Ministry for Primary Industries
Manatū Ahu Matua

Atmospheric Methane Modelling

Evaluating Regional Methane Emission Using Inverse Modelling

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1 Executive Summary

New Zealand's agricultural sector was responsible for nearly half of our greenhouse gas emissions inventory in 2016, and methane emissions from livestock make up the majority of these agricultural emissions. Due to the key role of agriculture in both our economy and our emissions profile, New Zealand has made a significant investment in developing technologies to mitigate methane emission from ruminant animals. Present methane emissions are thought to be relatively well known from estimates of animal dry matter intake and emission factors, but large-scale verification of the efficacy of mitigation technologies in the field will present a challenge. A possible solution is inverse modelling of emissions, based on atmospheric greenhouse gas observations from a network of observing stations, combined with models that describe the pathway the air took before arriving at the station to infer regional to national greenhouse gas emissions or uptake. The approach allows for improved estimates over the *a priori* (first guess) model input of emission by optimising the fluxes to observed atmospheric methane levels. Here, we present New Zealand's first national-scale methane inverse modelling study. We estimate regional to national emissions for the period 2011-2013, test the inverse methodology, and assess the value that might be added by additional measurement sites. Finally, we implement our findings in a study for 2018 and show that with improved modelling, measurements and infrastructure, we can significantly enhance the understanding of monthly, regional methane emissions in New Zealand.

The 2011-2013 case study using data from NIWA's observing stations at Lauder and Baring Head (used for a clean air background) identifies several prerequisites for consistent, realistic estimations of methane emissions from inverse modelling. For the principal methane emitting regions of the South Island (Canterbury, Otago and Southland), at best we can determine methane emissions a third of the time, predominantly during summer. Times of unsuccessful inversions are driven primarily by gaps in the Lauder time series, highlighting the need for further investment to ensure the quality and continuity of the data. The resulting emission estimates are also not ideal. Seasonal cycles are not well replicated and there is large variation from month to month. This is partly due to strong correlations between regions, suggesting that larger regions should be used. It was also due in part to incorrect meteorological fields (wind speeds and directions). The meteorological fields used in this case study only operate at a resolution of 12km and so were unable to replicate locally observed winds.

To investigate the meteorological limitations further, we then study 2018 using newer wind fields at 1.5km resolution. The new wind data was shown to be far more representative of the truth and gave greater confidence to our estimates of methane emissions. While there were still several months missing due to data gaps, and for a few months, particularly during the winter, emissions trends seemed unrealistic, the inversion has improved, with less uncertain and more realistic results. The main problems remain correlations between regions and gaps in data.

All of the understanding gained was combined in an inversion of 2018 using the latest model and additional, continuous data,from Baring Head. This additional data allowed us to fill in the gaps in our time series and to better resolve emissions from different regions. As a result the seasonal cycles across Otago, Canterbury and Southland were broadly reproduced and uncertainties greatly reduced. We were also no longer restricted to mostly summer months as in the 2011-2013 study because of the additional measurements at Baring Head and the improved modelling. The results for the South Island as a whole mirrored the emissions as estimated by MfE, even when the *a priori* estimates were inflated to 50% higher than the MfE values,and with a reduced uncertainty. This suggests that not only can we reproduce national emission inventories, but we can significantly reduce uncertainty in emission estimates (potentially to less than 0.05 Mt per year) throughout most of the year. With the imminent addition of further observing sites to the observing network and potentially the use of satellites, we will be able to further improve the results and to extend this to the rest of New Zealand and further afield.

2 Introduction

New Zealand's agricultural sector contributed 49% to our national gross greenhouse gas emissions in 2016 (MfE, 2018). Enteric methane emission from ruminant animals makes up 71% of these agricultural emissions, with agricultural manure management contributing an additional 3%. These methane emissions are currently estimated using an inventory method that has been specifically developed to suit New Zealand's pastoral agriculture and is driven by an estimate of animal dry matter intake. An uncertainty level of 16% in the enteric emission estimate of the national inventory has been determined through Monte Carlo analysis (Kelliher et al., 2009).

Independent verification of inventory estimates for New Zealand presents a challenge due to the wide spatial distribution of grazing and range of environmental factors (soil moisture, temperature, rain, irrigation, etc.) that affect pasture fodder. To date, verification has primarily centred around the sulfur hexafluoride tracer technique for individual freely-grazing animals (Lassey et al., 2001; Lassey et al., 2007) or micrometeorological techniques at paddock scale (Laubach and Kelliher, 2004). These techniques can only be applied at small scale, up to a few meters, and micrometeorological techniques are difficult to apply to constantly moving point sources like a grazing herd. Aircraft based measurements have shown the promise of using observations of methane in well mixed air to determine larger scale methane emissions over the Manawatu (Wratt et al., 2001.) However, this approach is limited by the fact that aircraft campaigns are only able to characterise emissions for snapshots in time and the technique requires consistent wind-flow conditions.

Given the dominance of enteric emissions in the national inventory and New Zealand's investment in mitigation technologies, there is significant value in developing verification techniques that can be applied at a regional or national scale. While methane emissions are reasonably well known at present, the efficacy of mitigation techniques will be difficult to verify at large scale. Atmospheric inverse modelling quantifies uptake or emissions of trace gasses at regional scales by using atmospheric trace gas data from a network of observing sites along with an atmospheric transport model that describes the pathway the air took before arriving at the station. Elevation (or suppression) of methane levels relative to an independently known background value can thus be translated into methane emissions or sink. This top-down form of verification is a recommended method in the International Panel on Climate Change good practice guidance for verification of national inventory reporting (Oliver et al., 2001; Winiwarter, 2004; IPCC, 2006). The inverse modelling approach has been used successfully to estimate methane emissions on global, continental, and national scales (e.g. Mikaloff-Fletcher et al., 2004, Bergamaschi et al., 2010, Manning et al., 2011). A model set-up that is specific to New Zealand has been piloted to estimate carbon dioxide exchange with the atmosphere (Steinkamp et al., 2017). Yet, this approach has never been applied to methane emissions in New Zealand.

In a previous study, we investigated the potential use for atmospheric measurements to detect agricultural methane emission reductions that would result from national mitigation strategies (Geddes et al., 2018). The study showed that it should be possible to detect reductions of 10-20% and perhaps as low as 5% with an intensive measurement campaign. To build on these findings we now shift our focus to attempting to quantify regional methane emissions using the inverse modelling methods described above. The study consists of four stages:

- Producing monthly varying methane emission maps for enteric fermentation, underpinned by national data inventories
- Perform initial inversions and model simulations using Lauder and Baring Head data for 2011-2013
- An investigation into the uncertainties and limitations of these inversions
- Assess infrastructure and scientific needs based on the findings of this study

There was an additional goal of using the inversions to compute emission maps for all of New Zealand. At this stage, without further development and measurement sites, this is unrealistic and would have only minor relevance as it would be unreliable outside of Otago and Canterbury. Instead we have made significant progress in improving the present state of the inversion with the results shown for 2018.

3 Methods

We have performed inversions for observations from 2011 to 2013 at Lauder, Central Otago, using supplementary information from another NIWA site; Baring Head near Wellington, where sampled air has travelled over the ocean and has not been in contact with terrestrial methane emissions or uptake. Lauder is NIWA's premier terrestrial measurement site and has been making observations of methane for over a decade. 2011 to 2013 was chosen as it coincided with the study period of Steinkamp et al., 2017 and so model data was readily available. We also compared two numerical weather models (NZLAM, and the newer NZCSM, described in 3.3) for the year 2018 in order to better understand the limitations of our initial inversions.

The inversions are underpinned by several key resources: (i) an initial estimate of monthly methane emissions and distributions, (ii) atmospheric methane measurements at an inland and a background (baseline methane levels) site, (iii) an atmospheric methane model, which itself relies on a numerical weather model, and (iv) an inversion method. These are described in the following sections.

3.1 MONTHLY EMISSION MAPS

Monthly agricultural methane emission maps were created by combining several sources of data. Firstly, annual regional production statistics are obtained and interpolated to cover the 2011-2016 time period. We also obtain the spatial map of carrying capacity of land for the "average farmer" (CCAV) from the Landcare land-use capability (LUC) dataset (Landcare, 2010a, Landcare, 2010b). The livestock production is then distributed across each region using only the land designated as agricultural (via the LUCAS New Zealand Land-use Map (LUM, Landcare, 2019)). The LUM also allows us to separate dairy from non-dairy land uses, but no further, therefore sheep, beef and deer all have the same spatial distribution. This results in the annual stocking rate for each class in each grid cell. From an unpublished data set of monthly emission totals for each category of livestock (MPI) and the annual production statistics, we are then able to estimate emissions per head, per month, for each grid cell. By combining this with the stocking rate, we obtain the monthly methane emissions per grid cell (1 ha). For the inversion this is then scaled down to a 0.1 x 0.1 degree (10km) grid in order for it to be compatible with the dispersion model.

The spatial distribution is of vital importance for the inversion model to calculate the effect of the sources of methane in a particular region on the observations. We also use the regional totals for each month as our first guess (prior or *a priori*) in the inversion model. This ensures we are starting reasonably close to the truth. The inversion will then optimise the overall emissions for each region for each month while maintaining the spatial distribution within each different region by matching computed to observed metane levels. We have assumed a conservative monthly uncertainty of 50%, which allows us to account for other non-agricultural sources of methane, mapping errors, and the additional uncertainty of using monthly, rather than yearly, emissions. When combined, the annual uncertainty would be approximately 15%, which is a reasonable estimate.

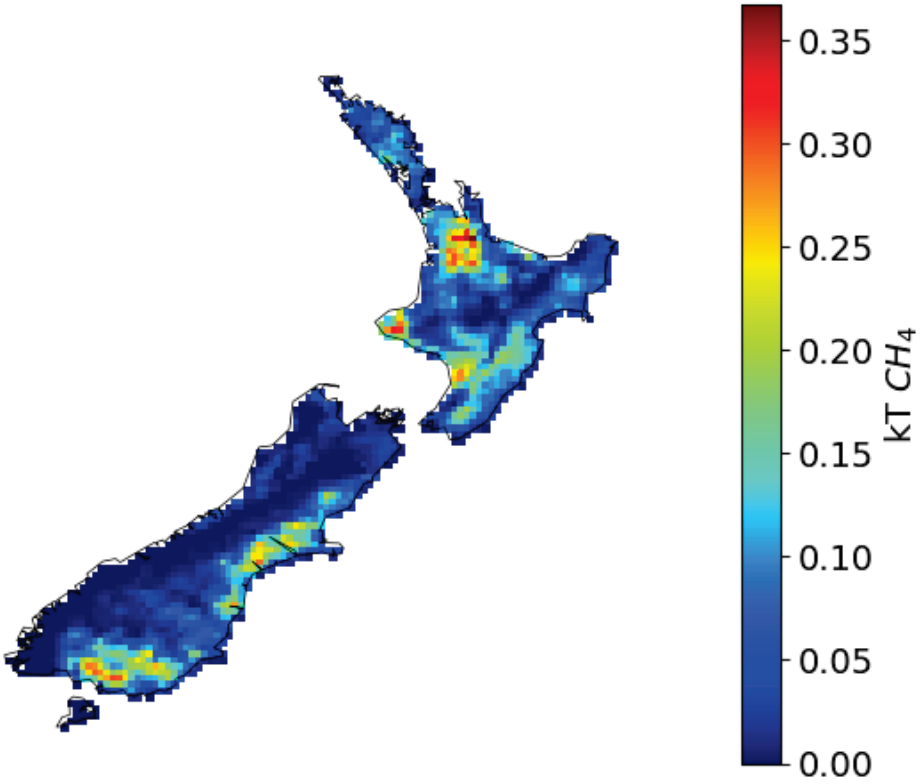

Figure 1: Prior methane emissions per grid cell (0.1° x 0.1°, ~10km x 10km) estimates for January 2011

3.2 OBSERVATIONS

NIWA's observation network includes 3 sites, Lauder, Baring Head and Maunga Kakaramea (central North Island). The latter is not used in this study as it has not yet been instrumented for methane (CH_4).

Continuous ground level in situ methane concentration measurements have been made at Lauder since 2007 (Smale et al., 2018). Measurements are calibrated to the WMO (World Meteorological Organization) reference scale via routine measurements of calibrated cylinder air prepared at the NIWA GASLAB facility at Greta Point, Wellington. The Lauder gas analyser (a Fourier transform spectrometer) has a precision of ~0.4 ppb and a reproducibility of ~1.2 ppb, which are within the Global Atmospheric Watch (GAW) recommended compatibility goals of 2 ppb (GAW, 2016).

In addition to the continuous measurements, regular (~weekly) flask samples are taken at Lauder and analysed at the NIWA GASLAB facility. This provides an additional data stream and an inexpensive method to check/validate the continuous measurements. Overall, the Lauder gas analyser and flask measurements agree to within ~1ppb.

The flask sample analyses made at Baring Head go back to 1989. When the air is coming from the south west or south east to Baring Head, it is very clean and contains no methane from local sources. Thus, such measurements make up our clean air baseline. Deviations at Lauder from this baseline, are caused by emissions within New Zealand.

In addition, a Piccaro (Tan et al., 2006) spectrometer was installed at Baring Head in 2011 that makes continuous measurements of atmospheric composition at surface level. From 2016 onwards, observations of CH_4 from this system have been possible, allowing Baring Head to be used in conjunction with Lauder, not only as a baseline but as a full measurement site.

3.3 ATMOSPHERIC METHANE MODELLING

The Numerical Atmospheric dispersion Modelling Environment (NAME) is an atmospheric dispersion model for short-range to global scales (Jones et al., 2007). Molecules or particles of a gas are released from a point source or area. Then the model can be run forward in time to model the dispersion of a pollutant plume or, as in this study, backward in time to determine the pathway a parcel of air took to an observing station.

NAME is driven by three-dimensional meteorological fields pre-computed by a numerical weather prediction model. This study employs meteorological fields from NZLAM-12, which has a 12 km spatial resolution and 70 vertical levels. NZLAM-12 is the New Zealand configuration of the UK Met Office Unified Model numerical weather model (Davies et al., 2005), which assimilates available weather data. These simulations cover a limited area domain around New Zealand of 146.8 to 185.8°E longitude, 53.4 to 26.0°S latitude.

NAME can also be driven by meteorological fields from NZCSM with 1.5km resolution, covering a smaller geographic area. This finer resolution improves the model's ability to understand and take into account complex topographic features, like the Southern Alps. This is crucial in accurately determining trajectories. NZCSM is however, only available for recent years (2017 onwards).

