

Uncertainty analysis – propagation of input climate data and soil uncertainties on nitrate-loss estimated by the Overseer science model

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Contents

Summary

Background

OverseerFM is a farm management decision tool that employs an agricultural science model to estimate 8 different nutrients loss and greenhouse gas emissions at both block and farm scale. Sensitivity and uncertainty analyses are necessary to provide information that aids in understanding the model's performance and estimates of N-loss in farming systems. An earlier targeted sensitivity analysis (Overseer Limited, 2022) identified key parameters impacting the N-loss output. The aim of the current study was to determine the uncertainty relating to the most sensitive parameters (rainfall, temperature, potential evapotranspiration (PET), profile available water (PAW)) for the three main farm systems in OverseerFM (dairy, beef and sheep, cropping) and to quantify the uncertainty in the N-loss estimates due to these key parameters.

Approach

In line with the sensitivity analysis, the uncertainty analysis was based on anonymised farm systems and conditions in Overseer (2175 in total). The parameter uncertainty represents the variability or dispersion of the values assigned to a parameter and is quantified by the standard deviation of the distribution of the assigned values. The uncertainty of the N-loss estimate(s) was quantified using the Monte Carlo technique to propagate the uncertainty of the rainfall, temperature, PET, and soil water holding capacity (from which PAW is calculated) parameters within the model by sampling the distributions of these input parameters to quantify the uncertainty for the N-loss estimate.

Findings

The combined uncertainty in the soil and climate input parameters resulted in an average relative uncertainty of 27±9% in the N-loss estimate across all the farm systems studied (dairy, beef and sheep, cropping). This value increased to $35\pm10\%$ at low values of N-loss (<10 kg N/ha/yr) and decreased to 15±5% at high values of N-loss (>100 kg N/ha/yr). Additional input parameters relating to management practices were estimated, based on their sensitivity indices in the absence of significant parameter interactions, to add an additional 1% uncertainty to the N-loss estimates. These calculated uncertainty values, and ranges, are comparable with other models in the field.

1. Introduction

To provide a better understanding of the N-loss estimates from the Overseer science model, it is important to understand the sensitivity of the model as well as the uncertainty in the model output, in relation to the uncertainty of key model inputs. A targeted sensitivity analysis was undertaken on the model that identified high model sensitivity to climate and soil water holding capacity input parameters common across dairy, beef and sheep and crop farms (Overseer Limited, 2022) i.e., parameters that significantly alter the N-loss estimate (kg N/ha/year) at the farm level when they are altered.

The aim of this study was to quantify the uncertainty of N-loss estimated by the Overseer science model (Overseer) at the farm level in relation to the uncertainty of the key climate and soil water holding capacity input parameters.

2. Propagation of the climatic data uncertainties

The model currently uses a long-term monthly average climate database at 500 m spatial resolution developed by NIWA for Overseer Limited (total monthly rainfall, total monthly PET, and monthly average temperature) covering the climate period 1991-2020. The climatic values are determined into a 500 m spatial resolution grid using a numerical model based on the 30-year statistics measured at climate station locations. This method is described in more detail in Wratt (2006). For the uncertainty analysis, NIWA provided long-term averages of climatic data alongside their standard deviations, which were then used to quantify the uncertainties of the climatic input parameters.

2.1 Climate input data uncertainties

The relative standard deviation (RSD), defined as the ratio of the standard deviation to the mean, was used to compare the uncertainties between different parameters whose values are variable. The RSD values for each annual climate input parameter are shown in Figure 1. On average, at the annual level, the RSD for annual rainfall was 16%, 6% for PET, and 5% for temperature.

The RSD values calculated with climate data averages and standard deviations provided by NIWA for each monthly climate parameter are presented in Appendix 1 (Figures 11-13). From these data, at the monthly level, the average RSD values were 55% for rainfall, 15% for PET and 12% for temperature.

The values of the climate standard deviations were based on the period 1991-2020 (current OverseerFM dataset). A comparison of the RSD values for monthly rainfall over a longer period is also presented in Appendix 2 (Figures 14 and 15). The RSD values for monthly rainfall show similar results over the different averaging periods, indicating that the 30-year period is an appropriate representation of average climate.

Figure 1: Map of relative standard deviation for annual rainfall (a), annual PET (b), and annual average temperature (c) with a 500 metres resolution. The median and the quartiles are indicated on each graph.

