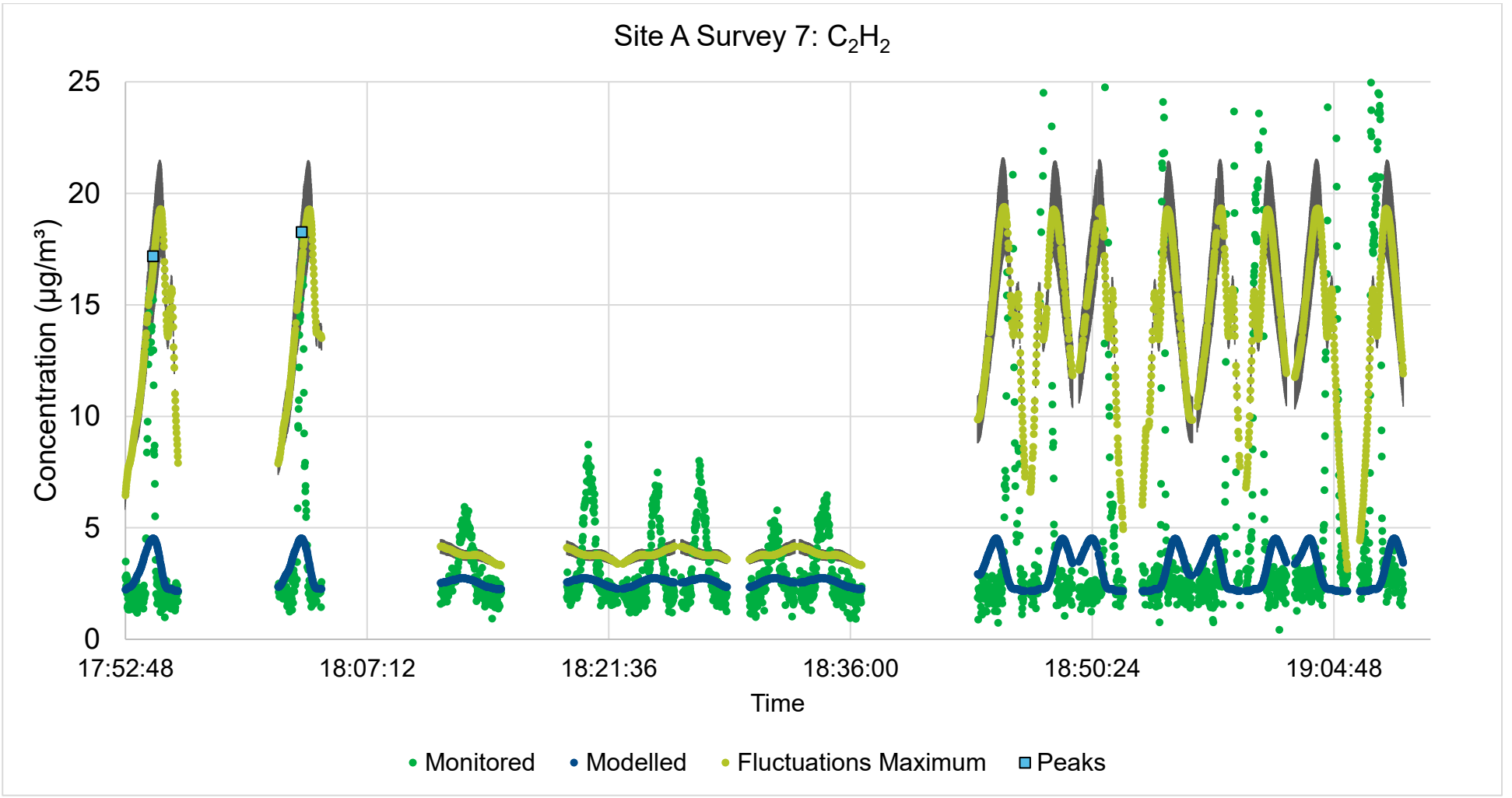

Figure 13 – Time series graph of hourly mean modelled (dark blue), modelled one-second fluctuations local maximum (lime green) and monitored (bright green) C_2H_2 concentrations for site A survey 7. The error bars represent the one-second fluctuations standard deviation of the modelled mean concentration. The 'Peaks' (blue squares) highlight the measured one-second peak C_2H_2 concentrations in the used transects (2 out of 16). The survey was carried out at dusk. The initial transects had measured peaks in line with the modelled wind direction, but then the wind direction changed.

7.1.3. Site B inputs

Site B was represented by 5 volume sources which were positioned over the location of the landfill site as shown in Figure 14. The total footprint area of sources was 205,115.0 m^2. Each volume source had a depth of 1 m.

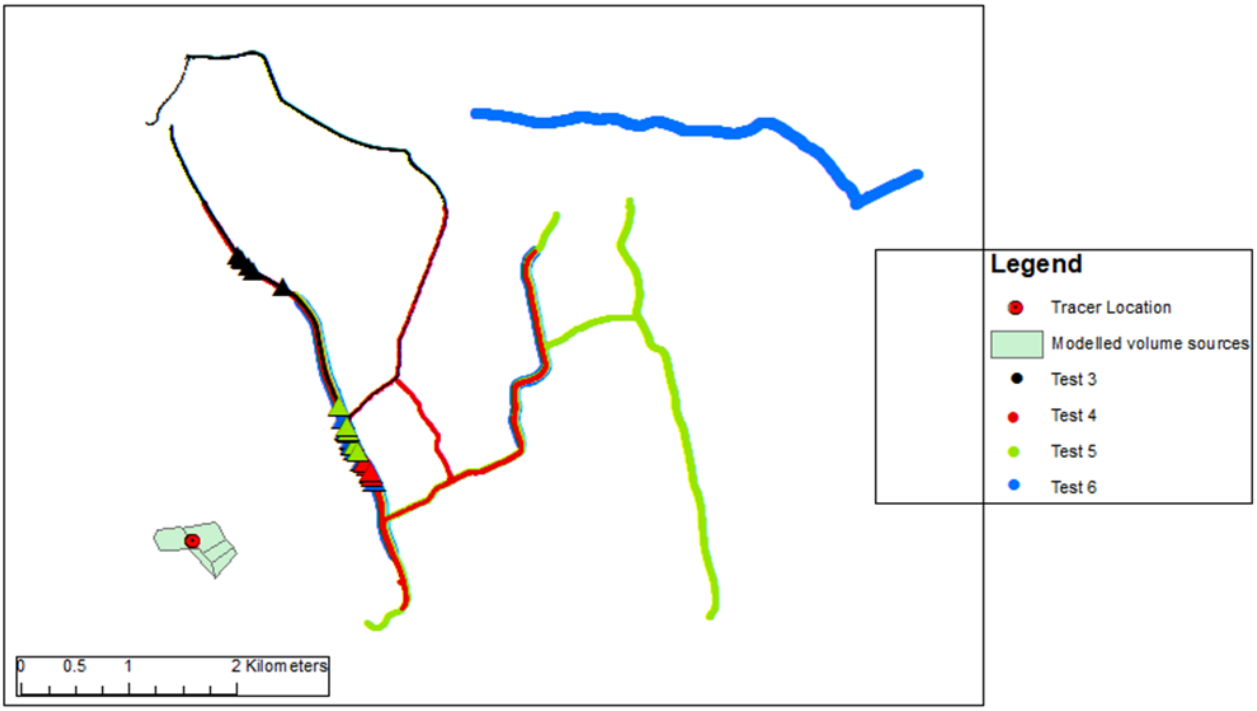

Figure 14 – Site B showing transect locations relative to tracer release site and modelled volume sources used to represent the landfill site. Receptor locations highlighted using a triangle symbol locate the position of the maximum values used for the inverse dispersion modelling.

The model domain used a latitude of 51.92°. All other site options, such as minimum Monin-Obukhov length were left as the model default values.

The tracer release was modelled as a point source with a height of 1 m, a diameter of 0.02m and a volume flow rate calculated using the release mass of pollutant, with the ambient temperature and pressure recorded on site for each survey. The emission rates and the tracer volume flow rates were calculated in the same way as for site A, the resulting input values are shown in Table 14.

Table 14 – Site B emission parameters for each survey.

Survey	Tracer emission rate of C_2H_2 (g s^{-1})	Tracer volume flow rate (m^3 s^{-1})
3	0.88	7.88E-04
4	0.74	6.59E-04
5	0.88	7.91E-04
6	0.86	7.91E-04

Sensitivity testing was carried out to find the meteorological parameters that gave the best agreement between modelled and measured tracer gas concentrations, leading to the minimum change in tracer gas emission rate using this inversion dispersion modelling method. Surface roughness values were selected separately for each survey as part of this process. The final set of input meteorological parameters used are shown in Table 15.

Table 15 – Site B meteorological parameters for each survey.

Survey	Surface roughness (m)	10 m height wind speed (m s^{-1})	Wind direction (degrees)	Cloud cover (Oktas)	Temperature (°C)	Wind direction variability (degrees)
3	0.25	6.2	189	4	8.9	5.0
4	1.25	5.7	240	8	11.4	3.5
5	0.20	3.6	230	8	10.3	3.0
6	0.70	12.9	230	6	9.6	5.0

Initial estimates of background concentrations of CH_4 were taken from monitoring data at the DECC background site at Tacolneston. These values were largely in agreement with the background concentrations suggested from the monitored data at site B. The initial background concentrations of C_2H_2 were assumed to be zero, however the monitored data baseline was above zero for some surveys, suggesting that a low background concentration should be applied in these cases.

Table 16 – Site B background concentrations.

Survey	CH_4 (mg m^{-3})	C_2H_2 (mg m^{-3})
3	1.343	0.000541
4	1.330	0.002162
5	1.316	0.001622
6	1.320	0

A subset of the TDM survey transects were used for each survey, to choose transects where the landfill signal was strong and the modelled wind direction was consistent with the measured values. The transects used for each survey are given in Table 17.

Table 17 – Transects used for site B

Survey	Total number of transects available	Number of transects used	Transects used
3	14	6	2,3,4,5,6,7
4	18	5	1,2,3,4,5
5	23	6	1,2,3,4,5,6
6	23	15	4,5,6,8,9,10,11,15,18,20,21,22,23,24,25

7.1.4. Site B evaluation

The modified Bayesian inversion approach was applied to estimate tracer gas emission rates for site B, to evaluate the model configuration. A perfect model configuration would lead to the inverse dispersion modelling input and output emission rates being equal.

The inverse dispersion modelling input and output tracer gas emission rates are compared in Figure 15 and Table 18. In general, the differences are small, only survey 4 gives a change of more than 0.1 g s^{-1}. The mean adjustment is -0.06 g s^{-1}.

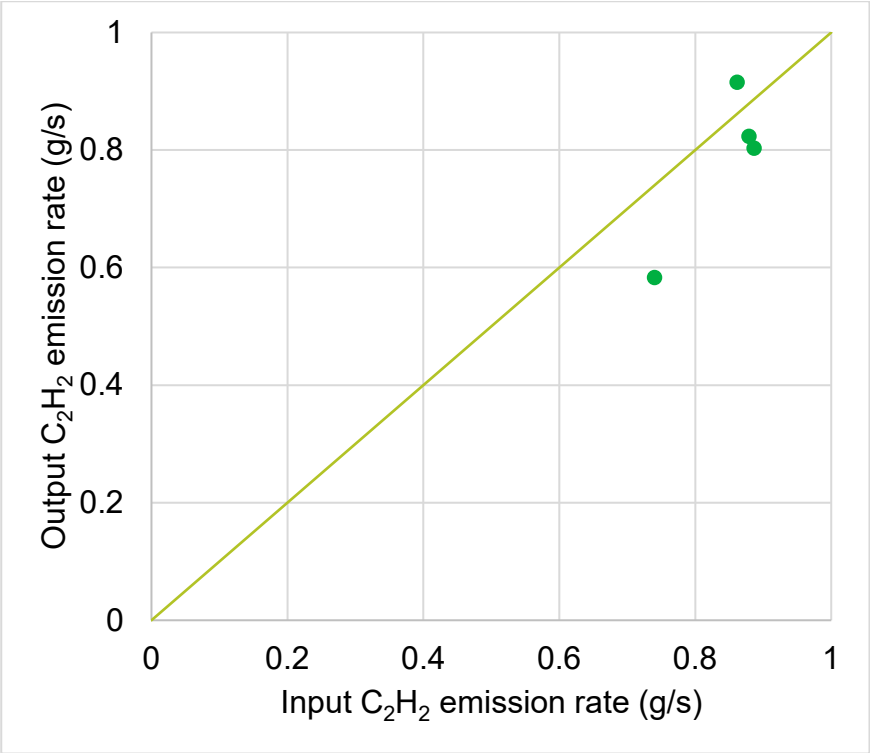

Figure 15 – Inverse dispersion modelling output C_2H_2 emission rate versus input C_2H_2 emission rate for the 4 surveys for site B.

Table 18 – Inverse dispersion modelling input and output C_2H_2 emission rate for the 4 surveys for site B.