We selected 2011-2013 as our trial period as it was consistent with our previous study (Geddes et al. 2018) and also with the carbon dioxide study by Steinkamp et al., 2017. For each day, 10,000 tracer particles/molecules were released at each station between 15:00 and 16:00, and NAME was run backward in time for four days to determine the back-trajectories of modelled air parcels. The 15:00 to 16:00 time window was chosen because analysis of diurnal variability at our existing observing sites shows that mid-afternoon data are the most representative over larger spatial scales. The four-day model simulation time was chosen because it is sufficiently long to transport most of the released tracer particles/molecules outside the NZLAM domain (Steinkamp et al., 2017). Methane was treated as a chemically inert gas in this study (i.e., no loss processes were considered), because its lifetime (~9 years, Prather et al., 2012) far exceeds the four-day time scale of the model simulations. The modelling allows us to link each observation of methane to upwind emission sources across the country, informing us on where the methane enhancement has come from. The model does not return estimates for regions that are downwind of the observing site over the four-day simulation.

3.4 INVERSION

The inversion is where we take all our existing data; the initial estimates of regional methane (*a priori*), observations and back trajectory modelling, and infer what the regional emissions of methane were. This is the core of this study and so requires a more detailed explanation. For a comprehensive description, refer to Rogers, 2000. Methane is emitted from different regions and arrives via atmospheric transport at the measurement site where it yields an observation. The amount of observed methane, y, depends then on the regional emissions of methane x and the modelled transport *f*. This can be written as;

$$y = f(x) + e$$

Where e is the uncertainty in the observation. The goal of the inversion is then to reverse this calculation: computing *x* given *y*. We begin with our initial guess at the regional methane emissions, known as the *a priori*, x_a, and then compute *y*, the modelled methane. We compare this to our observed methane y_0 and then repeat the process with different values of *x*, so that the difference between *y* and y_0 and between *x* and x_a is minimised. The resulting value of *x* is known as the *a posteriori* estimate - or retrieved statevector - and comes with an accompanying retrieved uncertainty. The latter is equally important as the *a posteriori* estimate. The inversion also takes into account the uncertainty in the observations and in the *a priori* and as such attempts to reduce the retrieved uncertainty compared to our initial uncertainty. We now describe several tools and metrics we use to interpret the results from an inversion.

3.4.1 Error Reduction

The percentage reduction in uncertainty from the *a priori* to the retrieved (*a posteriori)* is known as the error reduction and is a metric to assess the impact of the inversion. If the inversion cannot improve the uncertainty, it will return the initial value with its initial uncertainty, giving an error reduction of zero percent. This means the model and inversion scheme, together, are entirely dependent on the input emission maps, rather than the measurements. We gain no new knowledge.

3.4.2 Correlation

The nature of the atmospheric transport and the inverse method means that is impossible to perfectly isolate regions from one another, this means that there will always be correlations between different regions. This information is provided in the correlation matrix and is another tool to assess the inversion performance. A correlation of 1 between two regions for a particular month means that they are effectively indistinguishable from another; any change in one region is replicated in the other. Conversely a correlation of 0 means they act completely independently of one another. The correlation can be either positive or negative, if positive, when one region increases the other increases. When negative, if one region increases the other decreases and vice versa.

3.4.3 Averaging Kernel Matrix and Degrees of Freedom

The averaging kernel matrix contains information about the error reduction and inversion. It describes the sensitivity of the retrieved statevector to the true state, assuming perfect modelling. In our case, it is the sensitivity of each monthly regional emission estimate to the true value of every monthly regional emission. The diagonal of this matrix gives us the sensitivity of the retrieved value to its own true value. This is known as the degree of freedom, with the ideal value being 1 for each region per month. The elements of the matrix that aren't on the diagonal show the sensitivity of the retrieved value to the true value of another region or month (i.e. covariance), and so contain information similar to the correlation matrix.

The total degrees of freedom obtained is an excellent means of quantifying the usefulness of the inversion, it describes the total number of independent pieces of information. For instance, considering a single region, and our 3-year time period, the maximum degrees of freedom would be 36; one for each month. If in the inversion we obtained only 3 degrees of freedom, that might mean we have successfully obtained 3 individual months perfectly, or it could mean that we can combine different months to produce 3 averaged values, such as an annual mean for each year. By looking at where the degrees of freedom have come from, we can decide how to interpret them. The total degrees of freedom tell us how much information we have added by performing the inversion.

3.4.4 Regions

New Zealand and the surrounding area has been divided into a total of 25 regions, with 15 covering the land mass of New Zealand. The regions do not follow administrative regional boundaries, chosen for approximately equal sizes, the names assigned to each of our regions are for context only (Figure 2).

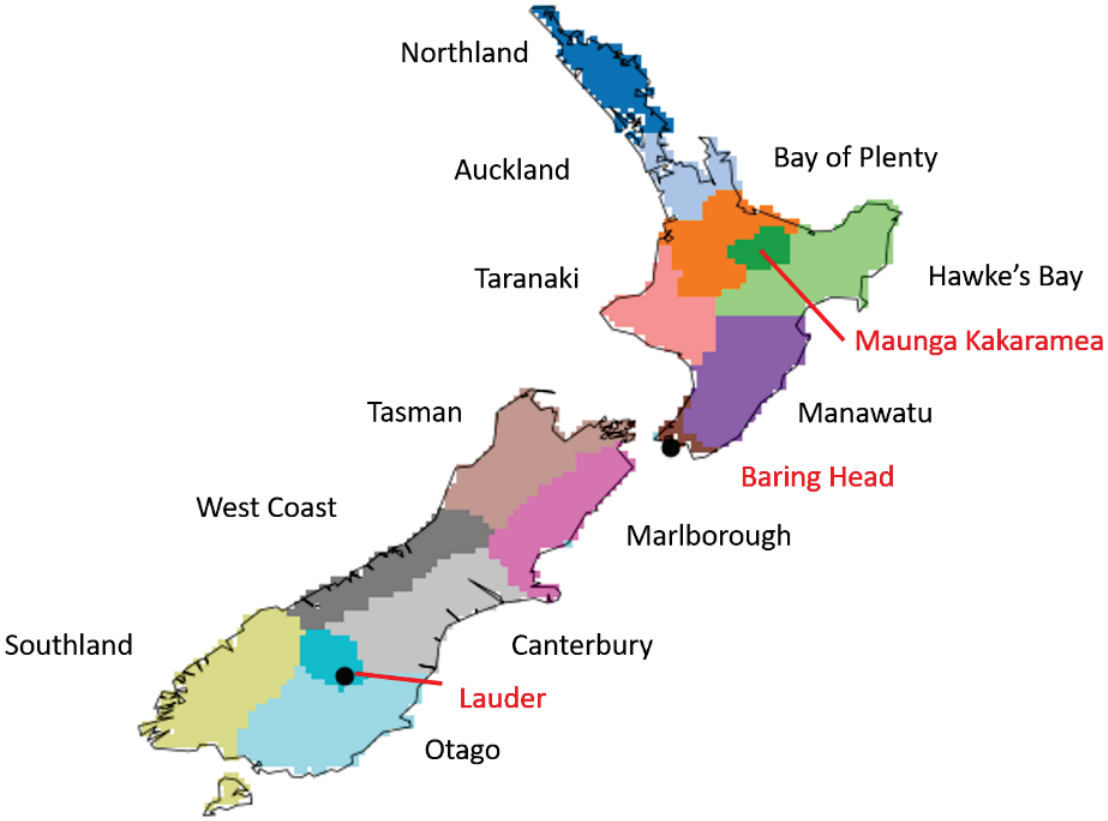

Figure 2: Inversions regions and measurements sites (red)

The small Lauder, Baring Head and Maunga Kakaramea regions are used to mitigate local variations so that false signals aren't attributed to other regions. For example, if there is a spike in the observed methane due to a source near the observation site, this will be accounted for in the retrieved value of the Lauder region, rather than being assigned to other regions such as Otago or Canterbury. Methane is measured at both Lauder and Baring Head.

4 Results

4.1 2011-2013 INVERSIONS FROM LAUDER

One of NIWA's two long-running in situ methane observing sites is at Lauder in Central Otago. NAME simulations show that Lauder observes a broad cross section of the southern half of the South Island. This region is characterised by substantial agricultural methane emissions, although these emissions are much more diffuse than emissions from the most intensive dairying regions such as the Waikato and Taranaki (Figure 1). Thus, emissions from the vicinity of Lauder may be more difficult to detect than from more intensively farmed regions. We will primarily focus on three regions: Otago, Canterbury and Southland. The other regions are either not adequately sampled at Lauder (i.e. The North Island) or do not have high enough emissions to be detectable (i.e. West Coast).

The inversion has been performed for 2011-2013 using the emissions maps shown in section 3.1 (Fig. 2) and observations described in section 3.2. The retrieved monthly regional emissions for Otago along with the uncertainty are shown below in Figure 3.

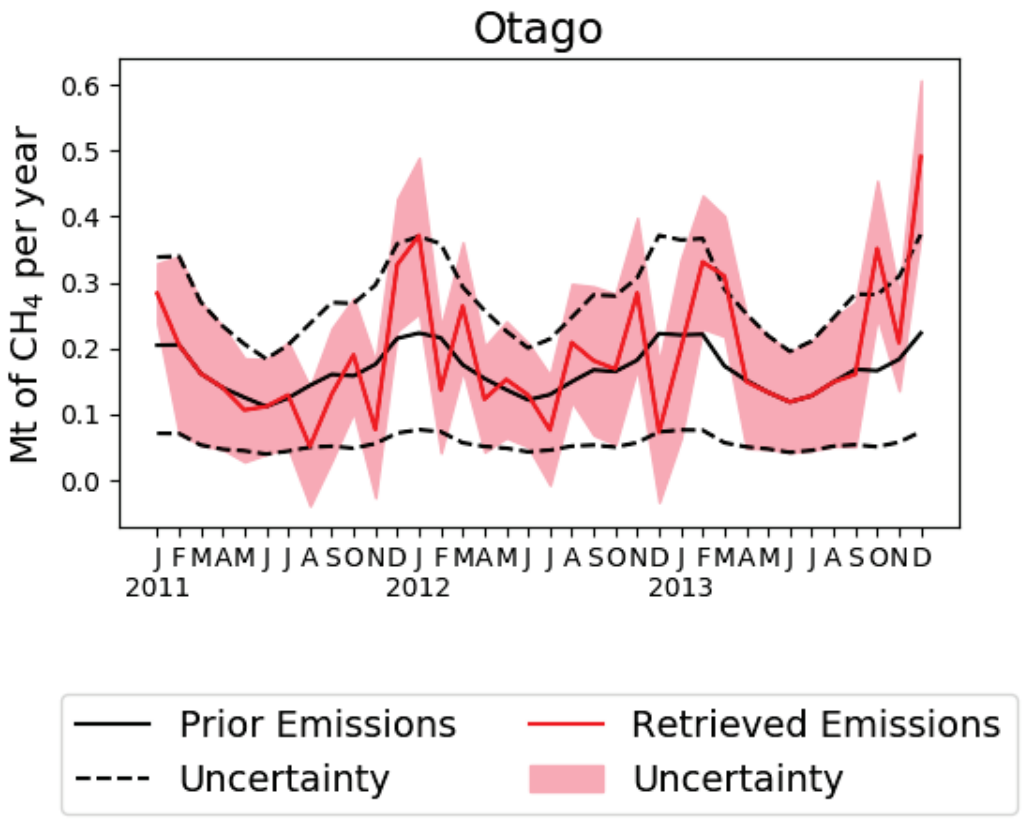

Figure 3: Retrieved and Prior Emissions for the Otago region, 2011-2013 with associated uncertainty

While it is tempting to draw conclusions about the seasonal cycle of methane emissions from these figures alone, it is important to understand the robustness of the results. For instance, in Figure 4 we display the error reduction for the Otago region and can see that while there are significantly high error reductions at certain times, approaching 70%, during the winter months there are periods with little or no error reduction, largely due to missing data (due to a combination of regular calibrations, updates and repairs) and low winds. The inversion is then adding no information in this time period, the retrieved estimates are equal to the *a priori* values. This must be taken into account when assessing differences between the *a priori* and the retrieved emissions so as not to draw false conclusions.

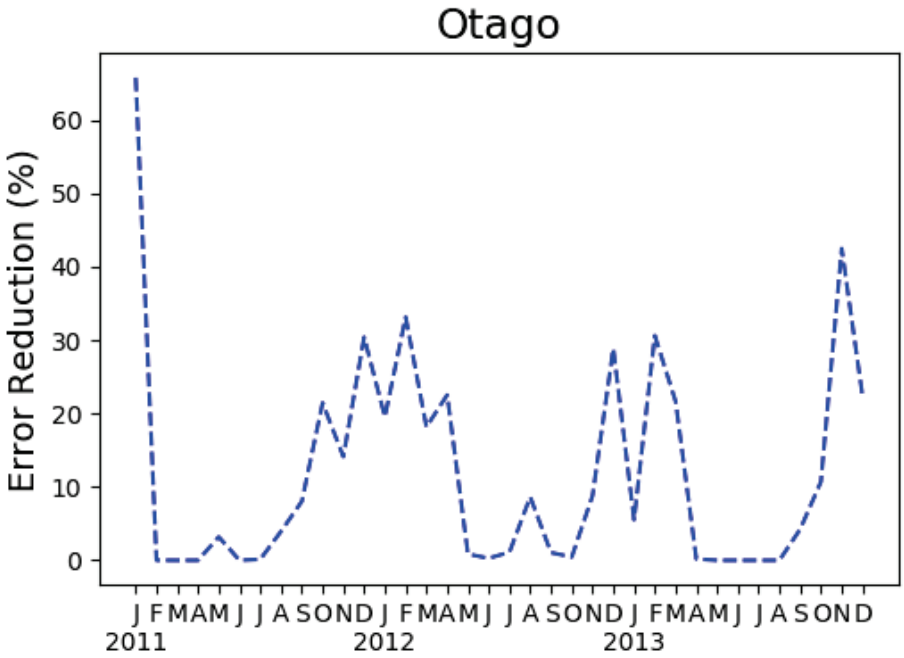

Figure 4: Error reduction for the Otago region, 2011-2013

In the following figures (Figure 5 to Figure 7) we show the results for Otago, Canterbury and Southland but filtered to only cases with error reduction greater than 5%. This leaves out emission estimates that are almost entirely dependent on our initial estimates, where the inversion has added no information.