2.2 Method – propagating N-loss estimates uncertainty due to climate parameters

The current version of the model code (6.4.1) was used for the analyses.

By quantifying the averages and standard deviations of the climatic input data it is possible to view each climate input parameter as a random variable normally distributed as a first approximation. The central limit theorem (30 monthly measurements over the period 1991-2020) allows us to create reasonable statistical models of sample averages debased on a normal distribution (Stirzaker, 2023).

The effects of climate data uncertainties on the N-loss estimates were evaluated by random sampling of the probability distributions and then deriving frequency distributions of the N-loss estimate i.e., the uncertainty analysis quantifies the variability of the estimate of the N-loss estimate due to the uncertainty of the climatic input parameters.

The model uses a monthly scale for input climatic data. Accordingly, each month was treated independently and represented by a normal distribution, a mean, and a standard deviation.

Each normal monthly distribution with average values was independently randomly sampled (Monte Carlo method) and used as an input parameter to calculate the estimate of N-loss and the process was repeated 100 times. The resulting replications were then used to assess the variance of the N-

loss distribution. The mean and the standard deviation of the N-loss distribution were used thereafter to assess the average uncertainty in the output due to the input uncertainty. For example, Figure 2 illustrates the process when the rainfall distribution is randomly sampled 5000 times for a location. The standard deviation of this N-loss distribution gives an estimate of N-loss uncertainty due to the uncertainty on rainfall.

Figure 2: (a) Distribution of the annual sum of the sampled monthly rainfall values for 5000 samples. (b) Total N-loss distribution at farm level.

To maintain consistency, the uncertainty analysis was carried out on the same anonymised farms used for the sensitivity analyses (Overseer Limited, 2022)

2.3 Results – N-loss uncertainties due to climate parameters

For each farm setup, the standard deviation of the N-loss distribution is estimated when the corresponding climatic data distribution is sampled separately. The final estimate of the standard deviation of the N-loss distribution is obtained when all climatic distributions are sampled independently and in combination. In this instance, the climate parameters were treated as uncorrelated. This was because the correlation between these parameters was considered weak, based on the climate data processing approach (Tait 2022). As such, the long-term monthly mean values for each climate parameter were determined separately.

The uncertainty of N-loss was assessed by calculating the RSD of N-loss distributions of each farm obtained by sampling the different climate parameters separately or all together. The RSD was calculated by dividing the standard deviation by the mean of the N-loss distribution.

Figure 3 shows the RSD of the N-loss distribution versus the N-loss mean for each studied farm when the monthly total rainfall distributions are sampled across all farming types. In total, 3080 farms were analysed across dairy, beef and sheep, and crop farms. The N-loss RSD values were then sorted by the mean N-loss at the farm level and stratified into 5 groups comprised of an equal number of farms.

The mean and the standard deviation of the N-loss RSD values for each group are represented by the red crosses (Figure 3).

The uncertainties of the N-loss estimated by Overseer due to the rainfall uncertainties were comparable for all farming types, including crop farms, over the N-loss range studied, with an average uncertainty of 24%.

The mean uncertainty on the N-loss estimate due to rainfall was ≤ 20% when the N-loss was greater than 50 kg/ha/yr. Although not statistically significant, there was a trend towards lower uncertainty as N-loss estimates increased.

Figure 3: Relative standard deviation (RSD) of the N-loss distribution versus the N-loss mean for all farms when rainfall distributions are sampled. Red crosses represent the mean and standard deviation of the RSD when farms are stratified into 5 groups with an equal number of farms.

Figure 4 shows the RSD of the N-loss distribution versus the N-loss mean when the monthly total PET distributions are sampled across all farming types. The mean and the standard deviation of the N-loss RSD values when farms are stratified into 5 groups with an equal number of farms are also represented by red crosses. Figure 5 shows the same distributions when average monthly temperature distributions are sampled. In total 3080 farms were analysed.

The impact of the PET and temperature uncertainties contributed 5% and 4%, respectively, to the Nloss uncertainty. These uncertainty values were statistically comparable across the whole N-loss range and for the three farm types.