Survey	Input C_2H_2 emission rate (g s^{-1})	Output C_2H_2 emission rate (g s^{-1})	Difference (g s^{-1})
3	0.89	0.80	-0.083
4	0.74	0.58	-0.156
5	0.88	0.82	-0.055
6	0.86	0.92	0.054
Mean	0.84	0.78	-0.060

Modelled and measured C_2H_2 concentrations for site B for each survey are compared in Figures 16 to 19. Transects used in the inverse dispersion modelling are identified by the blue squares marked ‘Peaks’ – these represent the measured peak values in the included transects. In general, the mean modelled concentration (dark blue) is considerably lower than the measurements (bright green), while the fluctuations local maximum concentration (lime green) is higher at most locations, but gives a reasonable match to measurements at

the measured peaks used. This is the expected behaviour, because the mean modelled concentration has an averaging time of one hour, and the fluctuations local maximum represents the maximum likely one-second concentration at all locations during a one-hour period, so at any given time should only be expected to match the measurement at the measured peak location, not everywhere.

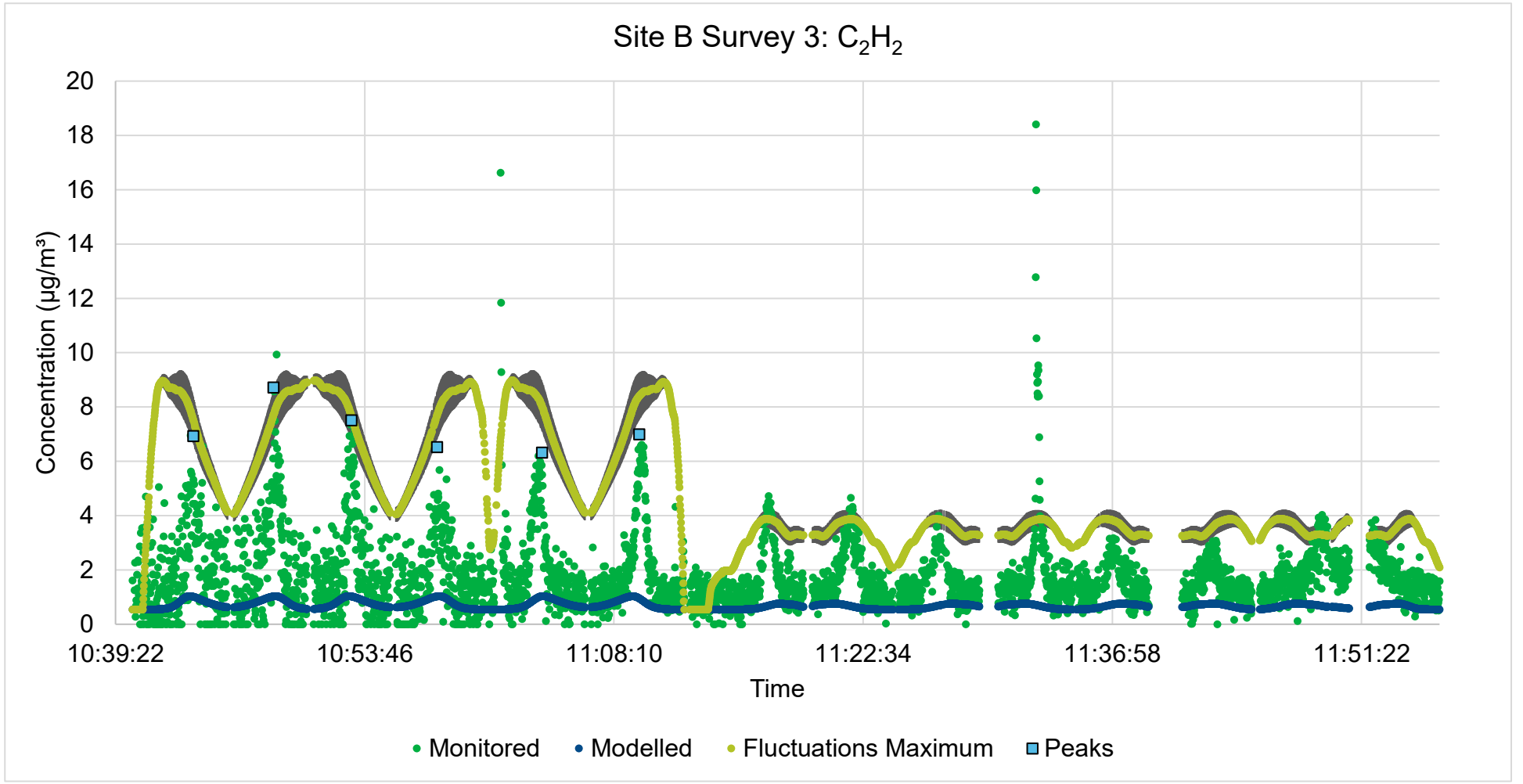

Figure 16 – Time series graph of hourly mean modelled (dark blue), modelled one-second fluctuations local maximum (lime green) and monitored (bright green) C_2H_2 concentrations for site B survey 3. The error bars represent the one-second fluctuations standard deviation of the modelled mean concentration. The 'Peaks' (blue squares) highlight the measured one-second peak C_2H_2 concentrations in the used transects (6 out of 14). The measurements were a little noisy. The wind direction was stable for the first few transects then gradually changed over the reminder of the time. The initial transects were 2.5 km from the site, moving to 4 km away for the final transects.

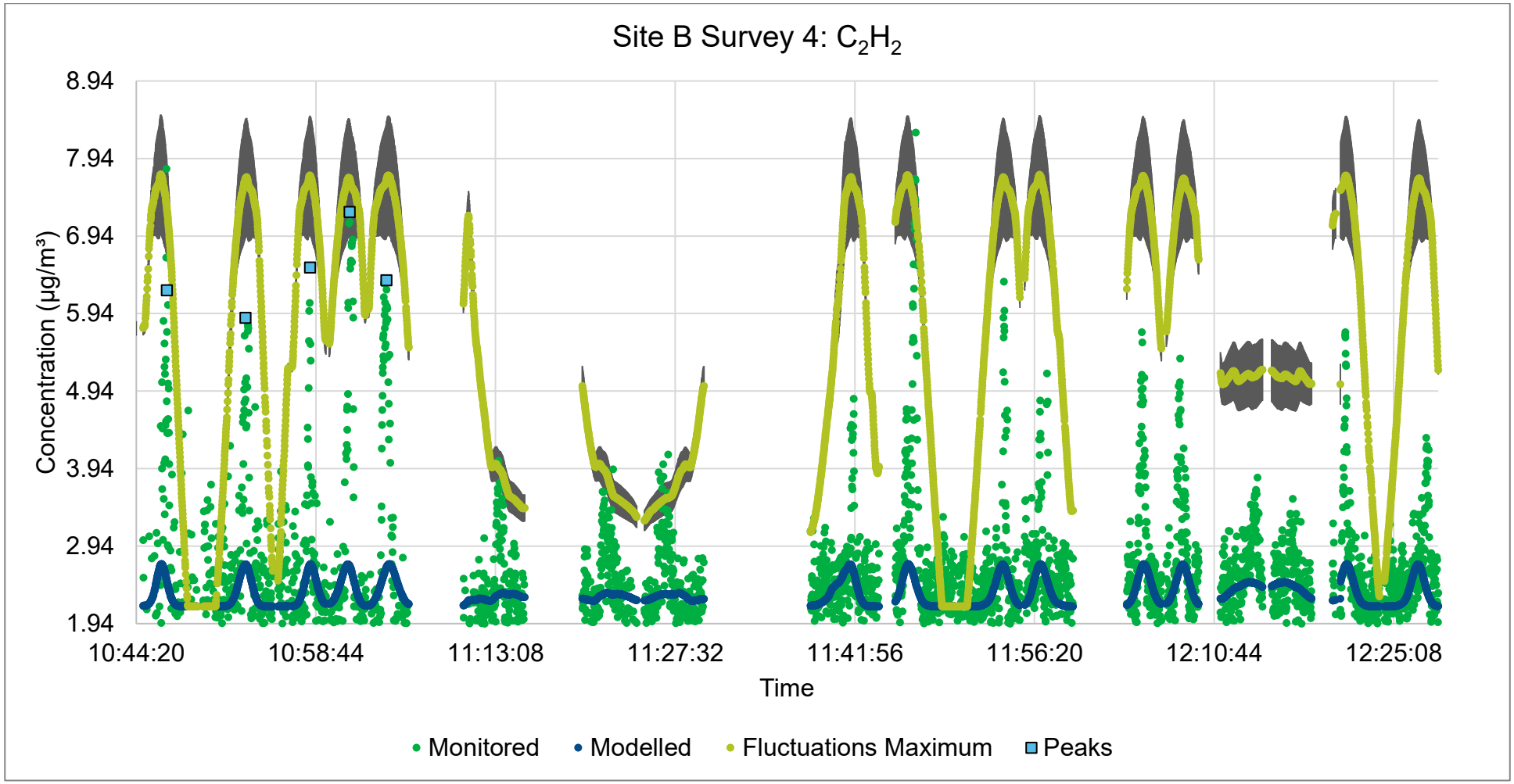

Figure 17 – Time series graph of hourly mean modelled (dark blue), modelled one-second fluctuations local maximum (lime green) and monitored (bright green) C_2H_2 concentrations for site B survey 4. The error bars represent the one-second fluctuations standard deviation of the modelled mean concentration. The 'Peaks' (blue squares) highlight the measured one-second peak C_2H_2 concentrations in the used transects (5 out of 18). The first 5 transects were along a road 1.5 km from the site, and the modelled plume aligned reasonably well with the monitored data. The transects then moved to 4 km away. These roads did not form a straight line transect so are more difficult to interpret.

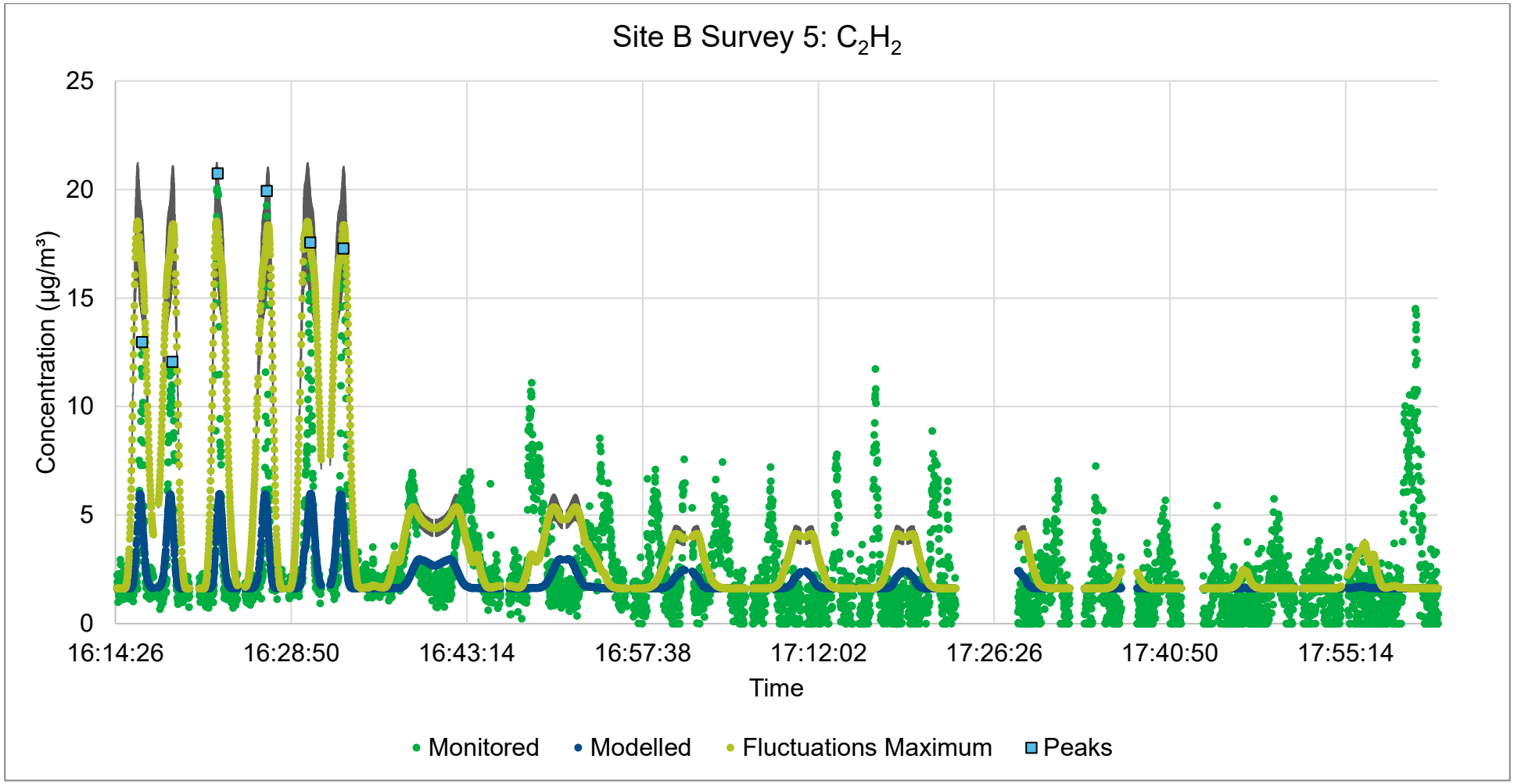

Figure 18 – Time series graph of hourly mean modelled (dark blue), modelled one-second fluctuations local maximum (lime green) and monitored (bright green) C_2H_2 concentrations for site B survey 5. The error bars represent the one-second fluctuations standard deviation of the modelled mean concentration. The 'Peaks' (blue squares) highlight the measured one-second peak C_2H_2 concentrations in the used transects (6 out of 23). This survey was similar to survey 4 in terms of location. The modelled wind direction aligned well with the measured peaks at the beginning of the survey, but then the wind direction changed. This survey was carried out at dusk.