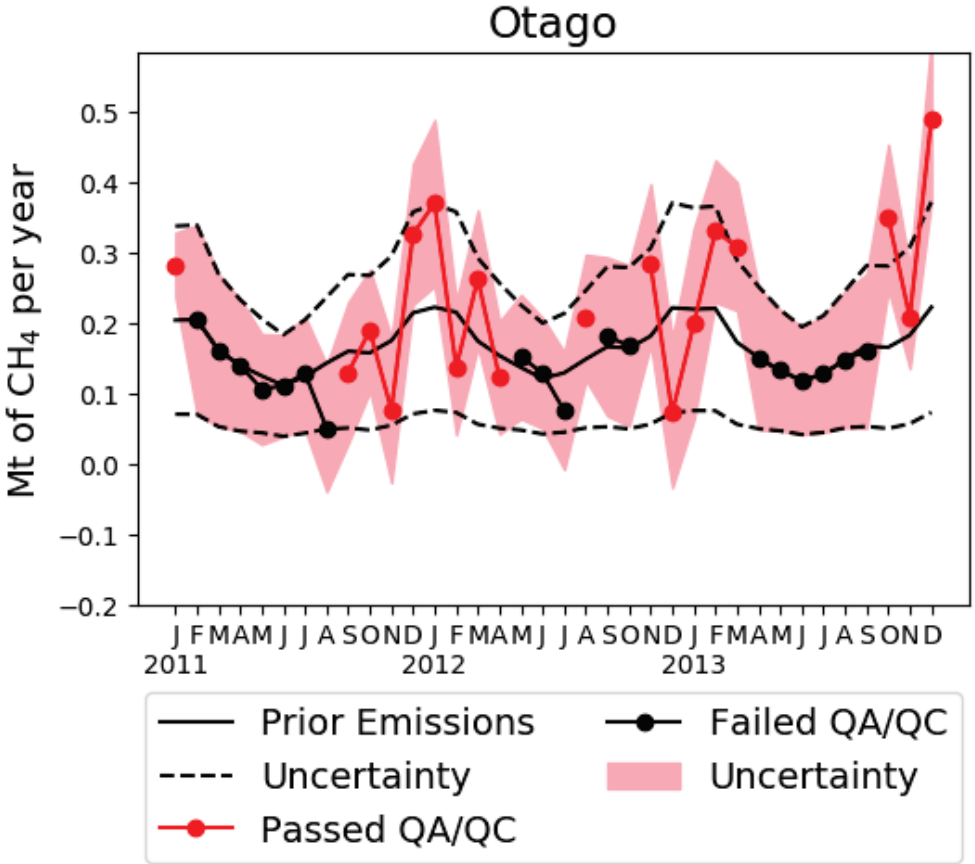

Figure 5: Inversion results for Otago, 2011-2013, filtered for cases where the error reduction is greater than 5%. Black markers denotes values that failed quality control and have been filtered out

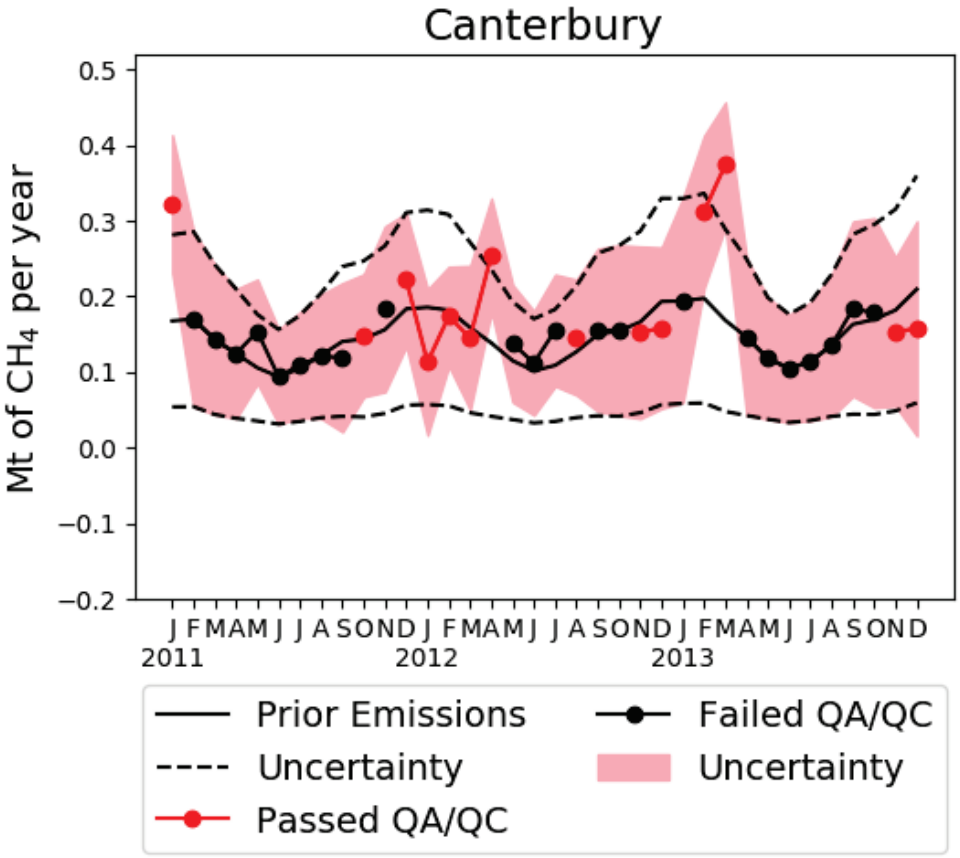

Figure 6: Inversion results for Canterbury, 2011-2013, filtered for cases where the error reduction is greater than 5%. Black markers denotes values that failed quality control and have been filtered out.

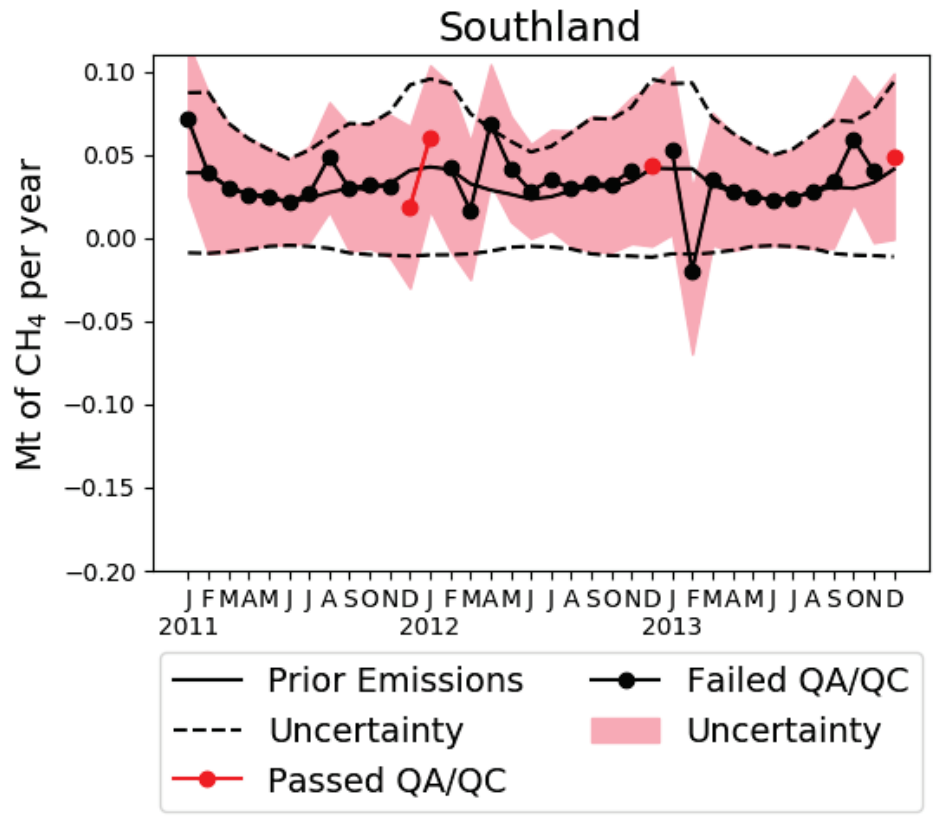

Figure 7: Inversion results for Southland , 2011-2013, filtered for cases where the error reduction is greater than 5%. Black markers denotes values that failed quality control and have been filtered out

The filtering process significantly reduces the number of available data points. For all regions we have the most success during spring and summer months, whereas autumn and winter are particularly poorly sampled. This could be due to several reasons, firstly the wind speeds are generally higher in spring and summer, and so the transport of methane should be stronger, increasing the robustness of the inversion. There could also be errors in the transport model itself that are not so noticeable at higher wind speeds but, when wind speeds are lower, could result in significantly different transport compared to reality. Lastly, as is the case in the winter of 2013, the instrument was not operational so no information could be added. In all cases, despite our filtering process, there are significant outliers, with often negative emissions, or emissions in excess of 100% more than the prior. These are driven by inter-region correlations and transport errors and are discussed in Section 4.2.

For Otago, with the exception of outliers such as in November 2011, the 2011 results are promising. The seasonal cycle from the prior is broadly reproduced but with steeper increase in emissions from spring to summer. Outside of 2011, the results are far less consistent and they are sparser for Canterbury and Southland. Southland may have more successfully retrieved months than Canterbury, but the uncertainty in its results is higher. This makes sense as the geographic isolation of Southland from Lauder means that the correlation between Lauder and Southland will be low, unfortunately the wind patterns mean that the Southland region is infrequently sampled compared to Otago and Canterbury.

Degrees of Freedom are 7.2, 5.6, 1.5 for Otago, Canterbury and Southland, respectively. This means that roughly, for every five months, we are able to retrieve one piece of information from Otago. In other words, roughly a half-year average. In contrast, for Southland it would be closer to an 18-month average. However, the distribution of the degrees of freedom throughout the year indicates that the averages would be weighted toward summer months.

Clearly, there are limitations on the applied inversion method and there is a need to investigate what is driving the uncertainties and potential systematic errors. We need to address why we are unable to obtain data during winter, how to overcome regional correlations and how to improve the consistency and quality of the inversions? These challenges aren't unique to New Zealand and our observing network but can be resolved by increasing the number of measurements sites and imporving the model resolution. In a recent study of methane emissions in Swizerland (Henne et al. 2016) , with similar topographical challenges, consistent results of national emissions were obtained by having 4 measurement sites and higher resolution modelling at 7 x 7 km,

4.2 UNCERTAINTIES AND LIMITATIONS OF THE INVERSIONS

4.2.1 Residuals

The residuals are the differences between the modelled and observed methane enhancement at Lauder (y and y_0 from Section 3.4) after subtracting the baseline methane as measured at Baring Head. This is shown in Figure 8, and barring several strong peaks, the residuals are generally below 0.05 ppm (50ppb) and close to zero. Ideally there would be no mismatch, but large differences indicate that despite the inversion's iterative process, it was unable to fully account for the observed methane values. These differences could indicate that we do not fully simulate the combination of sources and transport (in inversion terms, the smoothing effect is too high). They could also come from measurement errors and biases in our observations at Lauder or Baring Head.

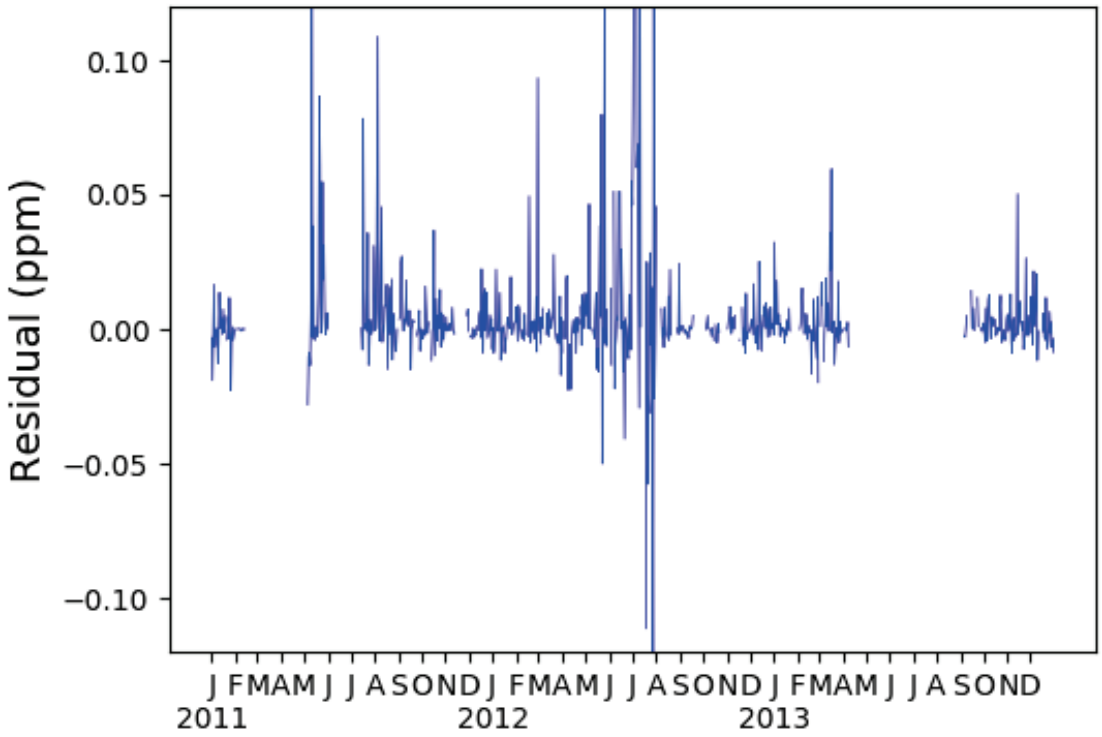

Figure 8: 2011-2013 residuals

If we compare the timing of the spikes in the residuals to the results shown in section 4.1, we can make a number of interesting observations. The large cluster of high residual values in mid-2012 has been screened out by the error reduction, which makes perfect sense; the aim of the inversion is to minimise this difference, if it is not minimised it will default to the prior. We can also see that for outlier values in the methane emissions such as December 2012, despite unrealistically low emissions in Otago and Canterbury, the corresponding residuals are good. Again, this makes sense; the inversion can arrive at unrealistic combinations of regional emissions while still minimising the residual. It means that a combination of things might be happening, firstly the transport might be incorrect. If the air came from markedly different areas than was modelled, the methane will be attributed to the wrong region. Secondly, the constraints on the inversion may be too loose, allowing the inversion too much free reign and so arriving at an unphysical result. Thirdly, there could be a bias in the measurement datasets, this would cause too much/little emission attribution in regions.

4.2.2 Correlations

The correlation between regions indicates how well we can separate them from each other. A correlation of 1 between two regions would mean they were completely unseparable, conversely, 0 would mean they were fully resolved. These correlations are dependent on the transport of methane. An air mass will pass over multiple regions before reaching Lauder, making them impossible to distinguish. We would therefore expect that for each of our considered regions, the Lauder region would give the highest correlation as the air has to pass over it. As shown in the following figures, this is indeed the case with neighbouring, strongly emitting regions also showing correlations at certain times of year. It is also worth nothing that when regions are not retrieved, due to either no sensitivity to them or due to lack of measurements and therefore default to the prior, the correlation will drop to zero, hence the zero correlations for all regions during the winter 2013.