Figure 4: Relative standard deviation (RSD) of the N-loss distribution versus the N-loss mean for all farms when PET distributions are sampled. Each point represents a studied farm. Red crosses represent the mean and standard deviation of the RSD when farms are stratified into 5 groups with an equal number of farms.

Figure 5: Relative standard deviation (RSD) of the N-loss distribution versus the N-loss mean for all farms when temperature distributions are sampled. Each point represents a studied farm. Red crosses represent the mean and standard deviation of the RSD when farms are stratified into 5 groups with an equal number of farms.

Propagating the input climate data uncertainties on the modelled N-loss resulted in an average uncertainty of 24% for rainfall, 5% for PET and 4% for temperature. The uncertainties on N-loss based on the climate parameters are also summarised in Appendix 3. The mean of the RSD of the Nloss distributions showed some variation over the N-loss range e.g., rainfall (Figure 3) however, this was not statistically significant and therefore the RSD is represented as a constant.

The RSD of N-loss distributions due to uncertainties of all climatic data was determined by random sampling of all monthly climatic data distributions (Figure 6). Uncertainties for the averaged climatic data resulted in an uncertainty of 24±10% for the N-loss across the 3080 farms studied. Although some variations in uncertainty were observed with different levels of N-loss, these were not

statistically significant. The uncertainties on N-loss due to all climate parameters are also summarised in Appendix 3.

Figure 6: Relative standard deviation (RSD) of the N-loss distribution versus the N-loss mean for all farms when climatic data distributions are sampled. Each point represents a studied farm. Red crosses represent the mean and standard deviation of the RSD when farms are stratified into 5 groups with an equal number of farms.

The mean uncertainty at the farm level on N-loss due to climatic data was 24±10%. For N-loss greater than 50 kg/ha/year, the mean uncertainties of the N-loss due to the climatic data decreases to 20±6%.

It should be noted that the square root of the sum of the squares of the uncertainty for each climatic parameter is close to the observed value when the parameters vary together (Appendix 3). As such, the total contribution of the parameter interactions to the N-loss variance can be considered low. This finding is consistent with the observation of low interactions from the sensitivity analyses (Overseer Limited, 2022).

3. Propagation of the soil data uncertainties

OverseerFM uses S-map soil data, where it is available, to provide users with soil property information (Lilburne et al., 2012). S-map provides soil information on various areas across New Zealand. Soil information is provided as a map of areas containing one or more soils (siblings). A sibling is a member of a soil family. Further information about S-map and soil properties is available on the Manaaki Whenua Landcare (MWLC) website. Each sibling has a defined set of soil properties or parameters. As the output parameters of the S-map model are strongly correlated, MWLC provided 100 parameter sets ('realisations') per S-map sibling, giving a reasonable and statistically valid representation of the soil water holding capacity parameters distributions.

3.1 Soil information uncertainties

Previous sensitivity analysis identified that of the soils properties investigated, the soil water holding capacity, represented by the profile available water (PAW), was among the most influential parameters for N-loss. The water holding capacity is characterised by the wilting point (WP), field capacity (FC) and saturation point (SAT) at different depths: top (0-30 cm), middle (30-60 cm) and bottom (>60 cm). These soil parameters are the results of mathematical modelling and were determined with uncertainties based on the variability in the inputs to the soil hydraulic model, model uncertainty, and variability of the other key soil properties (stone content, thickness) as described in Lilburne et al., (2016). In total, Landcare provided 100 soil properties realisations for 1752 S-map siblings. Figure 7 presents the maps of the RSD for the water holding capacity parameters provided for each S-map sibling.

The RSD of each soil water capacity parameter is \sim 15%, with an increase at low capacity (<10 mm) for certain S-map siblings.

Figure 7: Relative standard deviations (RSD) for each water holding capacity parameter: wilting point (WP), field capacity (FC) and saturation point (SAT) at the top, middle and bottom layers versus the parameter distribution average.

The PAW to 60 cm depth is defined as:

$$
PAW = 3 * ((FC_{top} - WP_{top}) + (FC_{middle} - WP_{middle}))
$$

The RSD of the PAW distributions plotted against the average PAW values are presented in Figure 8. On average, the relative uncertainty for the PAW value was 15±4%.

Figure 8: Relative standard deviation (RSD) on the PAW value versus PAW to 60 cm depth.