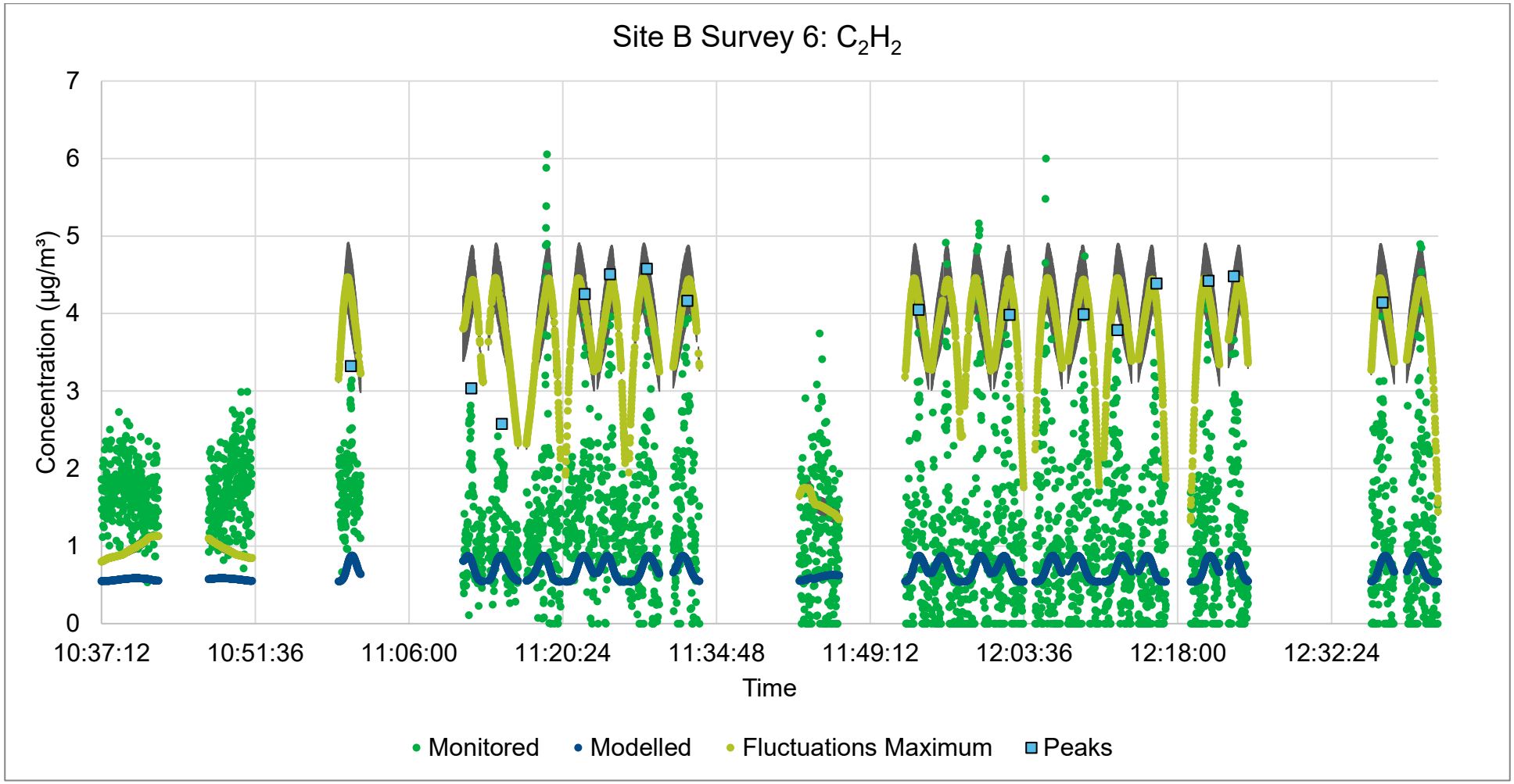

Figure 19 – Time series graph of hourly mean modelled (dark blue), modelled one-second fluctuations local maximum (lime green) and monitored (bright green) C_2H_2 concentrations for site B survey 6. The error bars represent the one-second fluctuations standard deviation of the modelled mean concentration. The 'Peaks' (blue squares) highlight the measured one-second peak C_2H_2 concentrations in the used transects (15 out of 23). The monitoring data is quite noisy. The measured peaks were in line with the modelled wind direction during most of the survey. The first transect was 6.5 km away, the transect at around 11:43am is 3.5 km away and the rest of the transects were 1.5 km away. The more distant transects were not used.

7.1.5. Site C inputs

Site C was represented by 8 volume sources which were positioned in the location of the landfill site, as shown in Figure 20. The total footprint area of the sources was 756,074.5 m^2. Each volume source had a depth of 1 m.

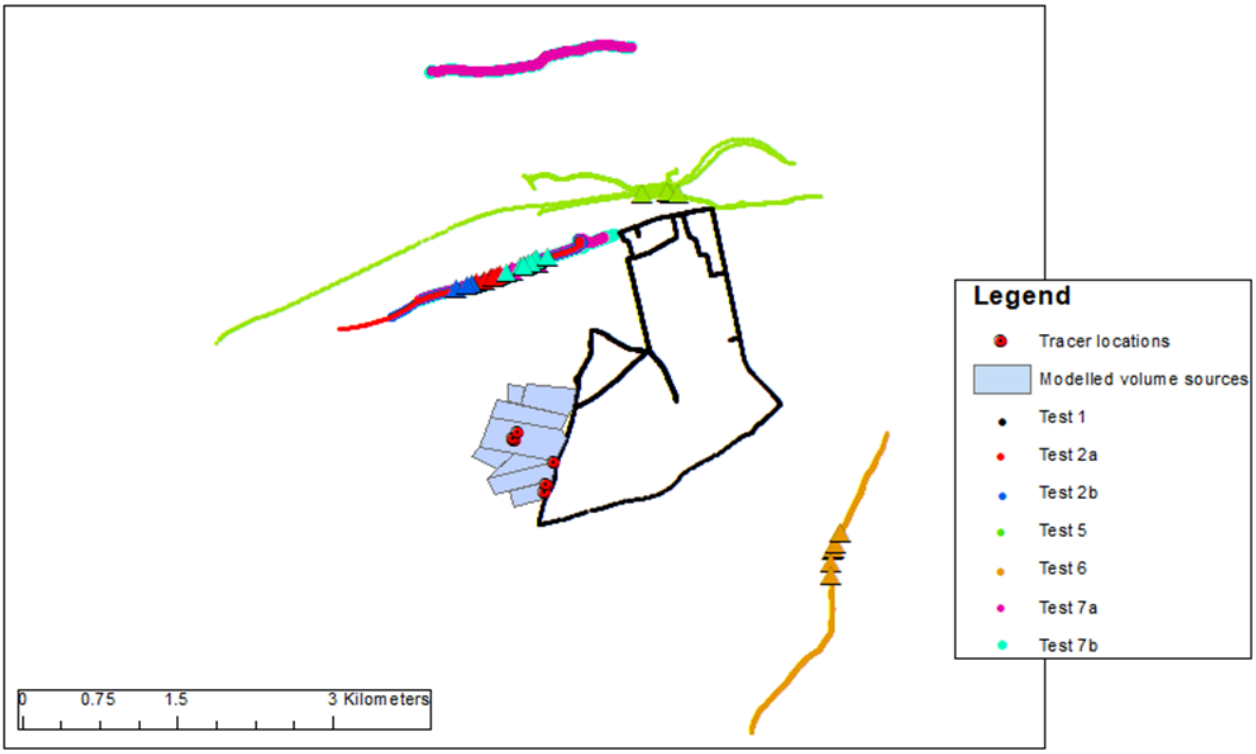

Figure 20 – Site C showing transect locations relative to the tracer release sites and modelled volume sources used to represent the landfill site. Receptor locations highlighted using a triangle symbol locate the position of the maximum values used for the inverse dispersion modelling.

The modelling used a latitude of 51.92°. All other site options, such as minimum Monin-Obukhov length were left as the model default values.

The tracer release was modelled as a point source with a height of 1 m, a diameter of 0.02 m and a volume flow rate calculated using the release mass of pollutant, with the ambient temperature and pressure recorded on site for each survey.

The emission rates and the tracer volume flow rates were calculated in the same way as for site A, the resulting input values are shown in Table 19.

Table 19 – Site C emission parameters for each survey.

Survey	Tracer emission rate of C_2H_2 (gs^{-1})	Tracer volume flow rate (m^3s^{-1})
1	0.71	6.38E-04
2a	0.74	6.64E-04
2b	0.58	5.22E-04
5	0.89	7.97E-04
6	0.90	8.00E-04
7a	0.86	7.99E-04
7b	0.86	8.02E-04

Sensitivity testing was carried out to find the meteorological parameters that achieve gave the best agreement between modelled and measured tracer gas concentrations, leading to the minimum change in tracer gas emission rate using this inversion dispersion modelling method. Surface roughness values were selected separately for each survey as part of this process. The input meteorological parameters are shown in Table 20.

Table 20 – Site C meteorological parameters for each survey.

Survey	Surface roughness (m)	10 m height wind speed ($m\ s^{-1}$)	Wind direction (degrees)	Cloud cover (Oktas)	Temperature (°C)	Wind direction variability (degrees)
2a	1.50	5.7	170	8	8.9	8.6
2b	1.00	6.7	160	7	8.7	4.0
5	0.10	3.6	210	7	7.0	1.0
6	0.05	3.5	290	7	6.2	5.0
7a	2.50	4.0	180	7	11.6	3.5
7b	2.00	4.0	180	7	11.0	3.5

Initial estimates of background concentrations of CH_4 were taken from monitoring data at the DECC background site at Heathfield. These values were largely in agreement with the background concentrations suggested from the monitored data at site C. The initial background concentrations of C_2H_2 were assumed to be zero, however the monitored data baseline was above zero for some surveys, suggesting that a low background concentration should be applied in these cases.

Table 21 – Site B background concentrations

Survey	CH_4 (mg m^{-3})	C_2H_2 (mg m^{-3})
2a	1.270	0
2b	1.270	0
5	1.350	0
6	1.343	0.000540
7a	1.316	0.001081
7b	1.316	0.001622

A subset of the TDM survey transects were used for each survey, to choose transects where the landfill signal was strong and the modelled wind direction was consistent with the measured values. The transects used for each survey are given in Table 22.

Table 22 – Transects used for site C.

Survey	Total number of transects available	Number of transects used	Transects used
2a	8	8	2,3,4,5,6,7,8,11
2b	4	3	1,3,4
5	15	4	13,14,16,17
6	16	7	2,3,4,5,6,7,8
7a	14	8	2,3,4,5,12,13,14,15
7b	15	10	1,2,3,4,5,6,14,15,16,17

7.1.6. Site C evaluation

The Modified Bayesian inversion approach was applied to estimate tracer gas emission rates for site C, to evaluate the model configuration. A perfect model configuration would lead to the inverse dispersion modelling input and output emission rates being equal.

The inverse dispersion modelling input and output tracer gas emission rates are compared in Figure 21 and Table 23. In general, the differences are small, only survey 7a gives a change of more than 0.1 g s^{-1}. The mean adjustment is -0.045 g s^{-1}.

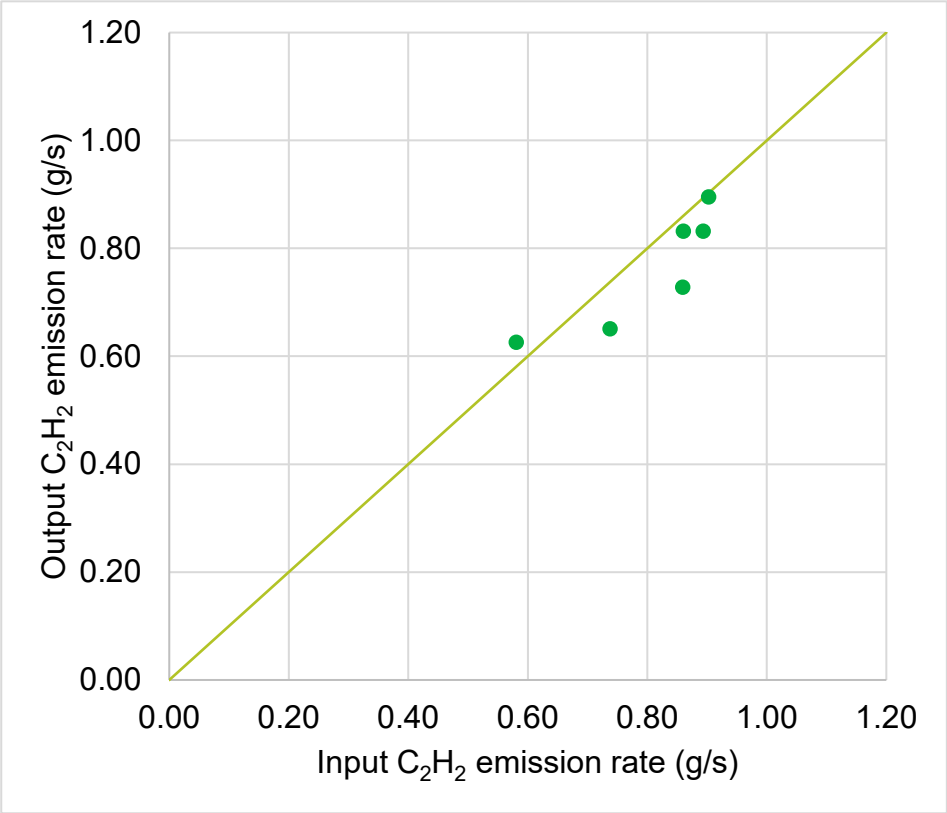

Figure 21 – Inverse dispersion modelling output C_2H_2 emission rate versus input C_2H_2 emission rate for the 6 surveys for site C.