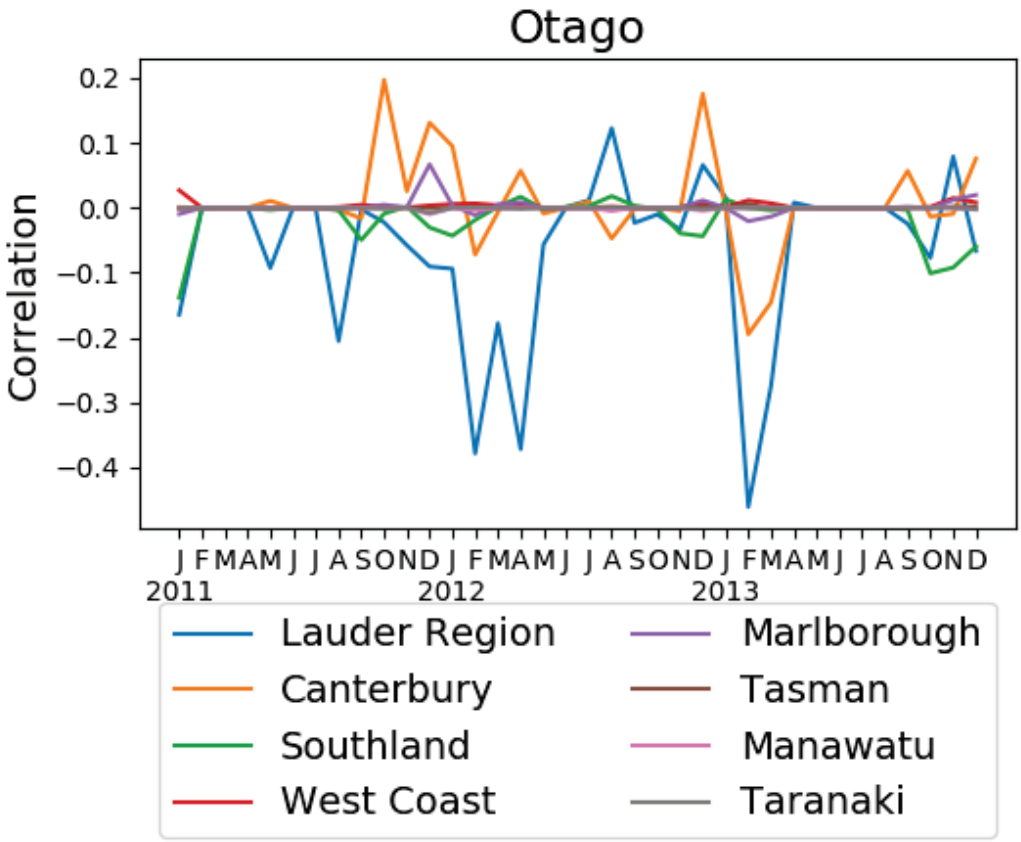

Figure 9: Otago correlations for 2011-2013

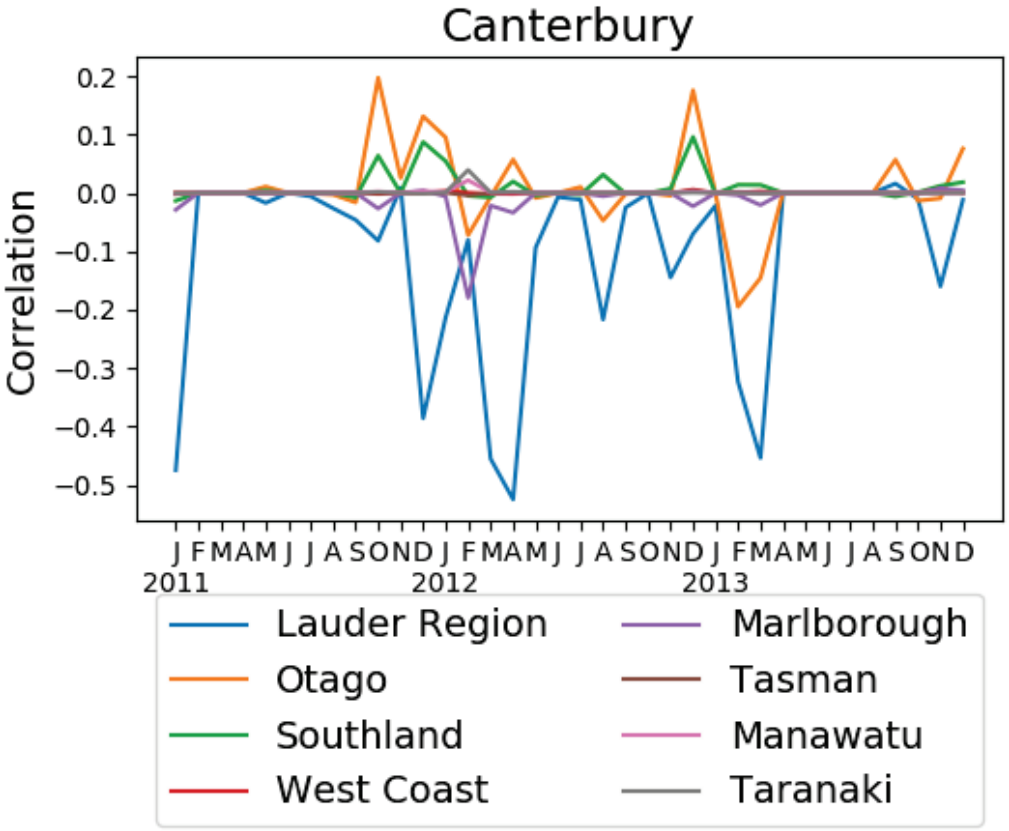

Figure 10: Canterbury correlations for 2011-2013

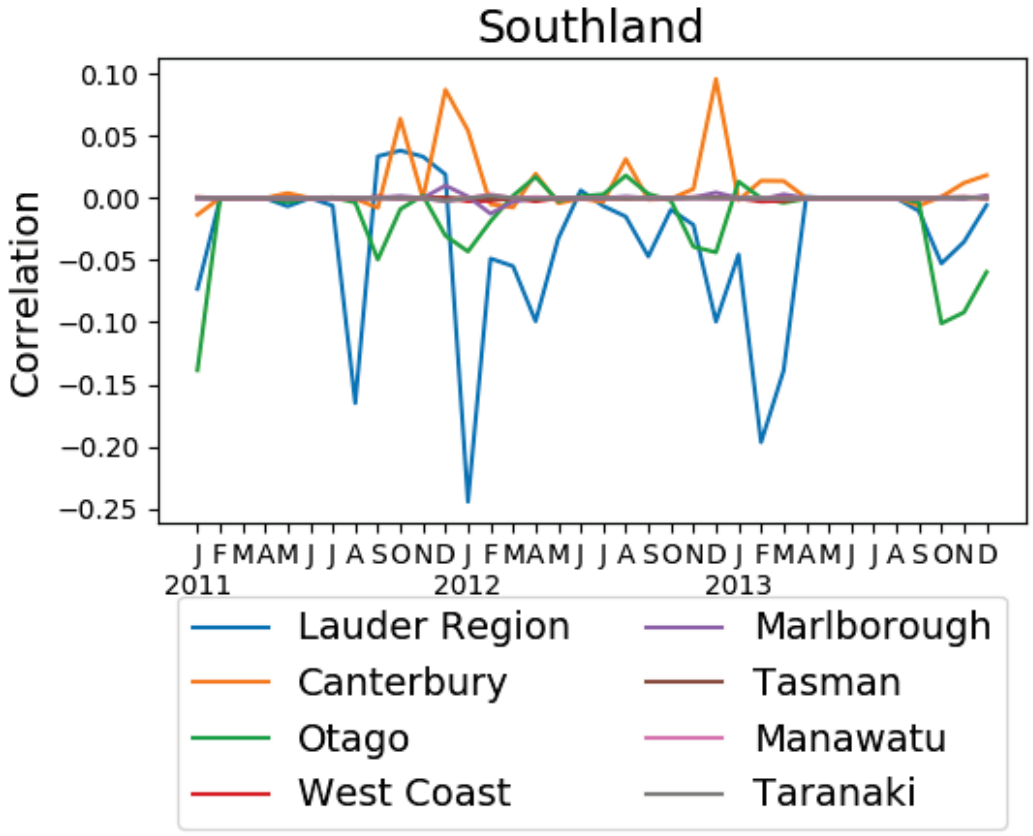

Figure 11: Southland correlations for 2011-2013

When there are strong correlations, greater than 50%, it becomes hard to separate out different regions with great confidence. Instead, it would be better to combine strongly correlated regions. We can also look to improve our *a priori* knowledge to constrain the values further or we can make additional measurements. If another measurement is made at a different site, the air flow to the new site would be different to the original site, and so have different correlations. By doing this we would then have different combinations of emissions at the same time, allowing us to constrain the regional emissions even further.

4.2.3 Simulated Results

Another test we can do is to simulate the inversion. In this we assume our model is perfect by creating a synthetic set of observations based on our *a priori* emission maps and dispersion modelling. Effectively saying the residuals are all zero and that;

$$y_0 = y = f(x_a)$$

This means that the inversion performance no longer depends on the modelling accuracy, and shows only the limitations of any measurement error, unavoidable correlations between regions and times (smoothing error) and prior constraints. In this simulation, we should then always replicate the *a priori*, x_a, and we will be able to determine the limiting factors in the quality of our inversions. The metrics described in Section 3.4 are still valid and are vital to the assessment of the simulation. Using a conservative fixed uncertainty of 2ppb for our synthetic observations and removing the times that in our real observations were unavailable we produce the following results.