To maintain consistency, the uncertainty analysis for N-loss was carried out as the same farm datasets used for the sensitivity analyses (Overseer Limited, 2022) excluding farms that did not use S-map to provide the block soil information. In total, 2175 farms out of 3080 were included in the uncertainty analysis.

3.2 Results – N-loss uncertainties due to soil parameters

The uncertainties on the N-loss due to the uncertainties of the soil properties were estimated by sampling the 100 realisations for each sibling at the block level of each farm.

Figure 9 shows the RSD of the N-loss distribution versus the N-loss mean when the soil properties were sampled across all farms. The RSD values were sorted by the mean N-loss at the farm level and stratified into five groups with an equal number of farms. The uncertainties of soil water holding capacity introduced an average uncertainty of N-loss of 11±4% for the farms studied. The uncertainties on N-loss due to the water holding capacity are summarised in Appendix 3.

The effect of the soil water properties uncertainties on the N-loss at the farm level was also found to be similar across all three types of farming.

Figure 9: Relative standard deviations (RSD) of the N-loss distribution versus the N-loss mean for all farms when water holding capacity distributions are sampled. Each point represents a studied farm. Red crosses represent the mean and standard deviation of the RSD when farms are stratified into five groups with an equal number of farms.

4. Propagation of the climate and soil data uncertainties

4.1 N-loss uncertainties due to soil and climate parameters

The uncertainties of the N-loss estimate due to the combined effect of the climate and soil information uncertainties were determined by sampling both the climate and soil information distributions for the 2175 farms with S-map data.

The standard deviation of the N-loss distribution for soil and climate combined was quantified by sampling different climatic data distributions and soil realisations in combination with 100 replications per farm. The RSD, which quantifies the N-loss uncertainty, was then determined by dividing the standard deviation by the mean of the N-loss distribution for each farm. Figure 10 shows the RSD versus the N-loss mean across all farm types. The mean and the standard deviation of the N-loss RSD values when farms were stratified into 5 groups with an equal number of farms are represented by red crosses.

Figure 10: Relative standard deviation (RSD) of the N-loss distribution versus the N-loss mean for all farms when climate and soil parameters are sampled. Red crosses represent the mean and the standard deviation of the RSD when farms are stratified into 5 groups with an equal number of farms.

The combined uncertainties of the soils and climate data resulted in an average uncertainty of N-loss of 27±9% across all farming systems. A small difference in the average uncertainty between dairy $(25±8\%$ on average) and beef and sheep $(29±9\%)$ farms was observed but was not statistically significant. There was a trend towards lower uncertainty for higher N-loss estimates (Figure 10, Table 1) however, this was not statistically significant. As such, the uncertainty results for N-loss were statistically equivalent across different types of farming.

The average and the standard deviation of the N-loss uncertainty calculated for different N-loss thresholds are shown in Table 1. For N-loss values less than 10 kg N/ha, the average relative uncertainty reaches 35% with a significant variability (±15%). This can be explained by the fact that Overseer is a threshold model. This means the model predicts no effect below a critical value based on a set of thresholds, while significant effects exist above this value. This effect leads to significant variability near the threshold values, i.e., at low N-loss values in the case of Overseer. In contrast, for N-loss above 100 kg N/ha/yr, the average uncertainty on the N-loss estimated by Overseer was 15±5%. The general trend is a decrease in N-loss uncertainty with increasing N-loss estimates (Table 1). This observation is similar for the variability (standard deviation) translating as higher confidence with higher estimates of N-loss.

Table 1: Cumulative uncertainties of the relative N-loss uncertainties due to soil and climate data uncertainties with the N-loss at farm level.

4.2 Soil and climate interactions

Table 2 summarises the average uncertainties due to climate and soil input data uncertainties, separately and in combination, across different ranges of N-loss for all farm types (represented in Figure 6, Figure 9, Figure 10 by the red crosses). Although there was trend towards a decrease in Nloss uncertainty with increasing N-loss estimates, it was not statistically significant.

It is worth noting that the square root of the sum of the squares of the uncertainty for each type of parameters (Table 2, column E) is in good quantitative agreement with the observed value when the parameters are sampled together (Table 2, column D). This means that the uncertainty of N-loss due to uncertainties in climate and soil data can be considered independent in a first approximation. This observation demonstrates that the interactions between these variables are weak compared to the direct effects of each parameter, consistent with the results of the sensitivity analyses (Overseer Limited, 2022).