Table 23 – Inverse dispersion modelling input and output C_2H_2 emission rates for the 6 surveys for site C.

Survey	Input C_2H_2 emission rate ($g\ s^{-1}$)	Output C_2H_2 emission rate ($g\ s^{-1}$)	Difference ($g\ s^{-1}$)
2a	0.74	0.65	-0.087
2b	0.58	0.63	0.045
5	0.89	0.83	-0.062
6	0.90	0.90	-0.007
7a	0.86	0.73	-0.131
7b	0.86	0.83	-0.029
Mean	0.81	0.76	-0.045

Modelled and measured C_2H_2 concentrations for site C for each survey are compared in Figures 22 to 27. Transects used in the inverse dispersion modelling are identified by the blue squares marked ‘Peaks’ – these represent the measured peak values in the used transects. In general, the mean modelled concentration (dark blue) is considerably lower than the measurements (bright green), while the fluctuations local maximum concentration (lime green) is higher at most locations, but gives a reasonable match to measurements at the measured peaks used. This is the expected behaviour, because the mean modelled concentration has an averaging time of one hour, and the fluctuations local maximum represents the maximum likely one-second concentration at all locations during a one-hour period, so at any given time should only be expected to match the measurement at the measured peak location, not everywhere.

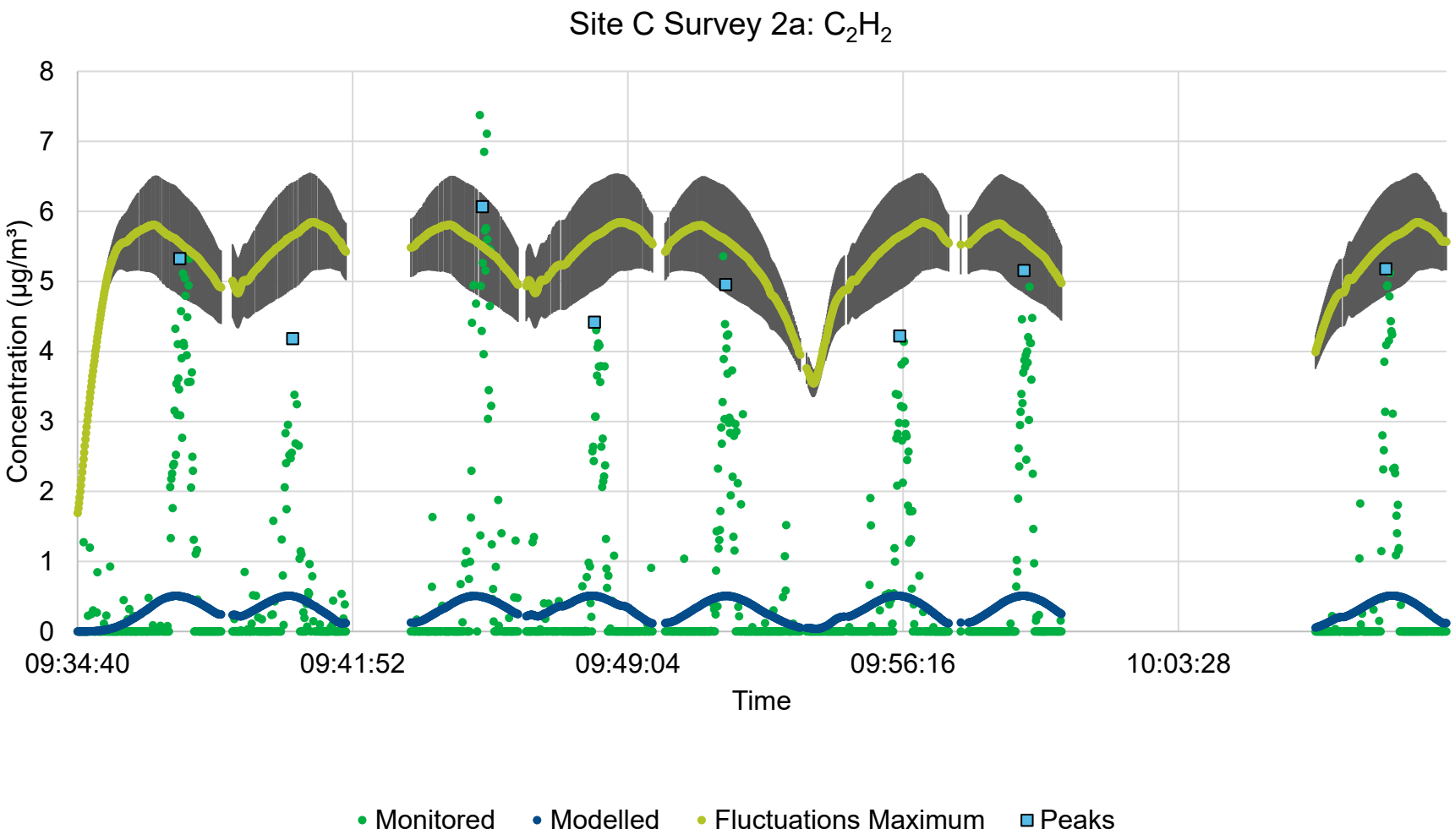

Figure 22 – Time series graph of hourly mean modelled (dark blue), modelled one-second fluctuations local maximum (lime green) and monitored (bright green) C_2H_2 concentrations for site C survey 2a. The error bars represent the one-second fluctuations standard deviation of the modelled mean concentration. The 'Peaks' (blue squares) highlight the measured one-second peak C_2H_2 concentrations in the used transects (8 out of 8). For this survey, all transects were in the same location, the wind direction was consistent, and all transects were used.

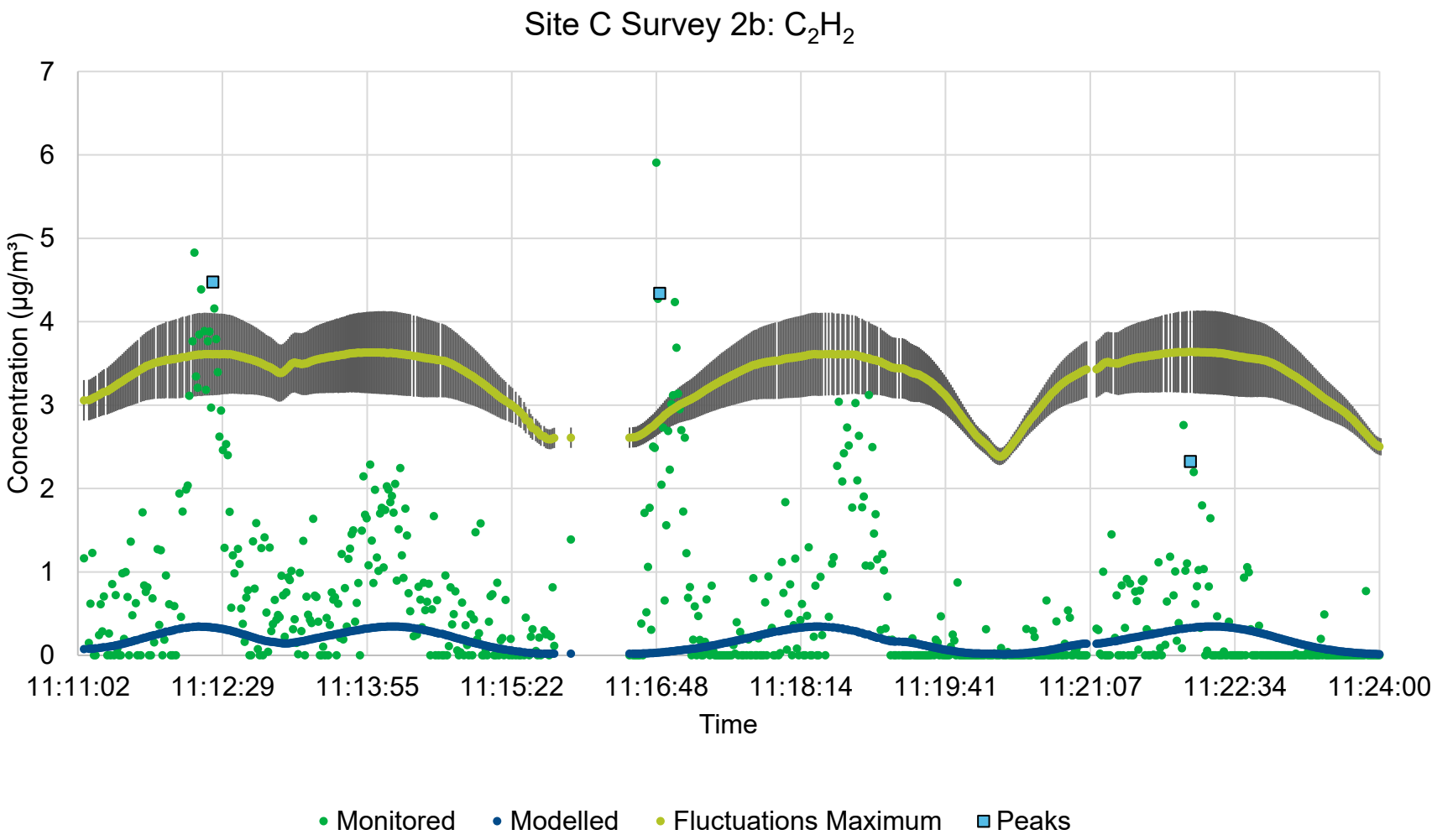

Figure 23 – Time series graph of hourly mean modelled (dark blue), modelled one-second fluctuations local maximum (lime green) and monitored (bright green) C_2H_2 concentrations for site C survey 2b. The error bars represent the one-second fluctuations standard deviation of the modelled mean concentration. The 'Peaks' (blue squares) highlight the measured one-second peak C_2H_2 concentrations in the used transects (3 out of 4). This was a short survey with 3 transects, each had a double peak, and the highest peak was in line with the modelled wind direction.

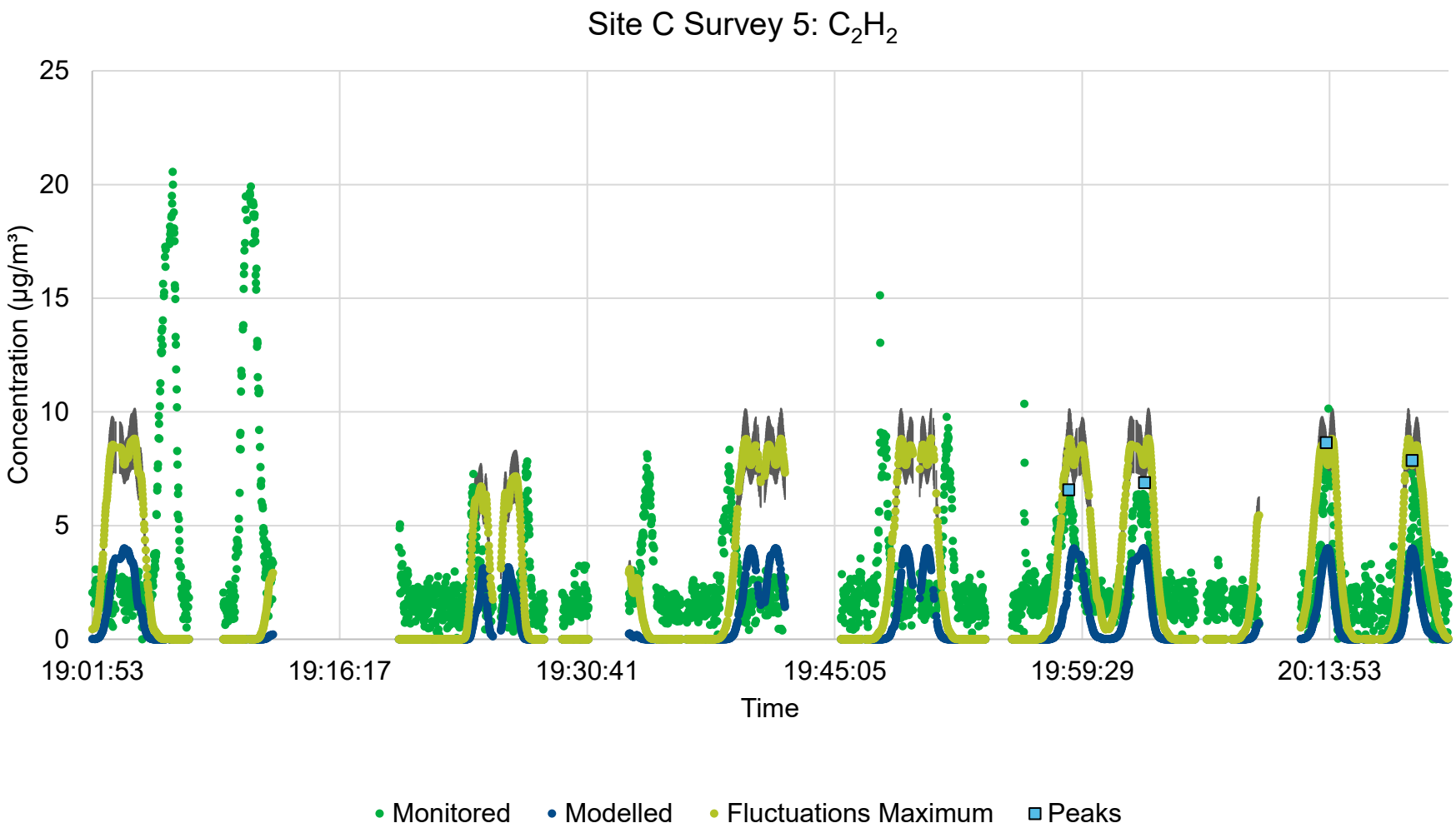

Figure 24 – Time series graph of hourly mean modelled (dark blue), modelled one-second fluctuations local maximum (lime green) and monitored (bright green) C_2H_2 concentrations for site C survey 5. The error bars represent the one-second fluctuations standard deviation of the modelled mean concentration. The 'Peaks' (blue squares) highlight the measured one-second peak C_2H_2 concentrations in the used transects (4 out of 15). All transects were 3km away, the wind direction shows variation, with only the last transects in line with the modelled wind direction.