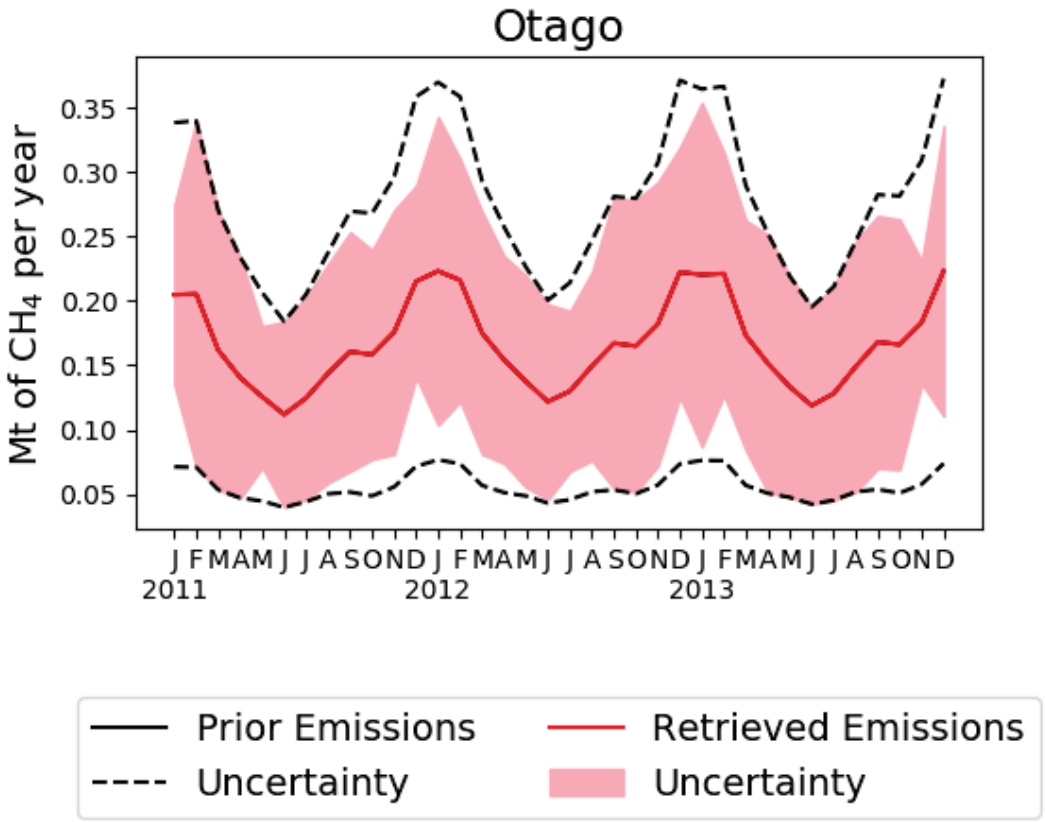

Figure 12: Simulated retrievals for Otago, 2011-2013

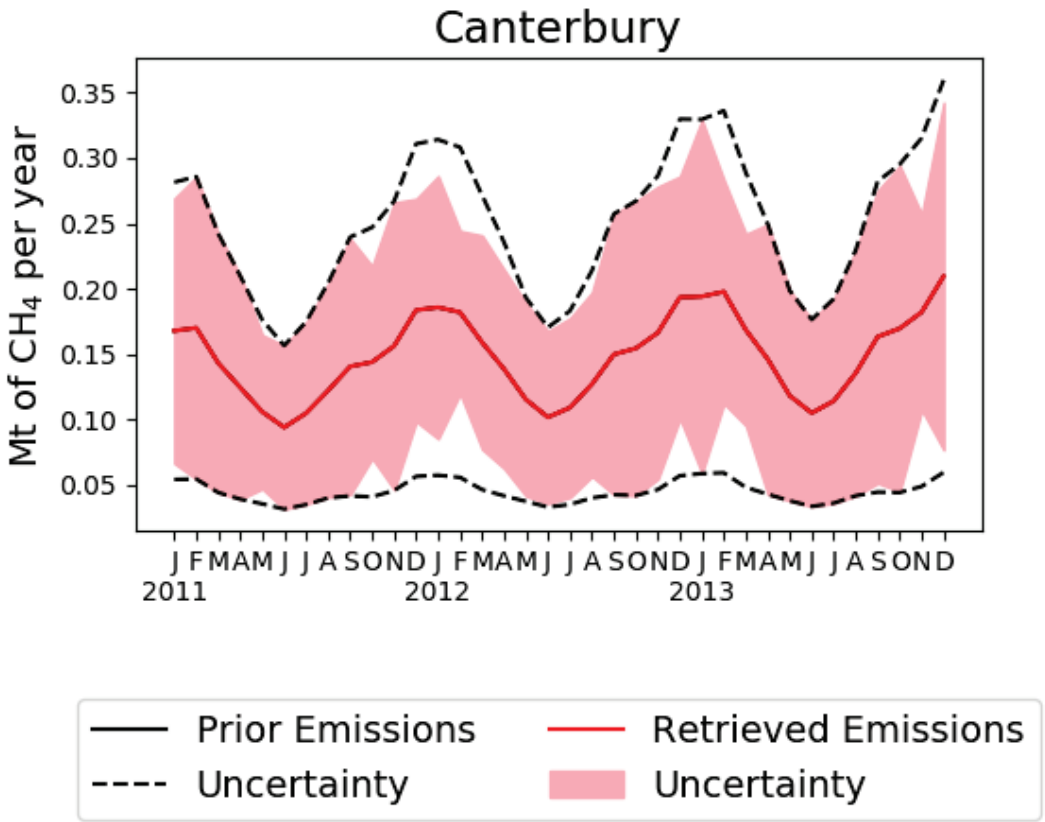

Figure 13: Simulated retrievals for Canterbury, 2011-2013

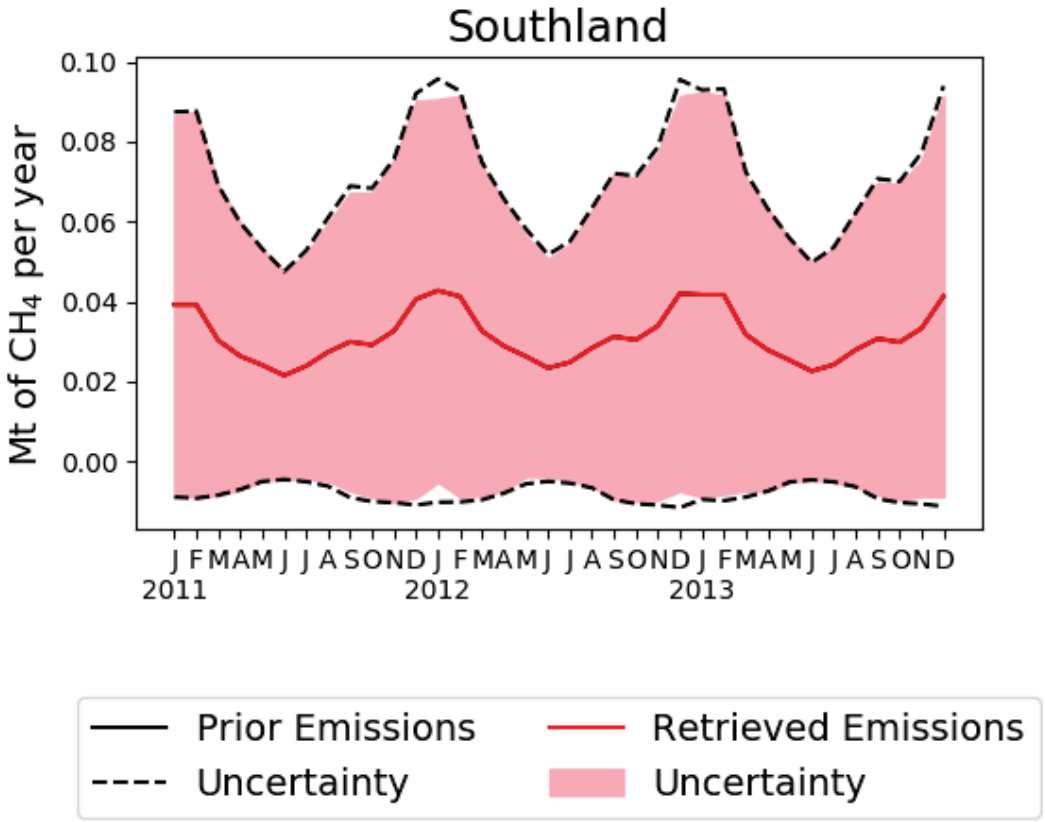

Figure 14: Simulated retrievals for Canterbury, 2011-2013

As can be see, the *a priori* is always retrieved, and the uncertainty reduced when possible, giving us confidence in the stability of the inversion. The degrees of freedom for Otago, Canterbury and Southland are 9.9, 7.2, 1.6 respectively. In each case, the error reduction between the real inversions and the synthetic ones are reasonably consistent with each other. This is born out in the similar degrees of freedom albeit with a slight increase, but for the purposes of this experiment, they are sufficiently close and show that our 2ppb uncertainty is a good approximation. We can use this synthetic inversion as a benchmark and investigate what would happen if we had a complete set of observations, i.e. no missing data during 2013.

If we now include the days were observations were missing, we can see the impact that would have upon the uncertainty and information content of the results. If we do this, using the same 2ppb uncertainty, we increase the degrees of freedom to 16.8, 11.2, 2.5 for Otago, Canterbury and Southland, respectively. The increase is stronger for Otago and Canterbury which is not surprising, we will always have less sensitivity to Southland compared to the other two regions. This highlights the need for a more consistent dataset with multiple observations for redundancy.

4.2.4 Measured v Modelled Windspeeds

The simulated results shown previously assume that the modelling is perfect. The dispersion modelling using NAME is driven by meteorological data from NZLAM, and although we have no control over NZLAM (in that we cannot perturb it until it matches our observations), we can assess its performance by comparing its output to the observed data at the Lauder site, the key parameter being wind speed. The windspeed at Lauder is routinely measured using our meteorological station and is compared to the model in Figure 15.

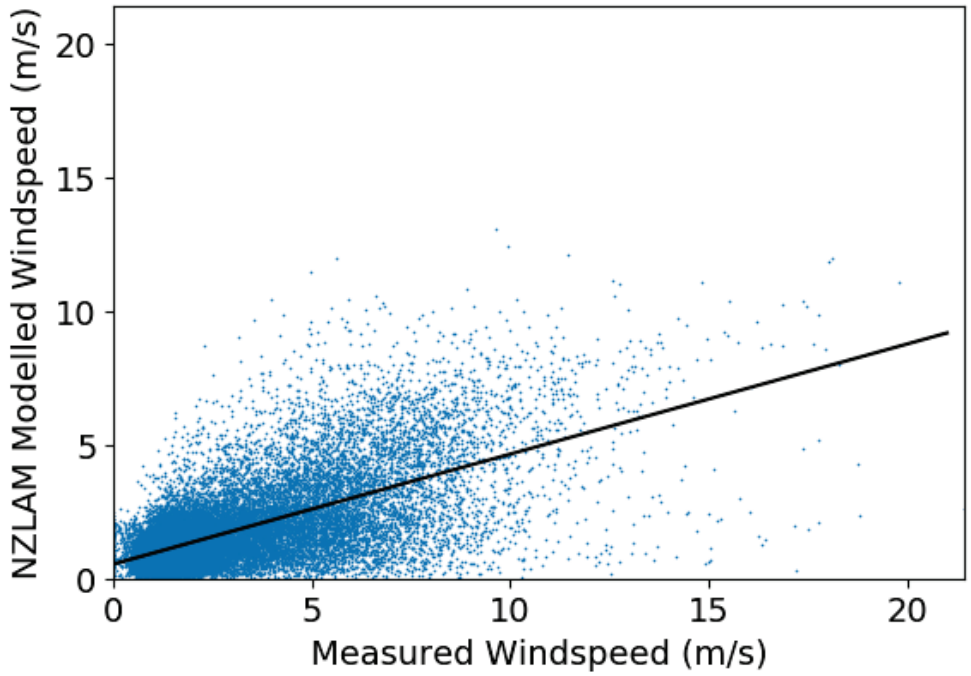

Figure 15: Measured vs NZLAM modelled windspeed at Lauder for 2011-2013, the black line is the linear regression between the two datasets.

While we do not expect the measured and modelled wind speeds to agree perfectly, the gradient of the regression line should be close to one. The gradient here is 0.41 with an intercept at 0.56 and r-squared of 0.4, meaning that NZLAM consistently underestimates windspeeds by approximately 50%. Although this observation doesn't necessarily apply over the complete 4-day back trajectory, it does show that there is a significant difference between the observed and modelled windspeeds. The impact at higher windspeeds is lessened as the difference in the footprint (i.e., the area influencing a given methane signal) would be smaller. At lower windspeeds, where the model significantly underestimates windspeed, the difference in the footprint could be profound.

This data could be used to filter down the inversion results, such as only using winds above a threshold, but for a robust treatment the differences between modelled and actual winds must be known over the whole NZ domain. There is no reason why the wind speeds from NZLAM would be more realistic elsewhere. Studying NZLAM in such detail is out of scope in this study and it has already been shown to underestimate peak windspeeds by Webster et al, 2008. However, we use newer, higher resolution wind fields that more accurately capture the dynamics of New Zealand.

4.3 IMPROVING THE INVERSION

4.3.1 Using NZCSM

We have shown that using NZLAM to drive our dispersion modelling could be leading to significant errors in our inversion that are hard to eliminate. Fortunately, NZCSM (a different weather model) has been generating the required data for 2017 onwards. By comparing inversions using NZLAM and NZCSM outputs over the same time frame we can see what impact the increased resolution of NZCSM has upon the windspeeds at Lauder and on the inversion results. Unfortunately, we only have data from 2018 for both NZLAM and NZCSM available at the time of writing, while the latest emission maps as prior are available for 2016. Nonetheless, a comparison of inversions using 2016 prior emissions and 2018 winds from either NZLAM or NZCSM provides an interesting case study. The wind roses for the three datasets are compared in Figure 16. As previously discussed, NZLAM consistently underestimates windspeeds compared to reality, what's more, it completely misses the strong north easterly winds routinely observed at Lauder, instead opting for gentle northerlies. NZCSM however, captures the prevailing winds much better, though it still slightly underestimates windspeeds at times, Figure 17.

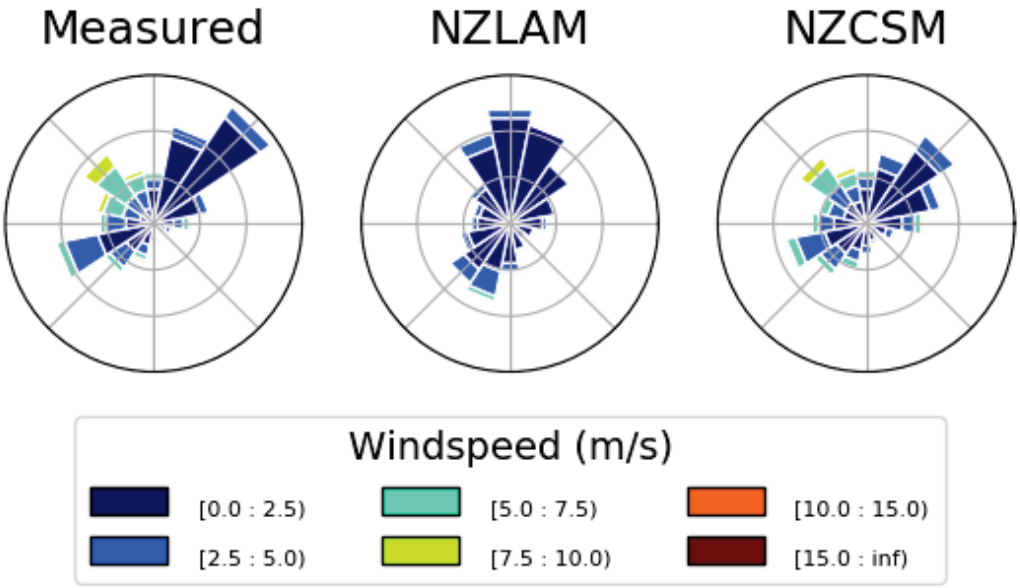

Figure 16: Wind roses for Lauder from measurements, NZLAM and NZCSM for 2018. Grey circles denote levels of 5%, 10% and with 15% (black outer ring) of the total number of records (8760)

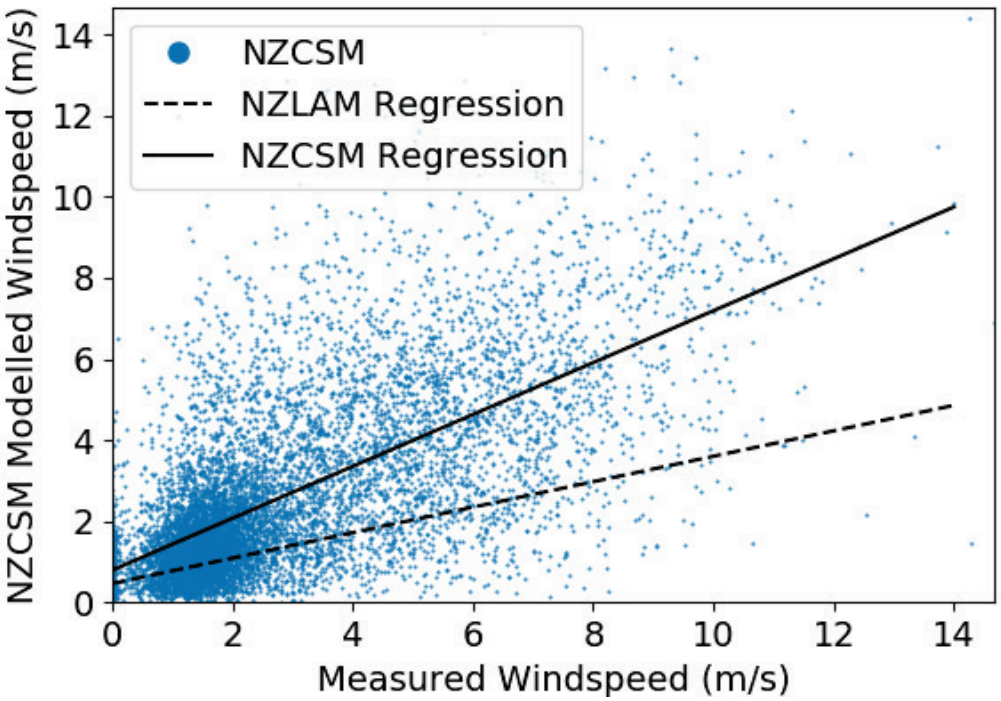

Figure 17: Measured vs NZCSM modelled windspeeds at Lauder for 2018. Black line denotes the linear regression between the two datasets, the dashed black line is the regression of the corresponding NZLAM data that is not shown for clarity.

The gradient of the regression in this case is 0.64, a far better value than the 0.31 from NZLAM over the same time period. The r-squared values are also improved from 0.36 to 0.43 the intercept has actually increased slightly but the overall agreement is far better.

We can assess the impact of the improved wind fields upon the dispersion modelling by comparing the total dosage maps of the models. The dosage is in effect the sensitivity of the measurement at Lauder to the emission map. Summing dosage over the year shows the areas from where methane emissions can be detected. The difference between the two maps is shown in Figure 18.