Table 2: Summary of the average values of uncertainties due to the uncertainties of climate information and soil.

5. Total N-loss uncertainty

The 10 most influential parameters on the N-loss identified by the earlier local sensitivity analysis (Overseer Limited, 2022) are presented in Table 3. The calculated uncertainties for N-loss due to the climate and soil parameters, separately and combined, are presented in bold.

The global sensitivity analysis on the 10 highest impact parameters identified from the local sensitivity analysis showed that the input parameters studied were uncorrelated (Overseer Limited, 2022). As such, it is possible to estimate the uncertainties on the value of N-loss due to given input parameters, based on their sensitivity indices. Under these conditions, the total variance of N-loss at the farm level can be calculated as the sum of the weighted variances of the input parameters (Stirzaker, 2003). Table 3 shows comparable values for the calculated and estimated N-loss uncertainties due to climatic and soil data, separately and combined (estimated combined uncertainty 24±6% versus calculated 27±9%). This indicates that the estimated uncertainty can be used with some confidence to predict uncertainties relating to the remaining parameters, for specific input uncertainties that were not available at the time of this study.

*Table 3: Top 10 of the most influential parameters with their calculated or estimated uncertainties. *The parameters' annual uncertainties were estimated and propagated using their sensitivity index from the sensitivity analysis.*

Using the sensitivity indices to estimate the combined uncertainty for N-loss due to all 10 parameters indicates that the predominant source of uncertainty was the 4 most influential climate and soil input parameters. The remaining 6 parameters were estimated to contribute approximately 1% uncertainty to the N-loss. The annual uncertainties for the remaining key paramaters (*) represent hypothetical values to be investigated further as part of ongoing sensitivity and uncertainty analyses, once specific annual uncertainty values are available.

6. Summary

- The combination of the soil and climate data uncertainties results in an average uncertainty on the N-loss estimated by Overseer of 27±9% across the farm systems analysed. There was a trend towards lower uncertainty for higher N-loss estimates with uncertainty ranging from 35±10% (<10 kg N/ha/yr), 25±7% (>40 kg N/ha/yr), 15%±5% (>100 kg N/ha/year).
- The patterns were consistent across the three types of farming investigated and the uncertainty distributions were all statistically comparable.
- The uncertainty relating to the N-loss estimate from the Overseer model $(27±9%$ calculated. 24±6% estimated), sits within the common range of uncertainties for this type of environmental modelling (Table 4).
- In the absence of significant parameter interactions, it is possible to use the sensitivity index to predict the contribution of a parameter's uncertainty to the uncertainty in the N-loss estimate. In this context climate and soil contribute the majority of uncertainty for N-loss, whereas the uncertainty with respect to the remaining parameters is minimal (~1%). This provides a certain degree of confidence in the changes in the N-loss estimate when those input parameters relating to management (e.g., fertiliser) are altered.
- Further work to test the potential to apply the proxy determination of uncertainty in instances where input uncertainty data is unavailable, and interactions are minimal, is warranted.

Table 4: Uncertainty for different environmental variables.

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9. Appendices

Appendix 1

Monthly relative standard deviations for individual climatic parameters.

Figure 11: Map of the relative standard deviation (%) for rainfall data per month on New Zealand grid 500x500 m. The average for each month is indicated in the graph.

Figure 12: Map of the relative standard deviation (%) for PET data per month on New Zealand grid 500x500 m. The average for each month is indicated in the graph.

Figure 13: Map of the relative standard deviation (%) for temperature data per month on New Zealand grid 500x500 m. The average for each month is indicated in the graph.

Appendix 2

Evolution of the climatic data standard deviations

The next graphs represent the map of the relative standard deviations of the monthly rainfall from different averaging periods. The standard deviations are constant across the two periods 1961-2020 and 1991-2020 and suggests that a period of 30 years is adequate to define an average climate.

Figure 14: Map of the rainfall per month relative standard deviation calculated over the period 1991- 2020.

Figure 15: Map of the rainfall per month relative standard deviation calculated over the period 1961-2020.

Appendix 3

N-loss uncertainty summary for the different types of farming systems

Average and standard deviation of the relative uncertainty on N-loss estimated by Overseer for the different types of farming systems and the different climate and soil water content parameters.

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