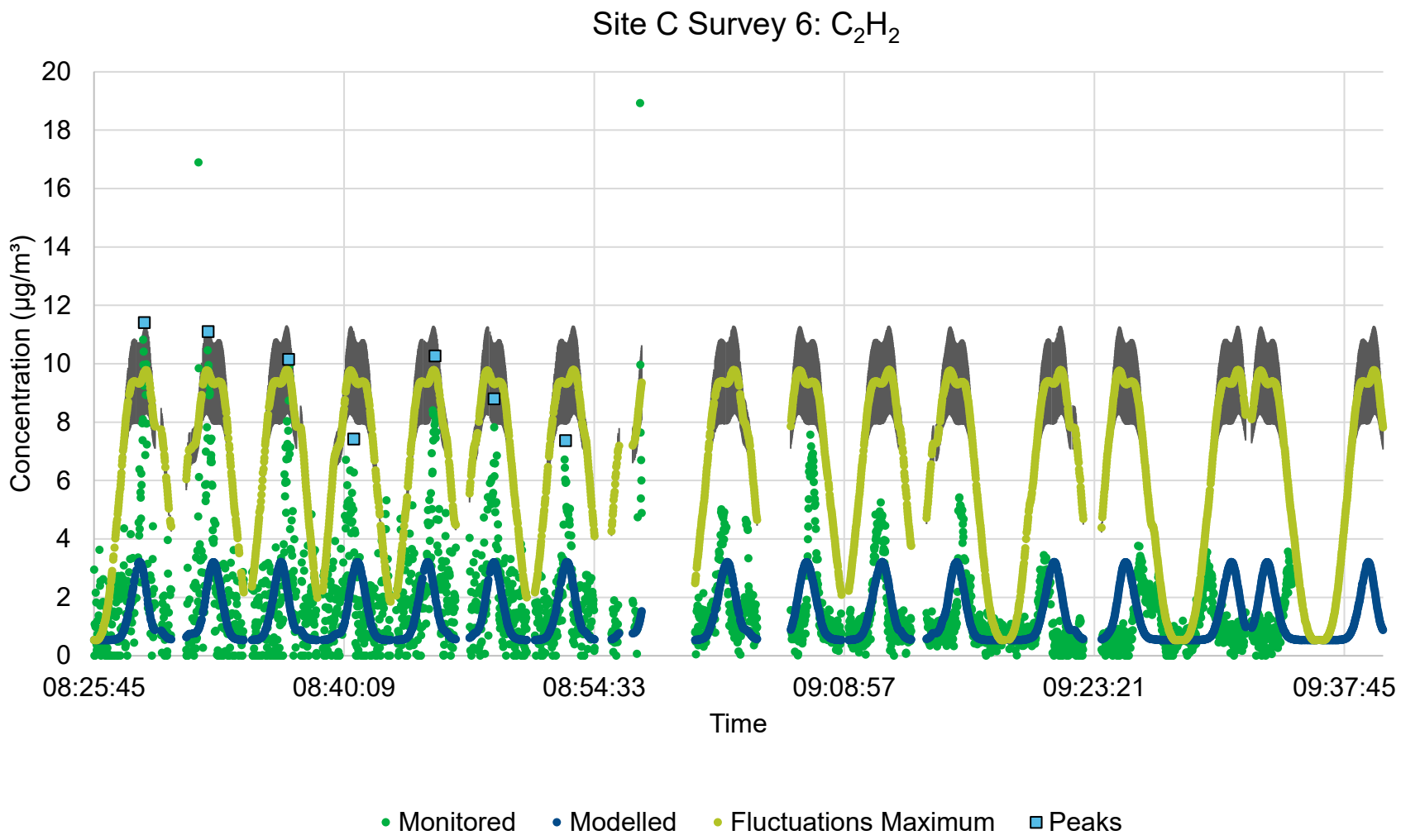

Figure 25 – Time series graph of hourly mean modelled (dark blue), modelled one-second fluctuations local maximum (lime green) and monitored (bright green) C_2H_2 concentrations for site C survey 6. The error bars represent the one-second fluctuations standard deviation of the modelled mean concentration. The 'Peaks' (blue squares) highlight the measured one-second peak C_2H_2 concentrations in the used transects (7 out of 16). This was a morning survey with the wind direction showing a shift half way through the survey.

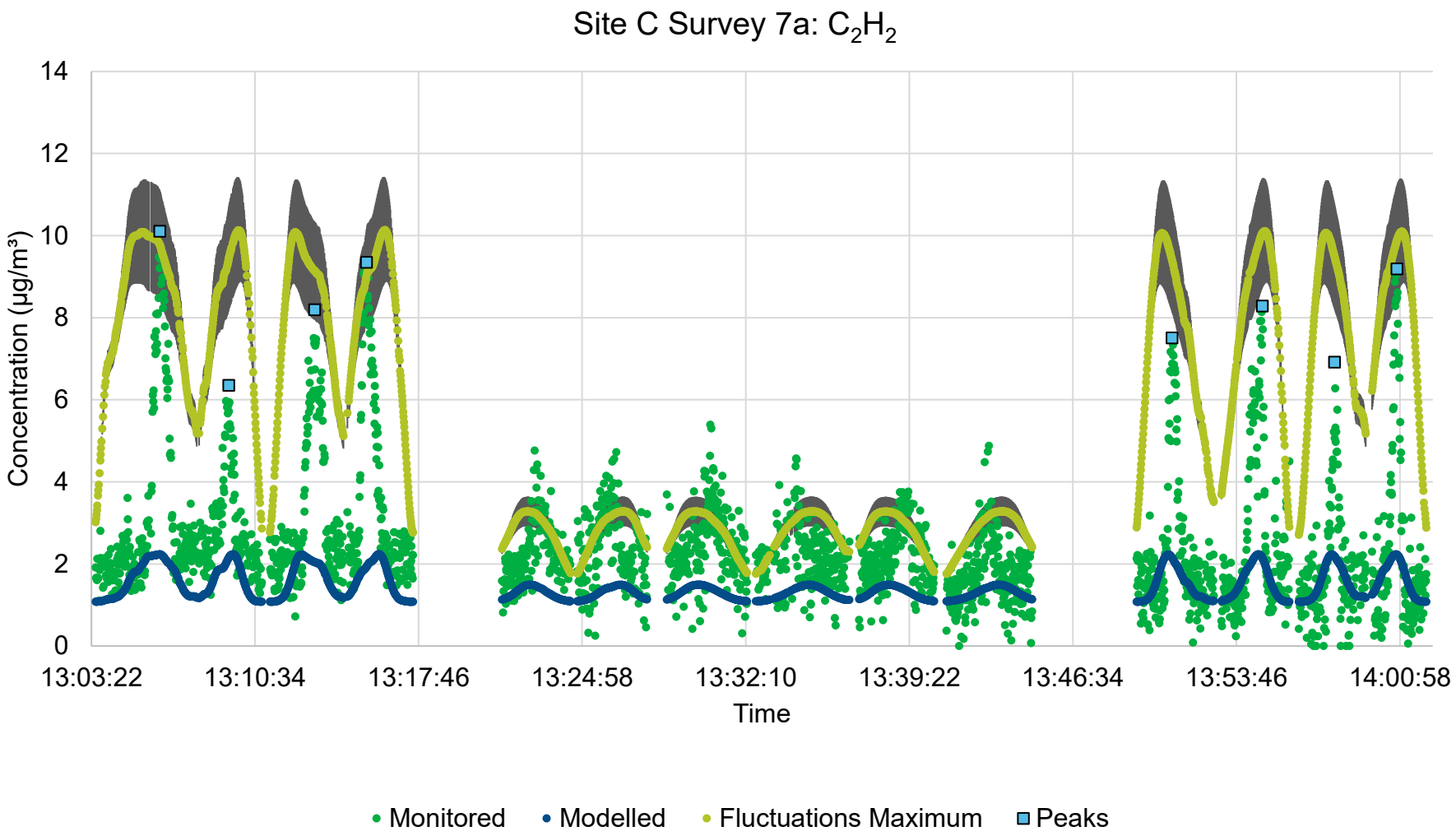

Figure 26 – Time series graph of hourly mean modelled (dark blue), modelled one-second fluctuations local maximum (lime green) and monitored (bright green) C_2H_2 concentrations for site C survey 7a. The error bars represent the one-second fluctuations standard deviation of the modelled mean concentration. The 'Peaks' (blue squares) highlight the measured one-second peak C_2H_2 concentrations in the used transects (8 out of 14). This survey measured 2 sets of transects, at 1.5 km and 3.5 km away. The measured peaks show consistency with the modelled wind direction throughout.

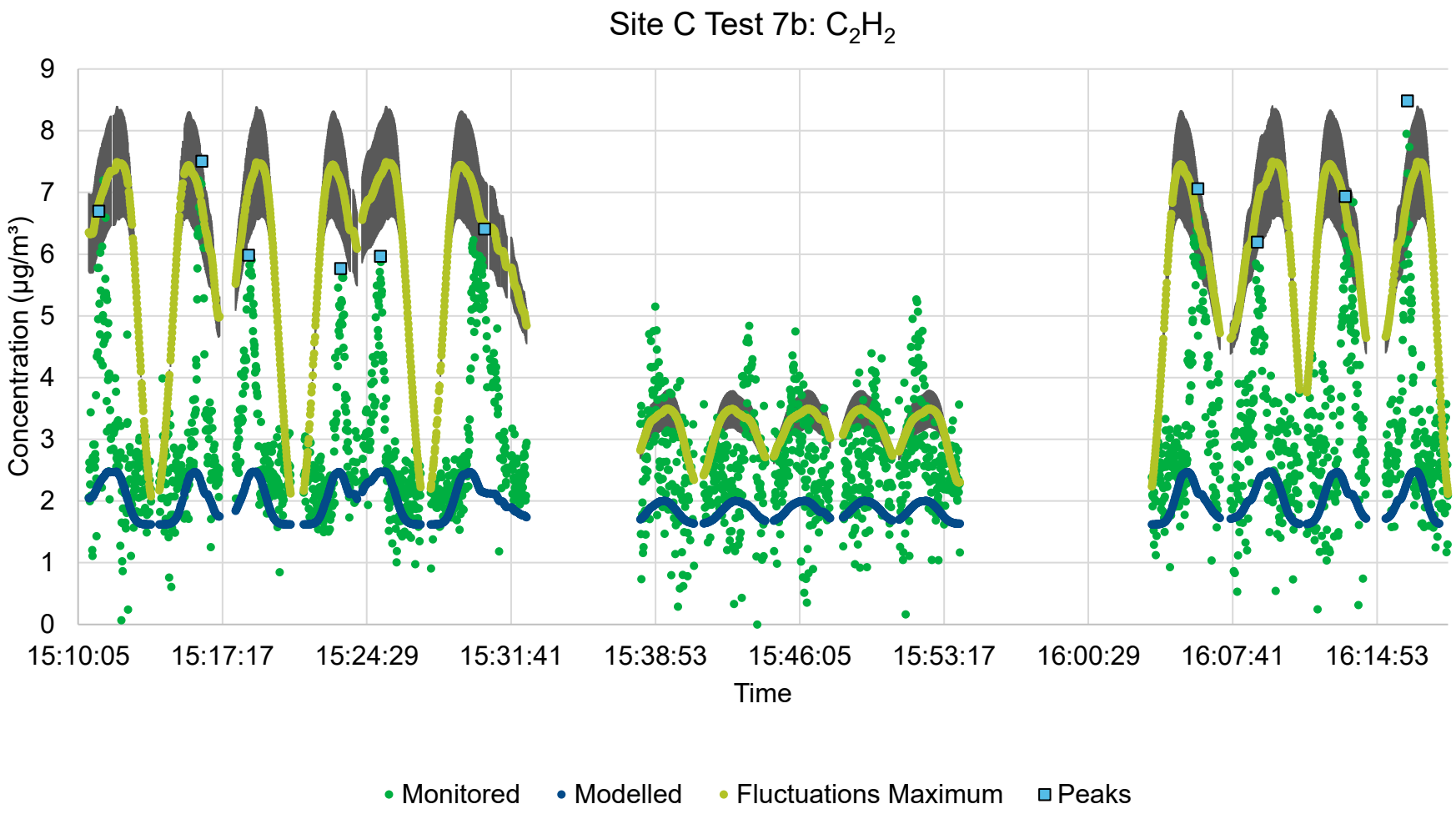

Figure 27 – Time series graph of hourly mean modelled (dark blue), modelled one-second fluctuations local maximum (lime green) and monitored (bright green) C_2H_2 concentrations for site C survey 7b. The error bars represent the one-second fluctuations standard deviation of the modelled mean concentration. The 'Peaks' (blue squares) highlight the measured one-second peak C_2H_2 concentrations in the used transects (10 out of 15). The transects measured in the middle of the survey were further away (4.1 km) from the landfill site than those at the start and end of the survey (2.1 km). This survey measured 2 sets of transects, at 1.5 km and 3.5 km away. The measured peaks show consistency with the modelled wind direction throughout.