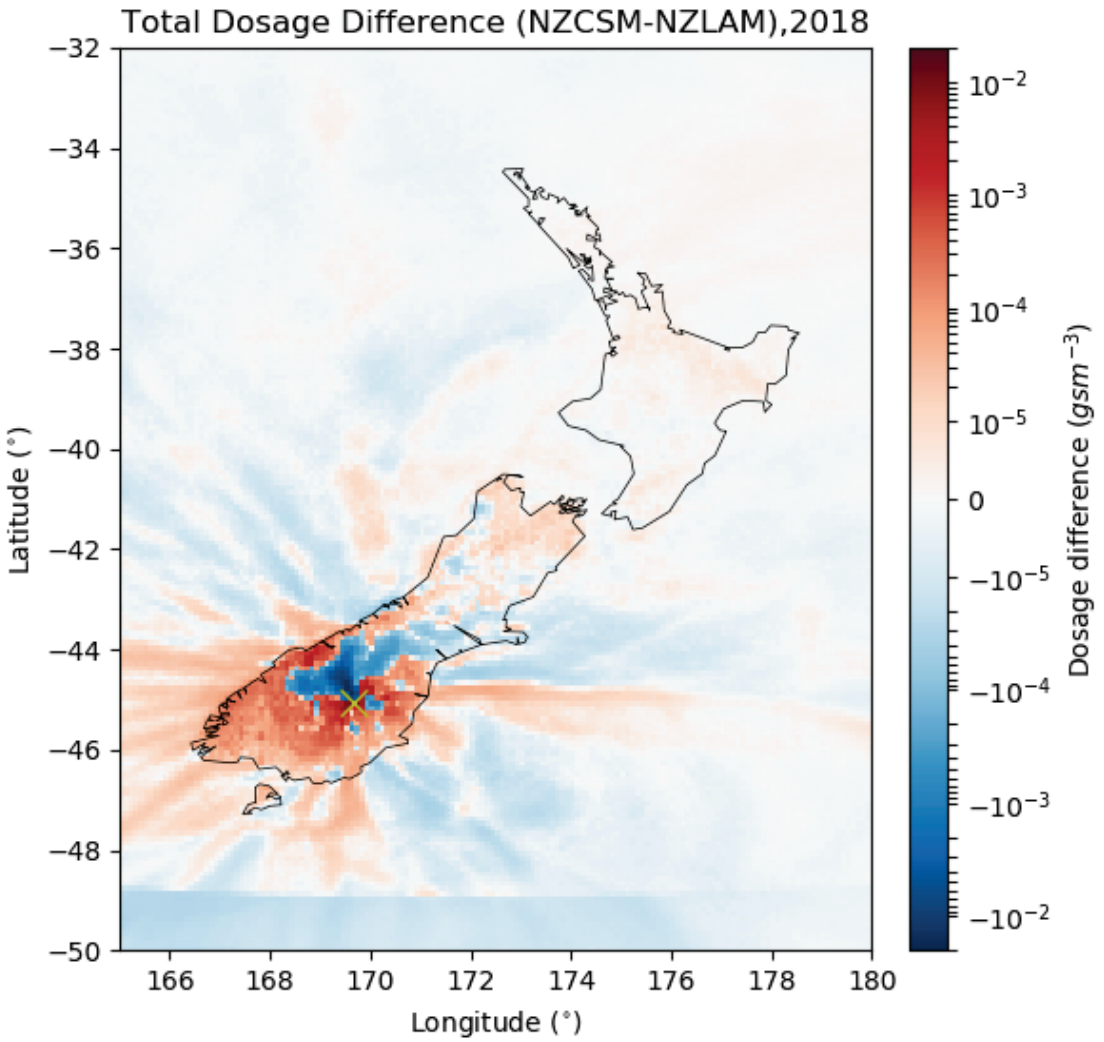

Figure 18: Dosage difference map (NZCSM-NZLAM) for 2018. Blue colours indicate NZLAM having higher sensitivity, red NZCSM. Yellow cross marks the Lauder observation site.

The most substantial differences occur near the observation site. NZLAM shows higher sensitivity to the north/north west of the site, with NZCSM showing higher sensitivity in north east and south west. If we refer back to the wind roses we can see why. NZLAM has modelled low winds to the north, with no strong north westerlies, meaning that the modelled air spends longer in the north / north west region. NZCSM however, has stronger north westerlies and more frequent lower winds from the north east and south west. These differences should then significantly alter the inversions in Otago and Canterbury. While there are differences in the rest of the country, particularly the West Coast, and Southland, the low dosage differences and low source strengths should mean that there are only minor changes. As hypothesised earlier, the impact of modelling with lower windspeeds only really affects short range transport.

With an improved transport model, we expect to see the residuals decrease as the transport better reflects the reality. The residuals for NZLAM and NZCSM are compared in Figure 19.

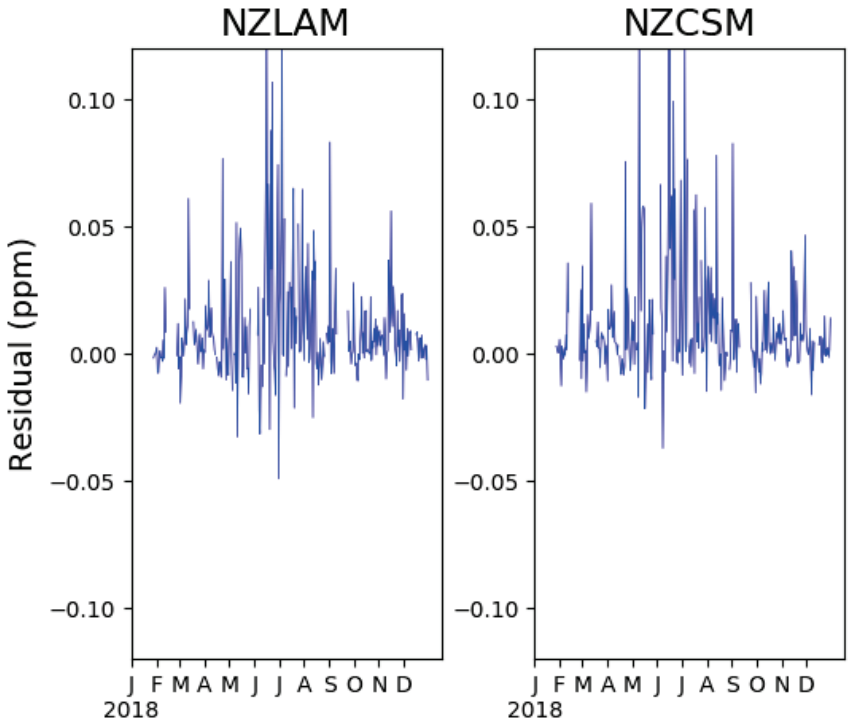

Figure 19: Residuals for NZLAM and NZCSM, 2018

The root mean square (RMS) of the residuals are 0.023 and 0.022 for NZLAM and NZCSM, respectively, indicating a slight reduction by using NZCSM. The remaining spikes, and in cases the strengthening of the spikes by using NZCSM, may indicate remaining problems with the modelled wind data, errors in emission maps or in the observational data.

If we now look at the inversion results using NZLAM and NZCSM we should see differences due to the differing footprints and reduced residuals.

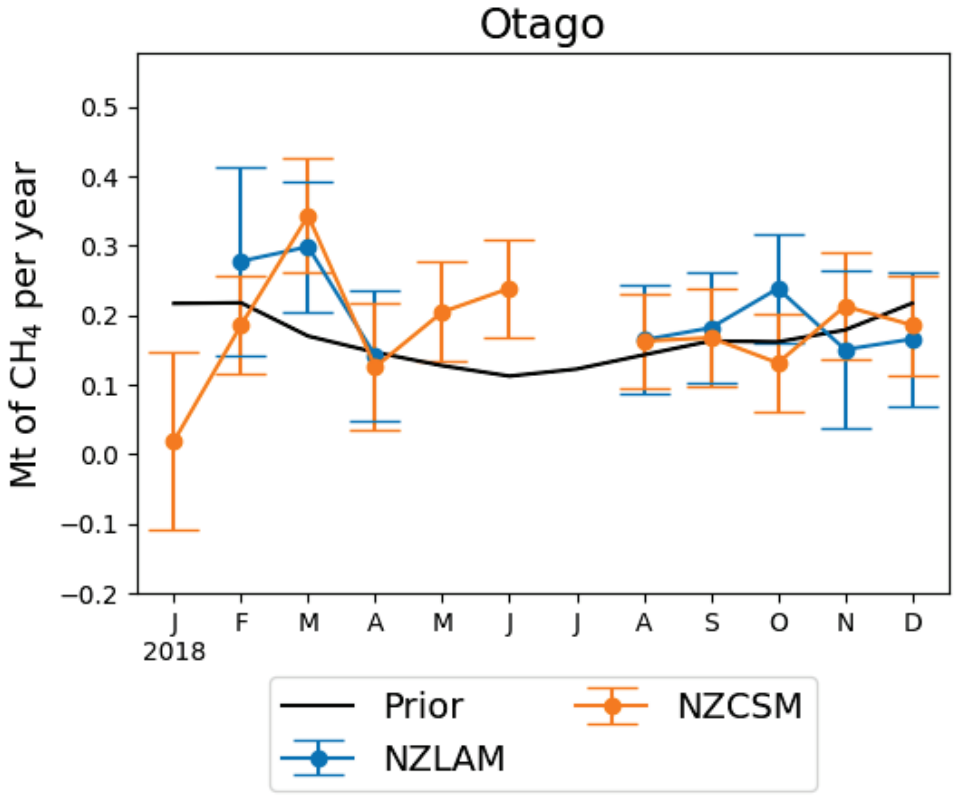

Figure 20: Inversion results for Otago, 2018, NZLAM compared to NZCSM, low error reduction months filtered out

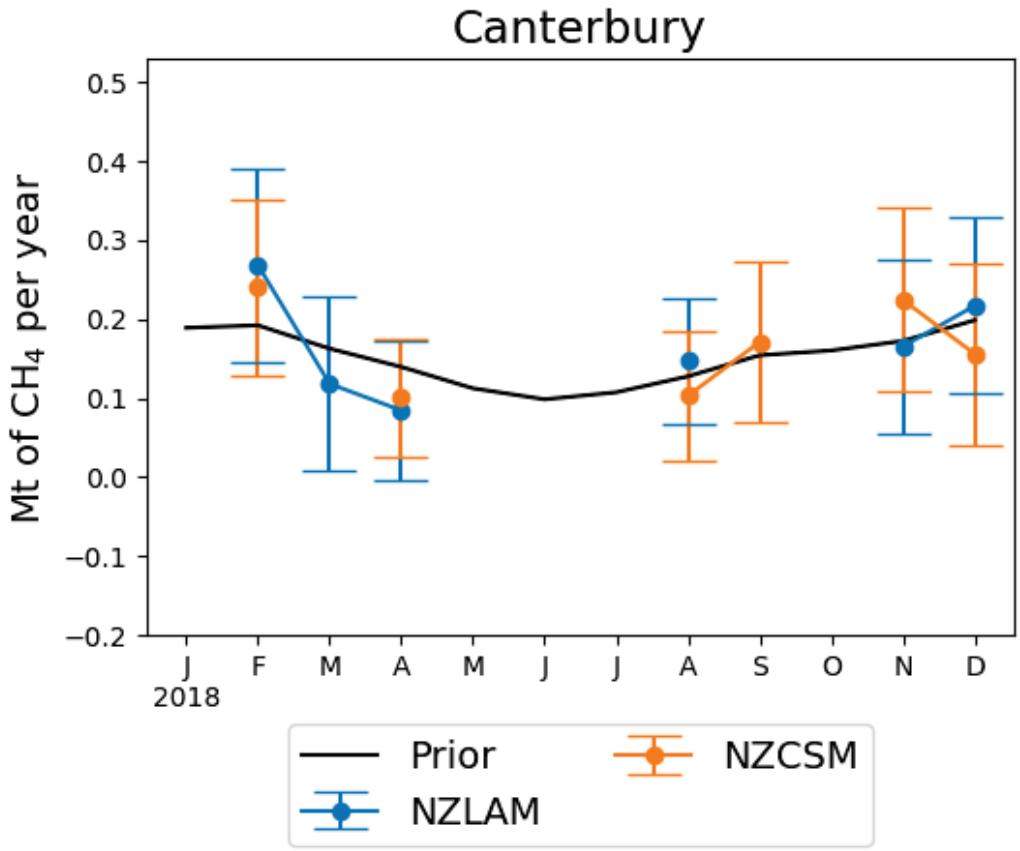

Figure 21: Inversion results for Canterbury, 2018, NZLAM compared to NZCSM, low error reduction months filtered out

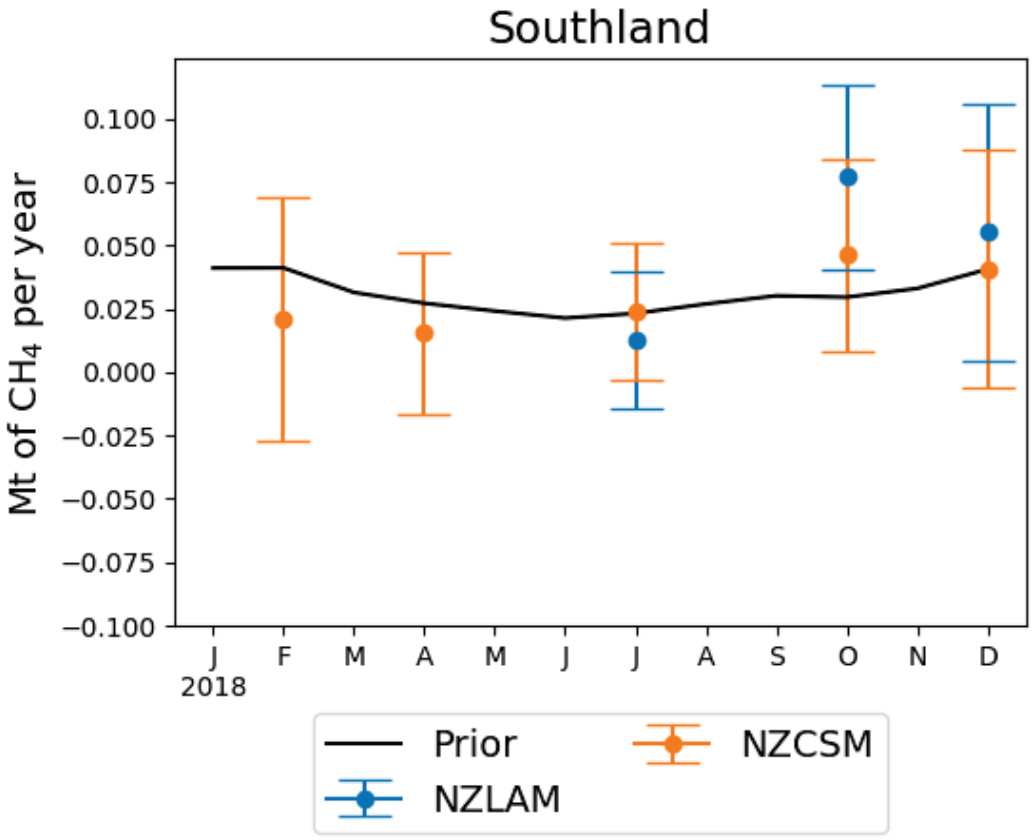

Figure 22: Inversion results for Southland, 2018, NZLAM compared to NZCSM, low error reduction months filtered out

All three regions show improvement in their results. For Otago, we obtain several additional months due to improved error reduction as a result of lower residuals. It also shows a consistent improvement in error reduction, with the mean error reduction increasing from 13% to 26% for Otago, 6% to 8% for Canterbury and 3% to 5% for Southland. The trends seem fairly consistent between wind models with similar outliers, such as March. The NZCSM results for Canterbury are similar, with one less data point but slightly improved mean error reduction and overall information content. For Southland we again see an increase in the months with valid results, perhaps due to the increase in south westerlies in NZCSM. The uncertainty is still significant across all months, but it has reduced from NZLAM.

The degrees of freedom for each region are shown in Table 1 and bare out the discussion above. Otago and Southland have significantly increased its information content, whereas there are only minor increases for Canterbury.

Table 1: Degrees of Freedom for 2018 using NZLAM and NZCSM. Totals for the South Island are give with (in brackets) and without the Lauder region.

Region	NZLAM DoF	NZCSM DoF
Otago	2.8	5.1
Canterbury	1.5	1.7
Southland	0.67	1.2
Total South Island (inc Lauder)	6.3 (11.2)	8.0 (13.24)

While information content has increased and uncertainty has been reduced by using NZCSM, it is far harder to assess the change in the retrieved emissions themselves. There are still vast gaps and shortcomings in the retrieved data. We need to improve the frequency and quality of the observations we are making, so that the retrieval can improve upon the *a priori* emissions estimate from the inventories.

4.3.2 Incorporating New Sites and Instruments

Using our synthetic inversion described in Section 4.2.3, we can assess the impact of improving the instrumental uncertainty and the distribution of instruments. A quick test we can do is to reduce our 2ppb uncertainty. This might not be possible for a single instrument, but with multiple simultaneous measurements, the uncertainty would decrease by the square root of the number of measurements. Doubling the instruments at Lauder, in our idealised scenario, would decrease the uncertainty to 1.4 ppb and increase the degrees of freedom to 21.7, 15.1 and 4.5 for Otago, Canterbury and Southland. The improved uncertainty allows us to increase the information content particularly from Southland where the absolute gain is larger.

A better strategy might be to have the additional instruments located in other regions. As an example, if instead of two instruments, each with an uncertainty of 2ppb at Lauder, we move one to Baring Head (there would be no reduction in uncertainty to 1.4 ppb) the degrees of freedom become 21.4, 18.5 and 3.5. While Otago remains unchanged, Southland has decreased and Canterbury increased significantly. In addition, significant information has been added to the Marlborough region, up to 7 degrees of freedom from less than 1 and 16.5 in the Manawatu region. These results are summarised in the table below. The strong impact of additional measurements at Baring Head on distant areas like Canterbury is due to the correlation between regions; constraints in one region result in constraints for another. This is well illustrated by Canterbury because it lies between the two measurement sites and is a strong source. Clearly then we can see the value of adding in additional observations to the network, and with sites in Winchmore and Maunga Kakaramea coming online for methane in the next few years we will have plenty of opportunity for further improvements.

Table 2: Simulated Degrees of Freedom from NZLAM, 2011 - 2013

Region	Original Simulation	No Data Gaps	Two instruments at Lauder	One Instrument at Lauder and Baring Head
Otago	9.9	16.8	21.7	21.4
Canterbury	7.2	11.2	15.1	18.5
Southland	1.6	2.5	4.5	3.5

4.4 2018 ENHANCED INVERSION

We can bring all our learnings together for an inversion of 2018 where we include observations of methane at our Baring Head site. Previously, we had used flask sample data (~weekly) to construct a baseline only. However, in recent years, hourly observations of methane are available at Baring Head using the Picarro system (continuous measurements) described in Section 3.2.

Using NZCSM for 2018, with 2016 as our a priori, *the results are further improved with degrees of freedom for each region of 7.5, 6.6, and 1.7 (Otago, Canterbury and Southland) compared to those shown in Table 1: Degrees of Freedom for 2018 using NZLAM and NZCSM. Totals for the South Island are give with (in brackets) and without the Lauder region.*

Region	NZLAM DoF	NZCSM DoF
Otago	2.8	5.1
Canterbury	1.5	1.7
Southland	0.67	1.2
Total South Island (inc Lauder)	6.3 (11.2)	8.0 (13.24)

The figures below also show emission estimates that are much more realistic and although there are some unexplained features, i.e. an apparent methane sink in Canterbury winter, they are extremely promising results.

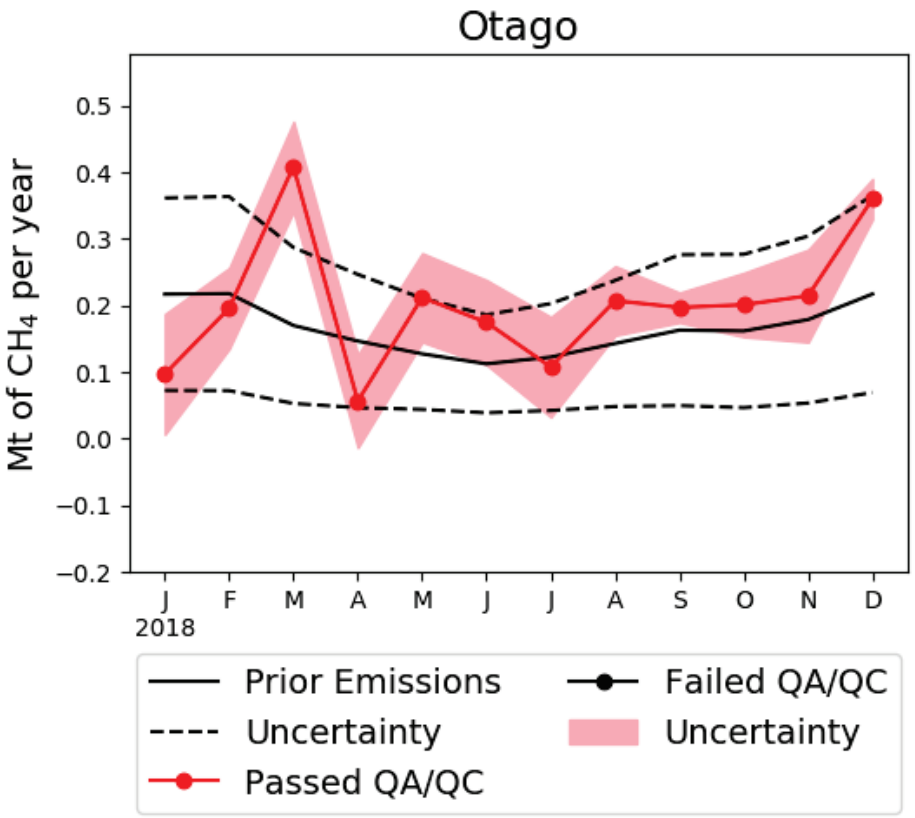

Figure 23: Retrieved emissions for Otago, 2018, using NZCSM and Baring Head data

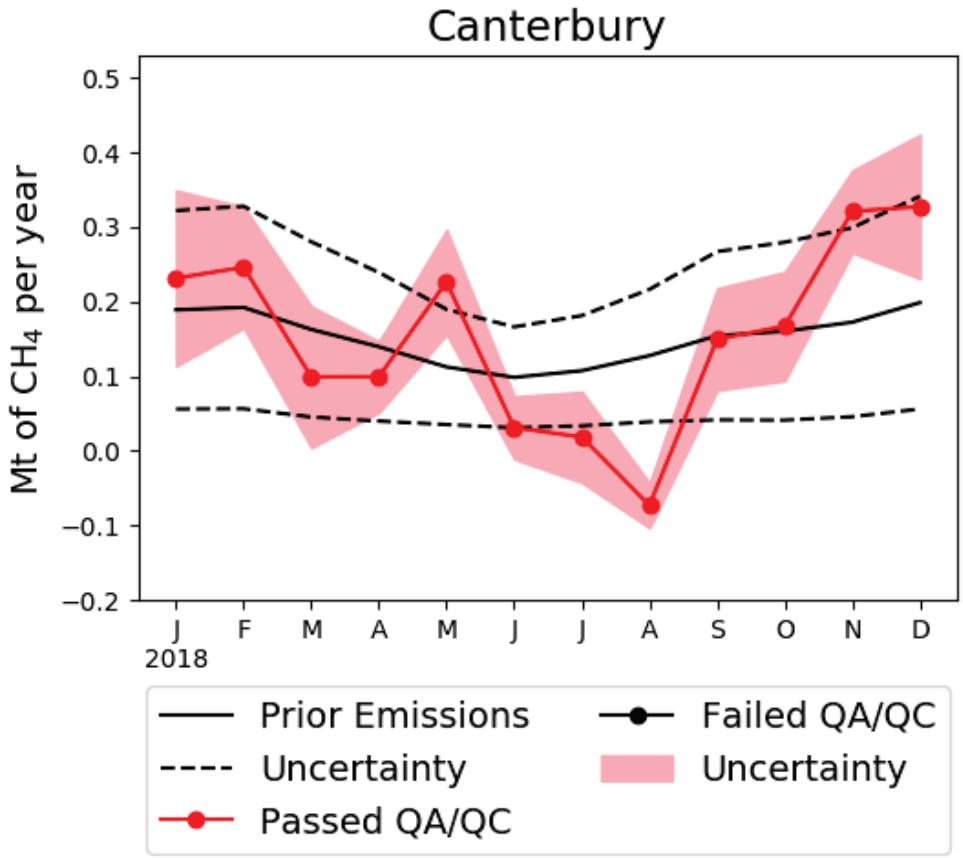

Figure 24: Retrieved emissions for Canterbury, 2018, using NZCSM and Baring Head data

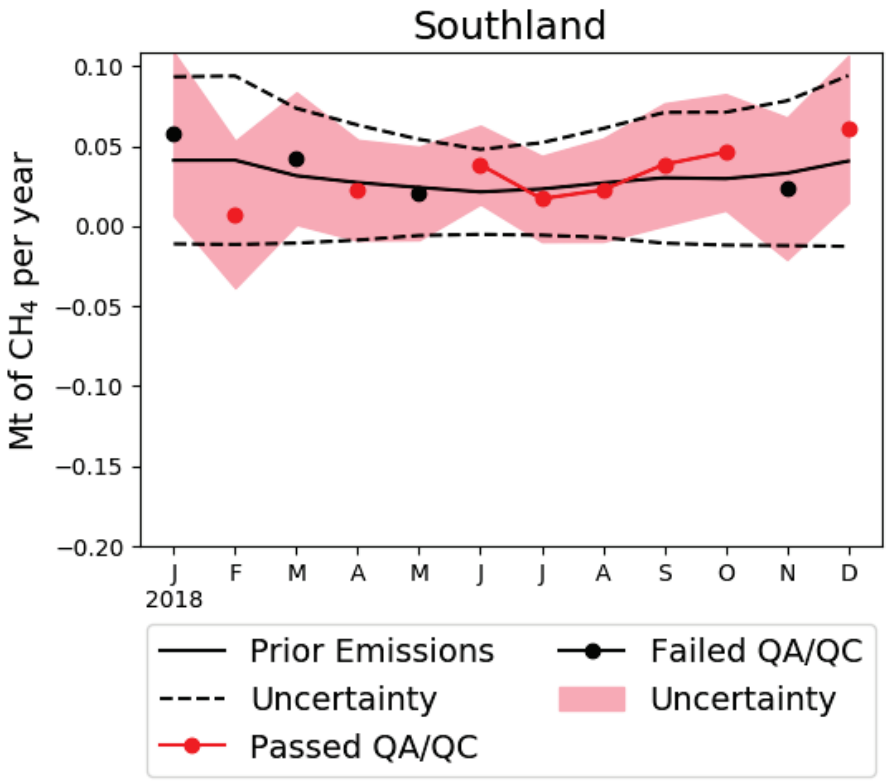

Figure 25: Retrieved emissions for Southland, 2018, using NZCSM and Baring Head data

A significant amount of information has been added to the northern part of the South Island and to the North Island by including Baring Head measurements. Such regions have virtually no impact upon the measurement made at Lauder and so in the retrieval, had zero information content. Marlborough has achieved a degree of freedom of 2.2, remarkable given its low emission strength. The Manawatu and Taranaki regions, reaching degrees of freedom of 7.4 and 3.5 respectively, are also promising but lack further constraints. The retrieved values are consistently lower than the *a priori* and follow the trends well, though the uncertainty is still appreciable.

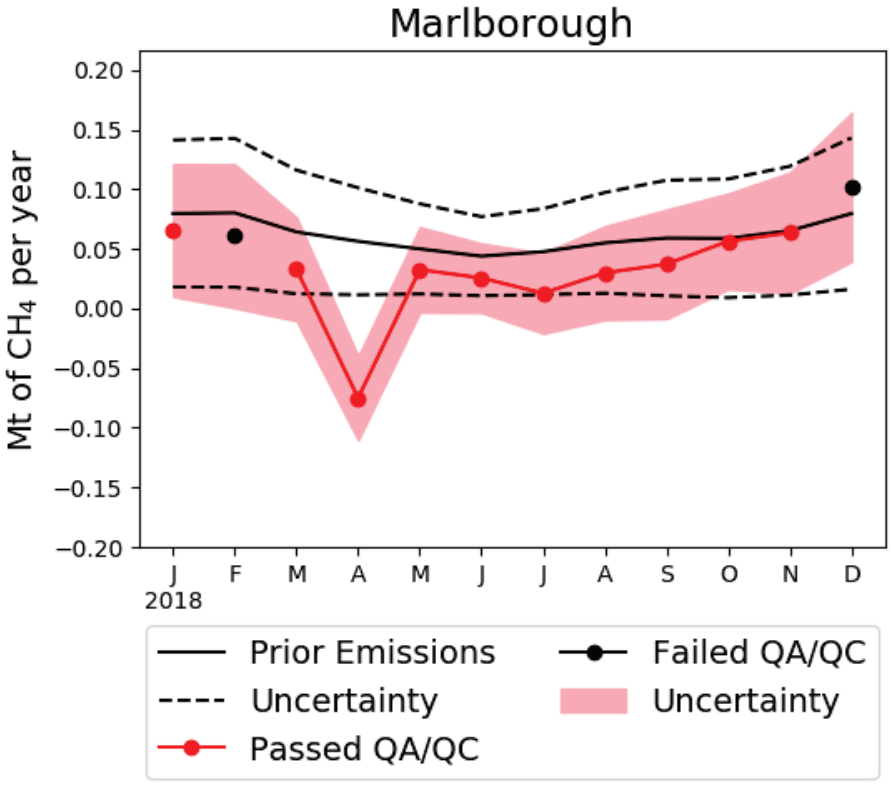

Figure 26: Retrieved emissions for Marlborough, 2018, using NZCSM and Baring Head data