7.2. Standard Bayesian inversion methodology

The standard CERC Bayesian inversion scheme (Carruthers and others (2019)) was applied with the same site characteristics, selected transects, meteorology and input CH_4 emissions as the modified methodology described above, with the following differences:

ADMS forward modelling:

- one second mean averaging time
- no modelling of concentration fluctuations
- default values for wind direction variability

Inverse dispersion modelling:

- all measurements for the selected transects were included in the inverse dispersion modelling

The uncertainty and covariance values that were used in the CH_4 inverse dispersion modelling with this methodology are given, with justifications, in Table 24.

Table 24 – Uncertainty and covariance values used in the standard Bayesian inversion scheme for all sites for CH_4.

Parameter	Value	Unit	Comment
Measurement uncertainty	50	μg m^{-3}	Estimate. Large enough to account for the instrument accuracy (1.3 μg m^{-3}) and model error.
Measurement uncertainty covariance	0		Set to zero to allow the error to vary between the different transect peaks.
Emissions uncertainty	0.01	g m^{-3} s^{-1}	Set to a high value to allow the initial nominal unit emission rates ($1x10^{-5}$ g m^{-3} s^{-1}) to be changed as much as necessary to obtain good model agreement.
Emissions uncertainty covariance	50%		Percentage of emissions uncertainty common to different sources. All sources represent part of the same landfill site, so have some interdependence.

7.3. 1D Gaussian profiles methodology

The CERC inversion scheme was applied to simulate a 1D Gaussian profile inverse dispersion modelling method, using the same selected transects and meteorology as the modified and standard Bayesian methodologies described above, with the following differences:

ADMS forward modelling:

- one hour mean averaging time
- landfill site represented as a single point source in the approximate centre of the landfill, with height 1 m, diameter 100 m and exit velocity 0.01 m s^{-1}
- no modelling of concentration fluctuations
- default values for wind direction variability

Inverse dispersion modelling:

- all measurements for the selected transects were included in the inverse dispersion modelling
- zero measurement uncertainty
- initial point source emission rate 1 g s^{-1}
- point source emissions uncertainty 5 g s^{-1}, a high value to allow the initial nominal unit emission rate (1 g s^{-1}) to be changed as much as necessary to obtain good model agreement

7.4. Backward Lagrangian Stochastic (WindTrax) modelling

WindTrax version 2.0.9.7 was used for the Backward Lagrangian Stochastic inverse dispersion modelling.

An overview of the WindTrax configuration for site A is shown in Figure 28. The background map was exported from ArcGIS with a visible 200 m resolution grid for matching with the WindTrax map grid. WindTrax runs in local coordinates, so the coordinate origin was set as the location of the tracer release for surveys 3 to 7.

The landfill source outline was digitised manually to match the combined ADMS source outlines, giving a total source area of 158,272 m^2. The mobile methane and tracer concentration measurements are represented by ‘truck’ measurement platforms, linked to files containing coordinates and associated concentrations. Ten virtual trucks were used, so each WindTrax calculation incorporates up to 10 measurements spread across a single transect. Measurements were assigned in blocks along the transect to each truck in turn, in order to ensure that each calculation uses measurements distributed along the transect. Figure 29 shows how measurements from survey 1, transect 11 were split between the trucks.

An anemometer and thermometer, nominally located at the northern edge of the landfill, are linked to a file of input meteorological data. The input meteorological data also includes the Monin-Obukhov length calculated by ADMS as an indication of stability, linked to the atmospheric profile. Input meteorological data values are shown in Table 25.

Background concentrations were input as an atmosphere property for each survey. The surface roughness length was set as 0.07 m to match ADMS. 1,000,000 calculation particles were used in both the backwards (landfill area source) and forwards (tracer point source) Lagrangian models for each measurement point.

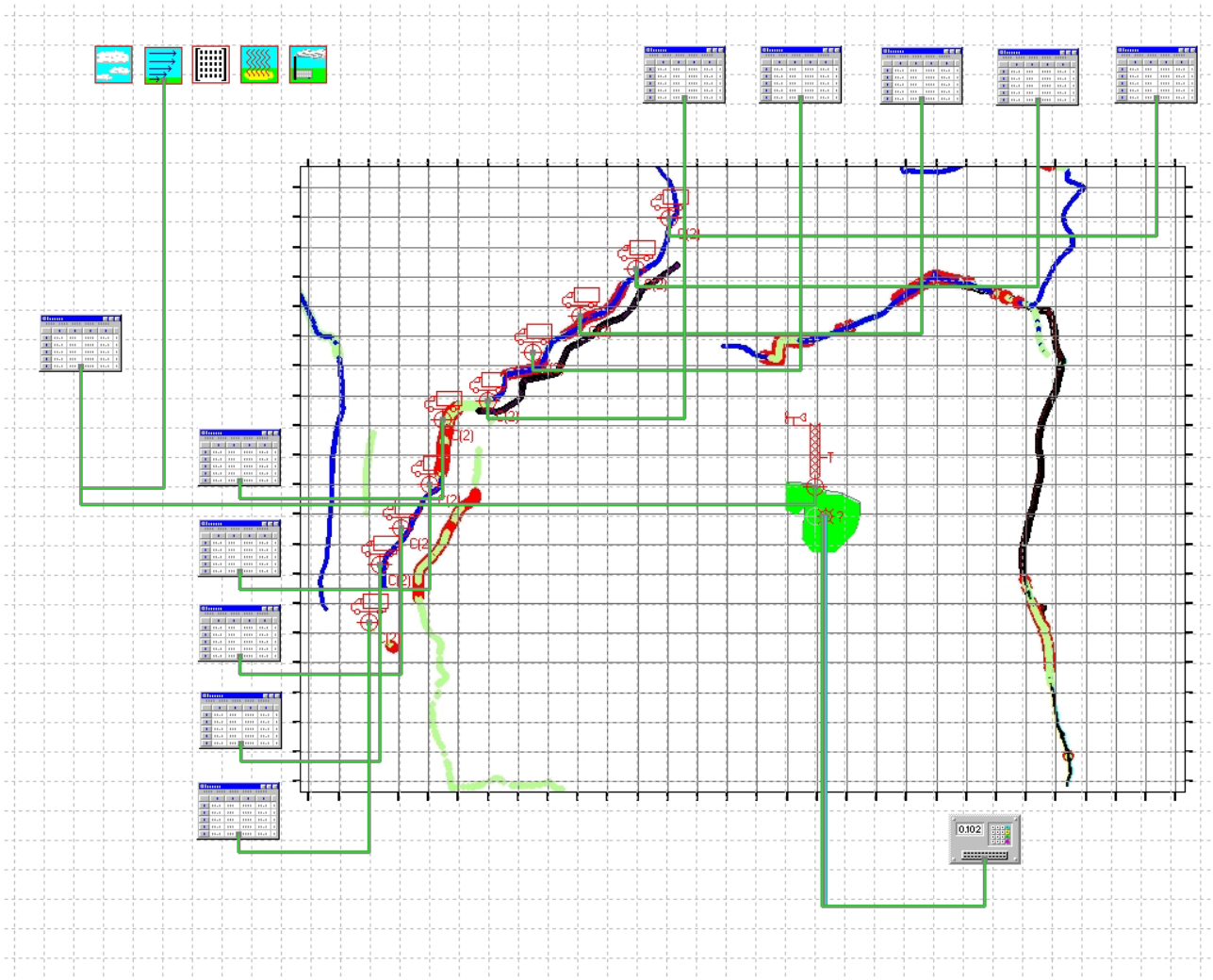

Figure 28 – Visualisation of WindTrax configuration. The bright green shape is the landfill area. Input files on the left are connected to each of 10 trucks (concentration measurements and locations), or anemometer and general atmospheric properties (meteorological data). An output file at the bottom gives the calculated emission rates. Coloured curved lines show the measurement data locations (background image). The grid lines are at 200 m resolution.

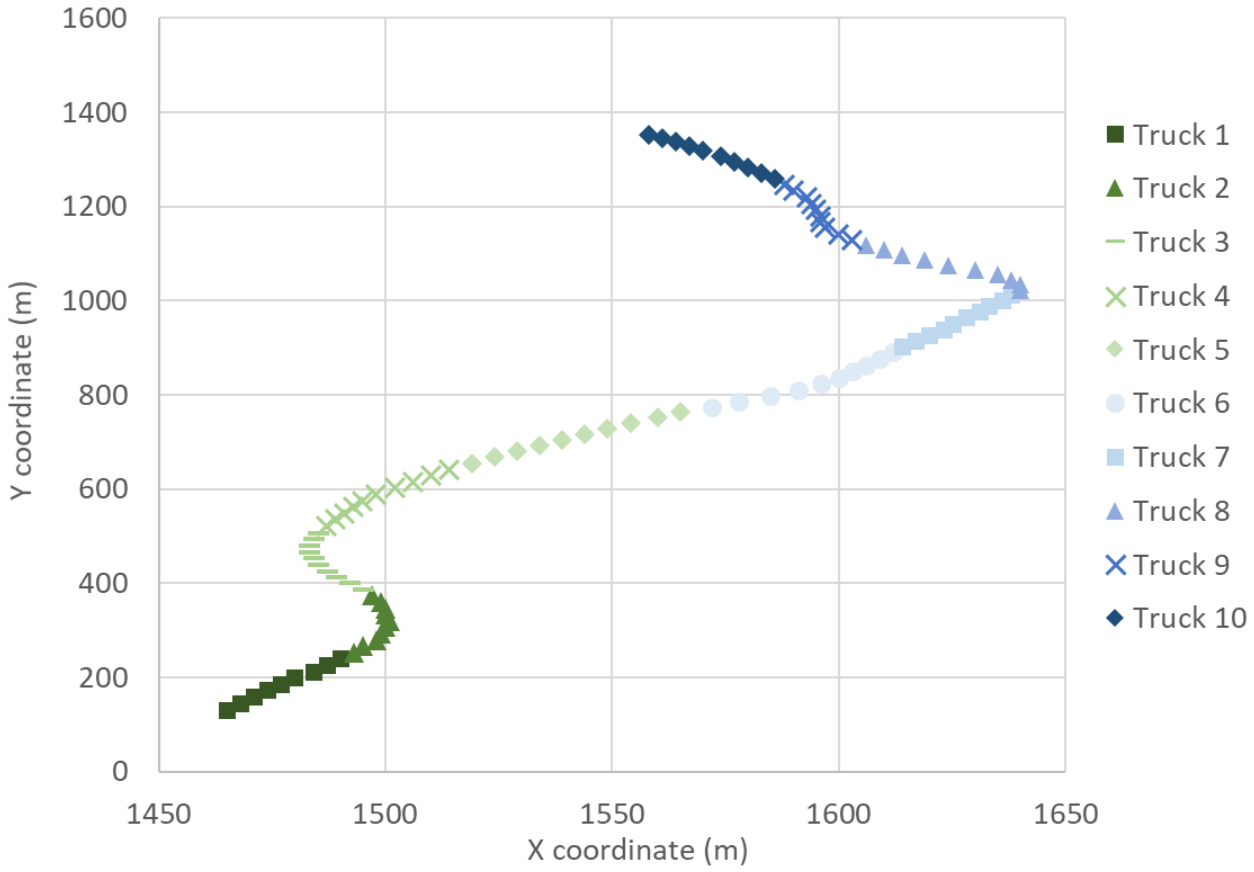

Figure 29 – An example of the distribution of transect data points split evenly between 10 trucks for survey 1, transect 11.

Table 25 – Input meteorological data used for WindTrax.

Survey	Wind speed (ms^{-1})	Wind direction (°)	Temperature (°C)	Monin-Obukhov length (m)	Background concentration CH_4 (ppm)
1	7.7	245	12.7	-2,500.0	1.92
2	3.6	85	2.8	46.9	1.99
3	2.1	290	3.8	-32.5	2.10
4	2.6	130	5.4	8.9	2.14
5	5.7	210	8.4	400.0	1.99
6	3.6	105	8.6	44.6	2.06
7	3.2	195	8.8	84.0	2.00

WindTrax is not recommended for use with source-receptor distances over 1 km. None of the TDM study measurements are within this limit and some are much further away. The measurements used for WindTrax in this study were limited to within around 3 km of the source, using only the closest transects in each survey. In addition, in initial runs a large number of points showed no influence from the source. This was reduced by removing points which lay more than ±20° away from a line along the modelled wind direction from the source centre. These distance and angle limits reduced the number of measurements available for each survey as summarised in Table 26. Figure 30 presents the WindTrax and TDM emission rates plotted against the number of measurements available for WindTrax. This graph shows a trend for the WindTrax results to be more closely matched to TDM with increasing numbers of available input measurements within the angular and distance thresholds.

Table 26 – Summary of measurement data used for input to WindTrax, with distance and angle limits applied.

Survey	Number of measurements	Transects included	Maximum distance (km)	Comment
1	528	2,5,7,9,11	2.07	No distance limit applied.
2	239	2,4,6	2.99	One distant transect excluded.
3	409	3,5,7	2.09	No distance limit applied.
4	939	3,5,7,9,16,18	2.55	One distant transect excluded, one wide angle transect excluded.
5	369	3,9	2.99	Four distant transects excluded.
6	501	3,5,7	2.68	One distant transect excluded.
7	474	1,12,14,16,18	1.86	Three transects beyond 3 km excluded.

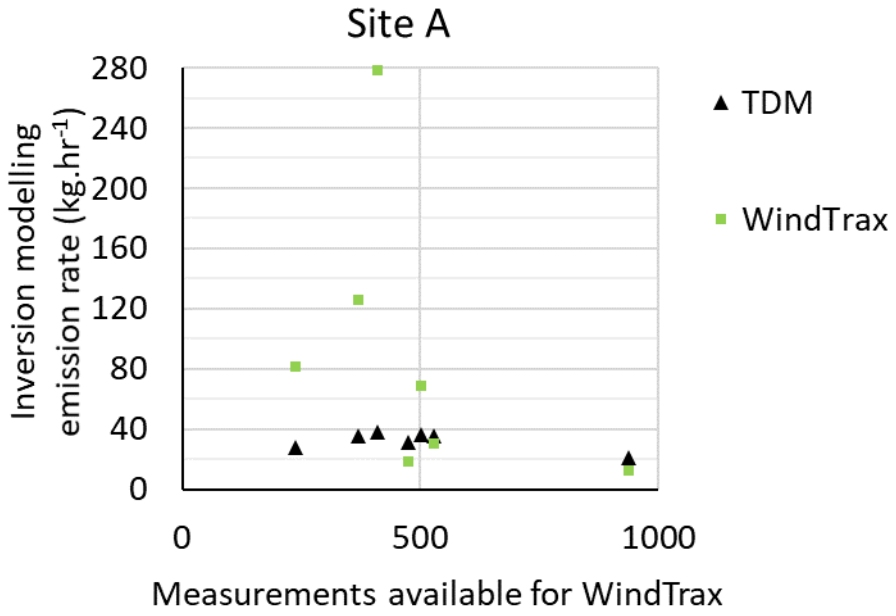

Figure 30 – Comparison of TDM and WindTrax calculated emission rates for site A, plotted against the number of measurements available for WindTrax.

The output from WindTrax included a separate emission rate estimate for each model calculation (based on up to 10 measurement points). It also provides the corresponding proportion of the landfill area which influenced the measured concentration and the ratio of the standard deviation of emissions to the mean emissions. Some of the output emission rates are negative. This may result from measured concentrations which are lower than the specified background concentration. High values of standard deviation/mean ratio indicate higher uncertainty in the emissions estimate. Post-processing was used to derive an overall emission rate estimate from the individual calculation estimates, by excluding:

- any negative emissions
- calculations with standard deviation/mean greater than 0.9
- calculations where the proportion of landfill area influencing the measured concentrations is less than 0.4

Survey 2 showed the lowest proportions of landfill area influencing the measured concentrations. This may indicate a mismatch between the modelled wind direction and transect location. An example of the emissions rates and standard deviation/mean ratio values for each model calculation within a single transect (survey 1, transect 5) is visualised in Figure 31. The number of model calculations included in the final emission rate averages is summarised in Table 27 for each survey.

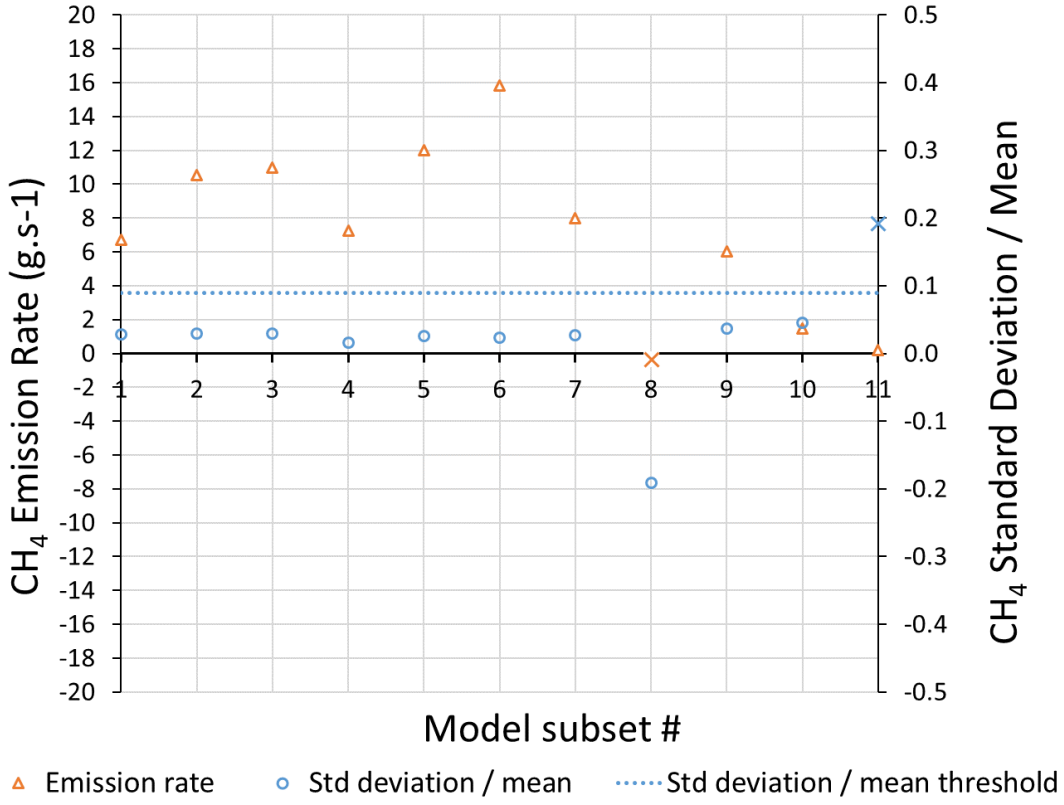

Figure 31 – WindTrax emissions and standard deviation/mean for individual model subset calculations within a single transect (transect 5) for survey 1. Excluded values are shown with a cross: one negative emission rate and one standard deviation/mean above the threshold value.

Table 27 – Summary of the number of model calculations included in average emission rate for each survey.

Survey	Number of model calculations included in average
1	42
2	10
3	43
4	95
5	37
6	51
7	48

Comparing Tables 26 and 27, it is clear that most surveys with higher numbers of available measurement points lead to high numbers of calculation subsets included in the output average. However, survey 1 has more points available for WindTrax than survey 3, but fewer valid calculation subsets. These discrepancies may indicate that some of the surveys generate a significant proportion of invalid model calculation subsets. Figure 32 compares TDM and WindTrax emission estimates, plotted against the number of model calculation subsets included in the WindTrax emission estimate. Comparing with Figure 30 shows a weak trend for WindTrax emissions to be closer to the TDM emissions when more calculations can be included in the output average.

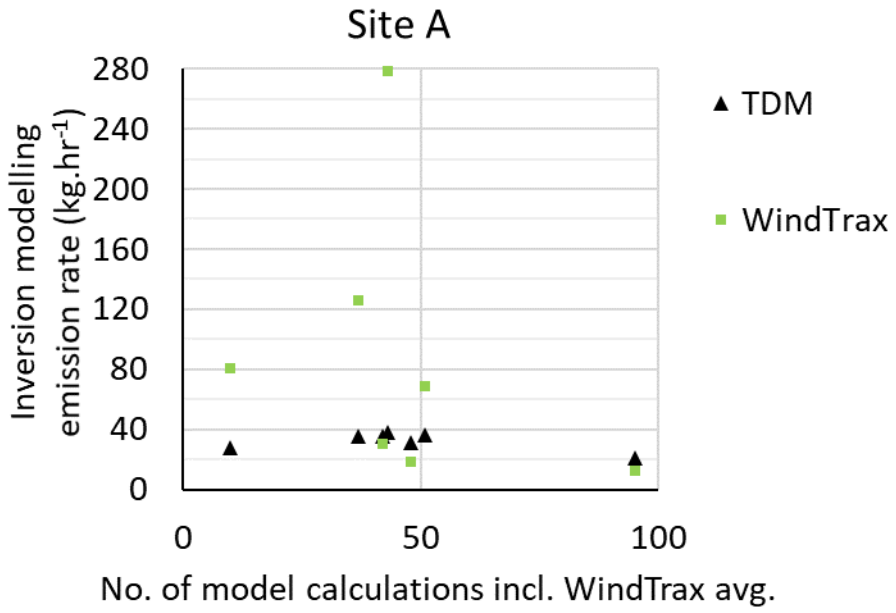

Figure 32 – Comparison of TDM and WindTrax emission rates, plotted against the number of model calculations used to derive the WindTrax average emission rate.

7.5. Inverse dispersion modelling CH_4 concentration results

The Modified Bayesian, Standard Bayesian and 1D Gaussian inverse dispersion modelling methods return the adjusted modelled concentration at the modelled receptors. The CH_4 results for these 3 methods for each site are given in Figures 33 to 35 as time series graphs for each site for each survey. The 1D Gaussian and Standard Bayesian methods return the adjusted modelled concentration at each measurement location; the Modified Bayesian method returns only the adjusted modelled concentration at the location of the peak measurement in each transect.

The results confirm that the same transects have been modelled with each method. The 1D Gaussian and Standard Bayesian methods capture some of the peaks but not others, whereas the Modified Bayesian method captures most of the peaks. In general, the differences between the 1D Gaussian and Standard Bayesian results are small. The 1D Gaussian plume is often wider and shallower than the Standard Bayesian plume because of the longer averaging time used in the forward ADMS modelling. The Modified Bayesian method gives the highest concentrations because these values represent the maximum likely concentration at the locations of the peak measurements, given the local short-term meteorological variability. The 1D Gaussian and Standard Bayesian method give the mean plume for the forward model averaging time used. The level of agreement between the adjusted modelled and measured methane concentrations gives varying levels of confidence in the inverse dispersion modelling methods' abilities to improve the modelled concentrations by adjusting the emissions. The methods' different treatments of the landfill plume result in differences between the resulting emissions (section 5.5).