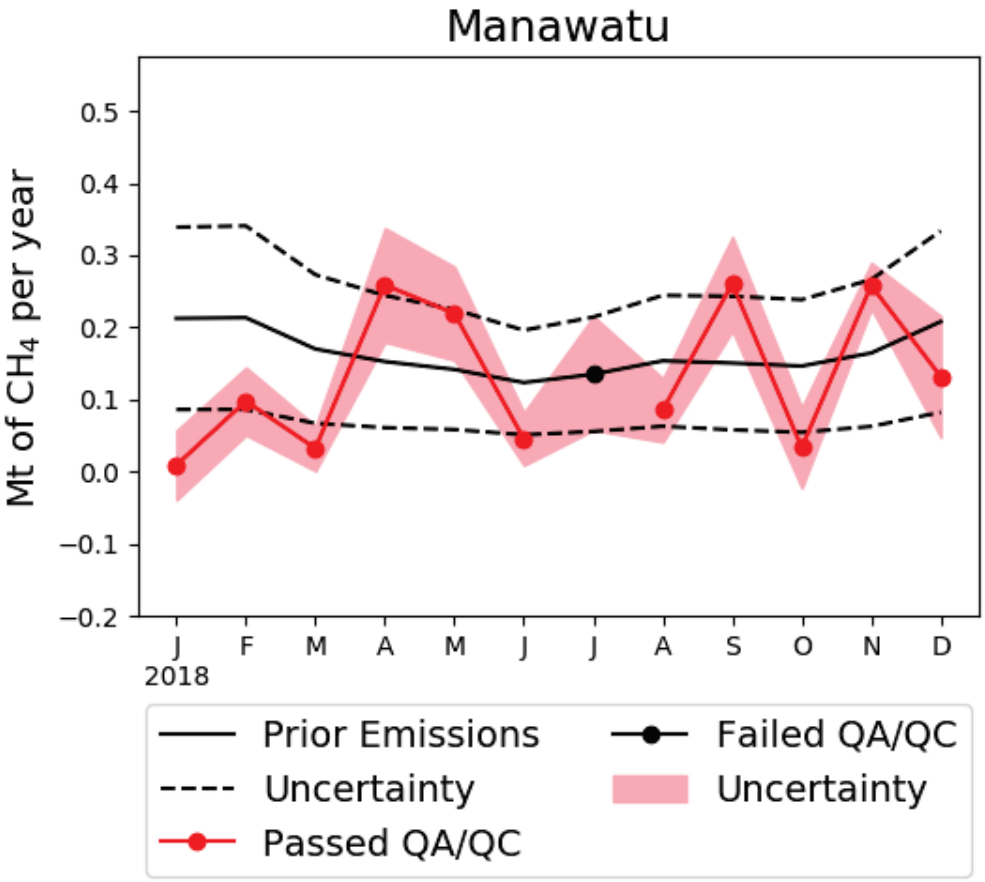

Figure 27: Retrieved emissions for Manawatu, 2018, using NZCSM and Baring Head data

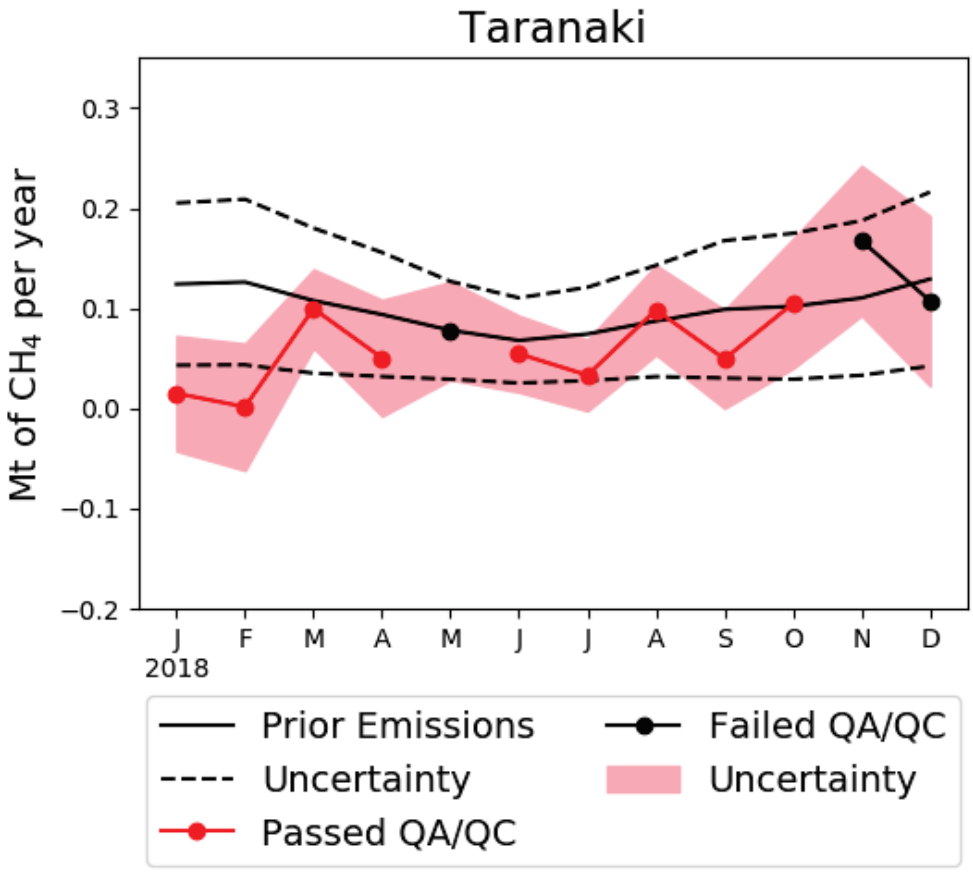

Figure 28: Retrieved emissions for Taranaki, 2018, using NZCSM and Baring Head data

Lacking further constraining measurements in the North Island, there are several extreme values in each region. With further sites and investigation this should improve, as was the case for Otago and Canterbury. To summarise the results, we can aggregate regions into North and South Island totals. This allows us to bypass inter region correlations, assuming that there is very little correlation between to the two islands, and also to compare directly to published inventories from the MfE;

Table 3 Summary of CH_4 emissions and uncertainty for 2018, noting that the emissions for MfE and MPI are from 2016, with MfE assuming the same distribution between the North and South Islands as the MPI dataset

Source	2018 CH4 Mt/y		
	South Island	North Island	Total
Ministry for the Environment (2016)	0.46	0.71	1.17 (1.37 All Sources)
MPI/Landcare (2016)	0.44 ± 0.05	0.69 ± 0.055	1.13 ± 0.074 (Agriculture)
NIWA - NZLAM	0.49 ± 0.045	0.69 ± 0.055	1.18 ± 0.071
NIWA - NZCSM	0.47 ± 0.042	0.69 ± 0.055	1.16 ± 0.07
NIWA - NZLAM (With Baring Head)	0.53 ± 0.037	0.65 ± 0.048	1.18 ± 0.061
NIWA – NZCSM (With Baring Head)	0.47 ± 0.033	0.58 ± 0.046	1.1 ± 0.057

The MfE and MPI agricultural emission estimates are shown above for 2016, split into North and South Island components based on the distribution from the MPI dataset. The MfE data is shown with its total for all sources of methane. The NIWA datasets are for 2018, based on 2016 priors and distributions and effectively measure the total methane from all sources. For the South Island this is going to be representative of the agricultural emissions. We have not included other methane sources into our *a priori* and distributions.

As can be seen, with successive improvements to our inversion, moving to NZCSM, and then including Baring Head we consistently reduce the uncertainty while not jeopardising the accuracy. The North Island shows a dramatic change with the inclusion of NZCSM and Baring Head, without further constraints from another measurement site to the north of Baring Head and additional understanding of other sources and sinks, it is too early to draw conclusions. We simply aren't sampling the North Island well enough yet.

4.4.1 Sensitivity to the Prior

In a test case, the prior emissions were set approximately 50% higher than the figures quoted by MfE due to a gridding error. This gave us an opportunity to see if, even with higher emission levels, we can still retrieve sensible emissions. In essence, are we or are we not, too sensitive to our *a priori* emissions?

Table 4: Summary of CH_4 emissions and uncertainty for 2018 but with 50% higher emissions in the MPI/Landcare dataset

Source	2018 CH4 Mt/y		
	South Island	North Island	Total
Ministry for the Environment (2016)	0.45	0.72	1.17 (1.37 All Sources)
MPI/Landcare (2016)	0.65 ± 0.08	1.02 ± 0.083	1.67 (Agriculture)
NIWA - NZLAM	0.67 ± 0.064	1.02 ± 0.083	1.7 ± 0.11
NIWA - NZCSM	0.63 ± 0.059	1.02 ± 0.083	1.65 ± 0.10
NIWA - NZLAM (With Baring Head)	0.61 ± 0.049	0.88 ± 0.07	1.49 ± 0.085
NIWA – NZCSM (With Baring Head)	0.53 ± 0.043	0.76 ± 0.067	1.29 ± 0.080

In the above table, the MPI/Landcare dataset is now approximately 50% higher than the MfE numbers. During our initial model efforts, the inversion struggles to bring these numbers down to more appropriate values. However, once we use NZCSM, coupled with the data from Baring Head, we drastically change the results. We are able to produce realistic emission levels regardless of the *a priori* so long as the spatial distribution and relative intensities are consistent, which they are in this case.

At the regional scale, results using inflated, erroneous prior are largely replicated, with slightly higher values, reflected in the last row of the above table. For instance, Figure 29, shows the correct and inflated priors and the resulting retrievals using NZCSM. The inflated prior has only had a minor impact upon the results. The retrieval can successfully deal with varying magnitude priors, suggesting it will have great utility in understanding New Zealand's past, present and future emission inventories, when the land use is well characterised but the stock numbers or feed quality is not.

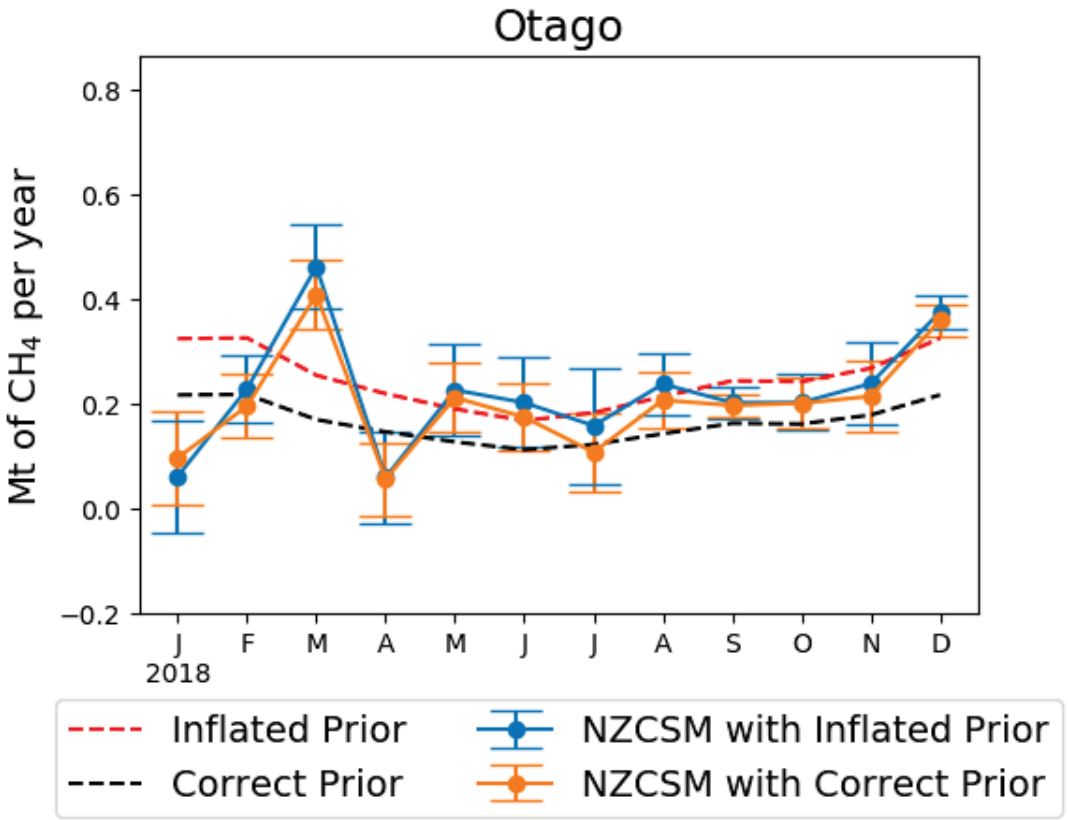

Figure 29: Comparison of the impact of the inflated prior and the correct prior upon the retrievals for Otago, 2018

5 Conclusions and outlook

Monthly regional methane inversions have been undertaken for 2011-2013. This preliminary case study showed promising results, particularly during the summer months, but was consistently hampered by large variations from month to month and region to region. It was identified that this was driven by gaps in the observations at Lauder, strong correlations between regions, and inaccurate wind fields.

Simulated inversions showed that with a complete time series, the information content would improve by approximately 50% over the 3-year time period. This highlights the need for a more robust dataset with multiple observations for redundancy. The impact of correlations can be dealt with by including additional measurement sites. This was also shown by the simulations with a strong increase in information content when using measurements at Baring Head as well as Lauder. Wind fields from NZLAM were shown to be significantly different than measured at Lauder and by comparing the resulting footprints to that from NZCSM (which showed far better agreement to reality), we have shown that there would be a significantly improved attribution of sources.

We applied these lessons to our 2018 time series using NZCSM as well as methane data from Baring Head, both not available for 2011-2013. The results showed a drastic improvement in accuracy and validity. The seasonal cycles, particularly for Otago, are generally reproduced, with far more consistency and accuracy. Otago and Canterbury achieved degrees of freedom over 6 in a single year, with an average uncertainty of 0.06 Mt/y (of CH_4) down from 0.11 Mt/y and 0.07 Mt/y from 0.11 Mt/y for Otago and Canterbury, respectively. The uncertainties for most other regions in the South Island as well as the southern North Island are also reduced to varying degrees.

In an additional trial, we successfully demonstrated that the retrieval is not too sensitive to the prior. The monthly emission maps used in this test were close to 50% higher than in reality. The resulting retrieval, when using Baring Head and NZCSM, was still able to simulate values that were close to those estimated by MfE for the South Island and North Island. At a regional level, the results were also consistent, further demonstrating the stability of the model. This suggests that, provided information on stocking density is reliable, we will be able to infer emissions even when historical and future emission factors are less well known.

To confirm this, we will need to perform further analysis on well understood years where we have the data from Baring Head to supplement those made at Lauder. By increasing our data set to multiple years, we will also be able to improve our quality control, allowing us to filter out days when the windspeeds and boundary layer are low. Looking ahead, with additional sites coming online, such as Winchmore in Canterbury, Manakau Heads (Auckland), and Maunga Kakaramea, we should be able to add further constraints to our regional emission estimates, particularly in the North Island where it is really needed.

A theme throughout has been the need for consistent data sets. While this has improved over time, there are still gaps in the time series. This can be remedied by increased funding so that more time is dedicated to each instrument and or additional instruments for redundancy. Another avenue that could be explored is satellite observations. Long methane time series such as that from GOSAT (Yokota et al., 2009) could be used in the inverse model in place of ground based modelling, such as in Turner et al., 2015. The temporal resolution of such data would be poorer, but its spatial coverage could be extremely useful in filling in the blanks, when surface measurements at our observing sites are not available or are observing an unusefull footprint. This would require a substantial amount of model development but has been shown to be useful in constraining regional to national emissions. With newer satellites such as Sentinel 5 Precursor and the upcoming MethaneSat, the potential for improvement in this area is vast.

To summarise, regional estimates of monthly methane emissions have been shown to be possible using NIWA's ground based network of measurement sites. There is significant room for improvement with the installation of additional sites and further quality control. Satellites could also be a useful adjunct to allow further analysis of historical emissions and to constrain emissions where ground based measurements are challenging.

6 Acknowledgements

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