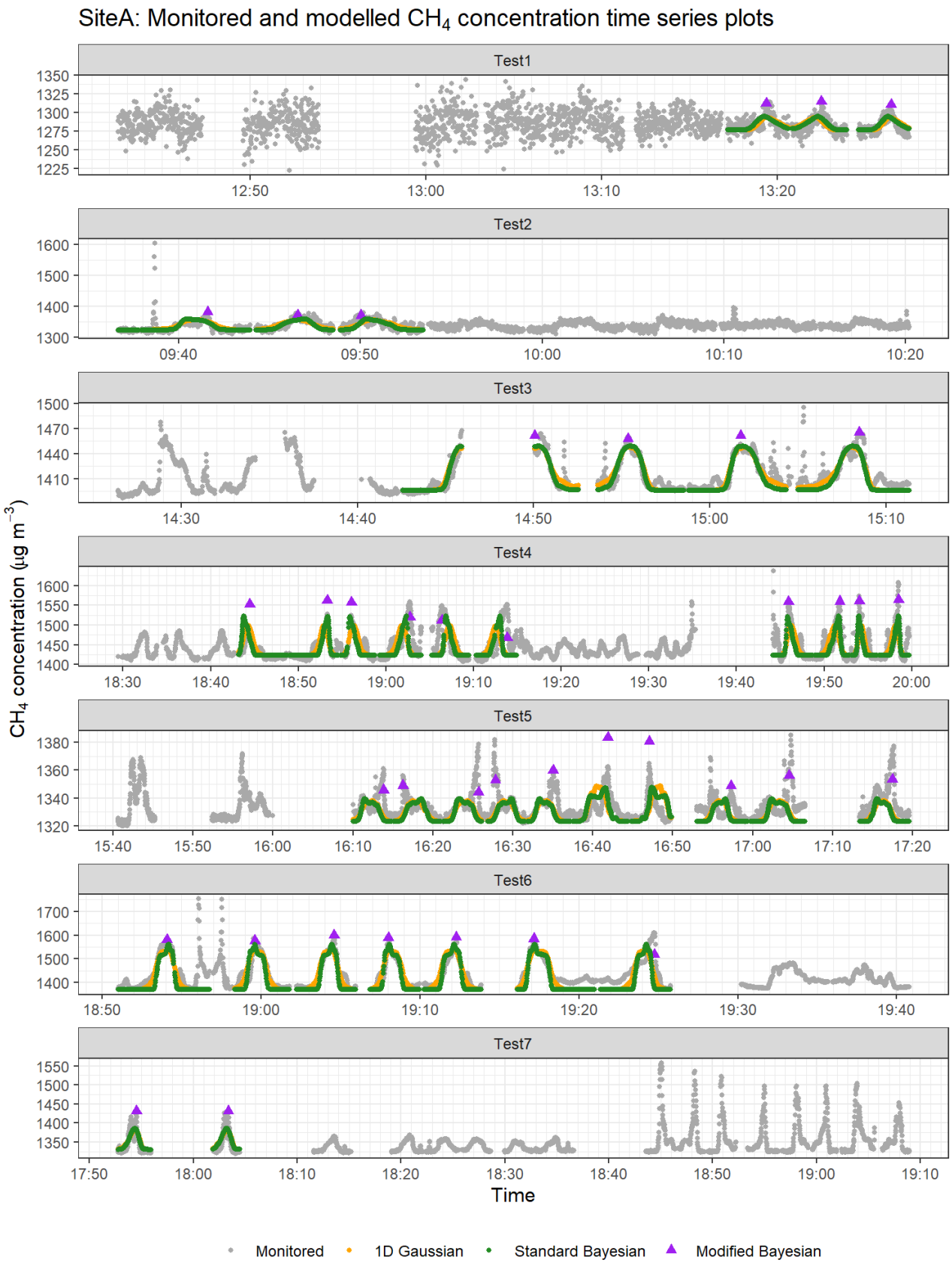

Figure 33 – Time series plots comparing site A monitored CH_4 concentrations (grey) with inverse dispersion modelling CH_4 concentration results using the 1D Gaussian (orange), Standard Bayesian (green) and Modified Bayesian (purple) methods. Surveys were carried out on different days and at different times. Inverse dispersion modelling results are shown for transects selected for inclusion.

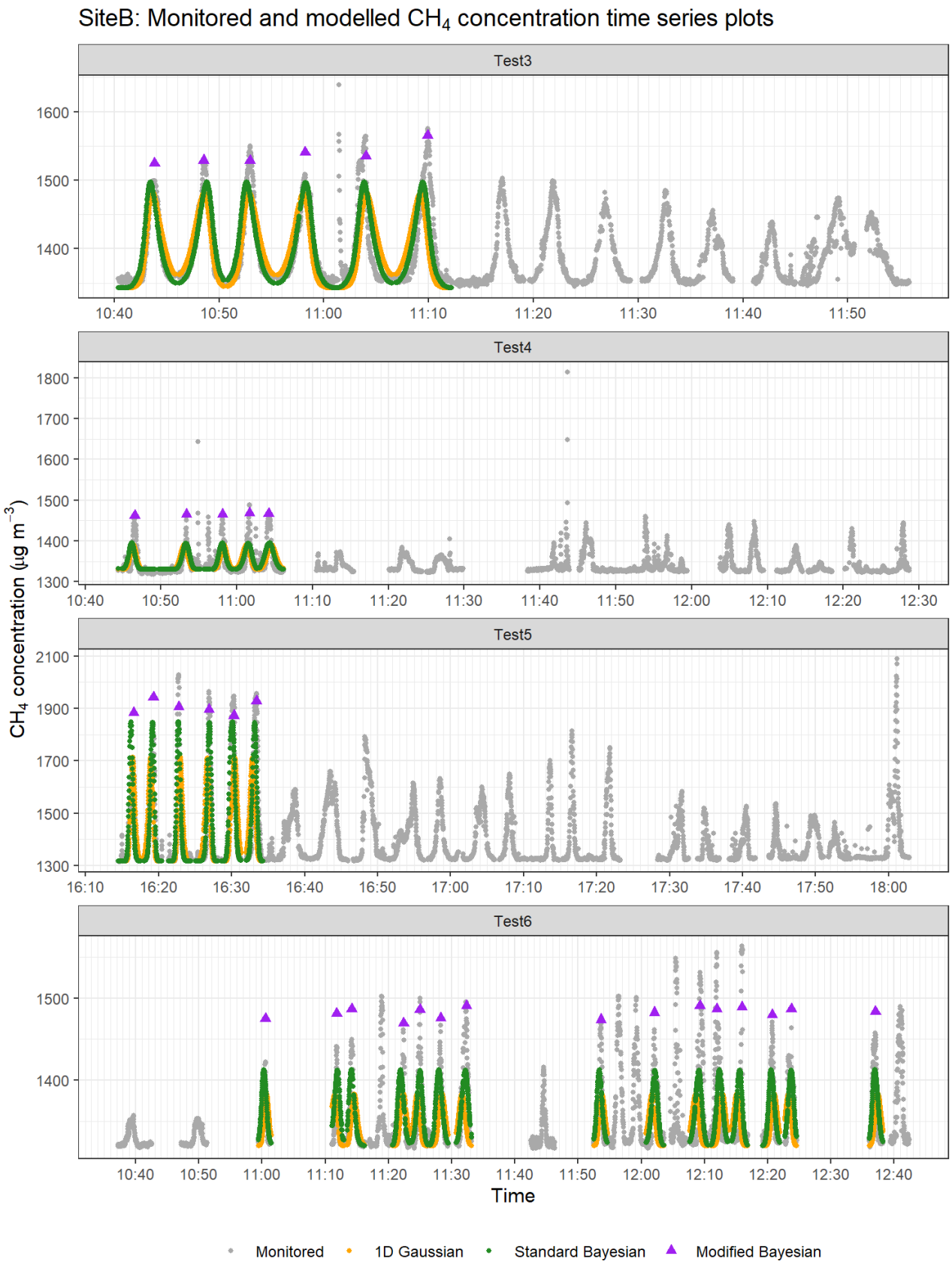

Figure 34 – Time series plots comparing site B monitored CH_4 concentrations (grey) with inverse dispersion modelling CH_4 concentration results using the 1D Gaussian (orange), Standard Bayesian (green) and Modified Bayesian (purple) methods. Surveys were carried out on different days and at different times. Inverse dispersion modelling results are shown for transects selected for inclusion.

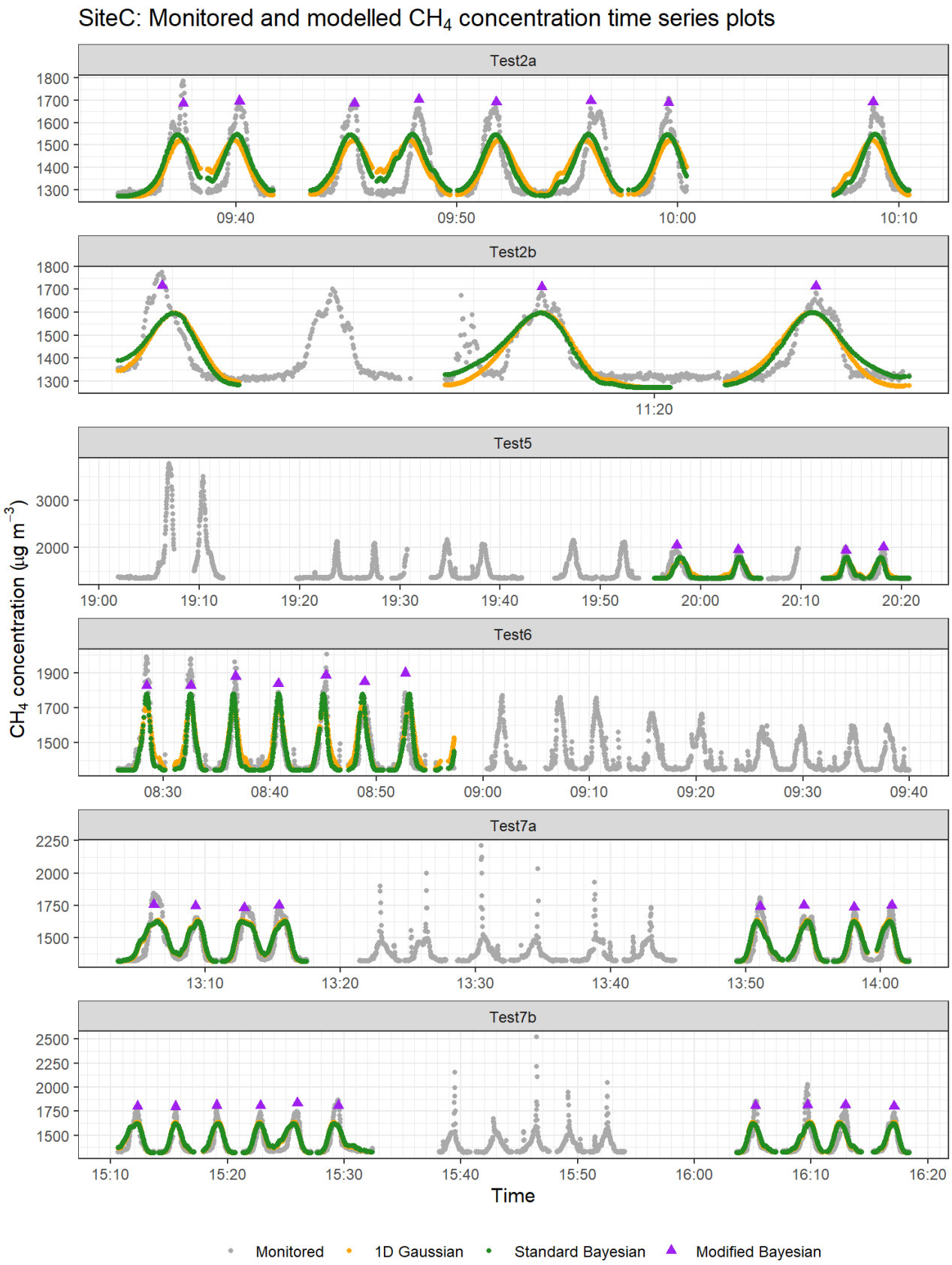

Figure 35 – Time series plots comparing site C monitored CH_4 concentrations (grey) with inverse dispersion modelling CH_4 concentration results using the 1D Gaussian (orange), Standard Bayesian (green) and Modified Bayesian (purple) methods. Surveys were carried out on different days and at different times. Inverse dispersion modelling results are shown for transects selected for inclusion.

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Glossary

Adjoint modelling - Running a model with the time direction reversed, for example, to follow advection/dispersion backwards from receptor locations towards source areas from which concentrations could have originated.

Anaerobic digestion - A process for the controlled decomposition of biodegradable materials, which captures the methane and other gases produced. Feedstock materials include food waste, agricultural waste and/or sewage sludge.

Bayesian - Statistical frameworks and methods which use Bayes' theorem; Bayes' theorem describes the conditional probability of an event given prior knowledge and observed data, this probability is updated in light of new data.

Biogas - Fuel gas produced through anaerobic digestion.

Cost function - A measure of model performance which quantifies differences between predicted and actual outputs, the aim of optimisation processes is to minimise this cost function to find the best solution.

Fluctuations local maximum concentration - Maximum likely ADMS modelled concentration at a given location, given the plume meandering caused by wind and turbulence variations that occur on sub-hourly timescales, when using the ADMS fluctuations module.

Fugitive emissions - Emissions from poorly-controlled sources, such as leaks from pipework or landfill coverings.

Gaussian - A probability distribution that is symmetric and bell-shaped. Also known as a normal distribution. Gaussian dispersion models use Gaussian-shaped plume concentration profiles in the vertical and crosswind directions.

Inverse dispersion modelling - Modelling techniques which estimate the location and/or emission rate of pollutant sources based on measured pollutant concentrations at known locations under known meteorological conditions.

Lagrangian - A function which combines the kinetic and potential energy of the system. The Lagrangian at each point along a path over time gives the 'action'; the action between 2 points will be minimised and so the path taken may be determined. Lagrangian dispersion models follow a large number of individual simulation particles through a flow field, with random perturbations representing smaller-scale turbulent motions.

Mass balance - Based on the Law of Conservation of Mass; if the mass of a specific substance entering a defined spatial volume (for example, airborne measured upwind background and source emissions) and the mass exiting the volume (for example, airborne measured downwind plume) are known, then the amount of mass emitted from the source can be calculated as the difference (balance) of the 2 measured masses.

Measurement plane - A 2D vertical surface where concentrations are measured downwind from the source. This surface aims to cover the crosswind and vertical extent of the target plume. Either optical or airborne methods can be used to measure concentrations across a vertical plane.

Monin-Obukhov length (LMO) - A measure of the scale of atmospheric mixing, influenced by the balance between thermal and mechanical parameters.

Simulated annealing - An optimisation algorithm which works in analogy to the metallurgy technique of annealing, where metals are heated to above their recrystallisation temperature before cooling to optimise the structure and physical properties of the final material.

Stochastic - A random process for which the specific outcome cannot be precisely determined, only described statistically.

UAV - Unmanned aerial vehicle, for example, quadcopter drones, model aircraft.

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