



# HOKKAIDO UNIVERSITY

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**Modeling soil CO<sub>2</sub> and N<sub>2</sub>O emissions and estimating carbon  
budget in agro-ecosystem at regional scale**

(土壌からの CO<sub>2</sub> および N<sub>2</sub>O 排出モデルの構築と地域レベル  
での農業生態系炭素収支の見積もり)

Hokkaido University      Graduate School of Agriculture  
Division of Environment Resources      Doctor Course

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## **List of Abbreviations**

|                  |                                   |
|------------------|-----------------------------------|
| C                | Carbon                            |
| N                | Nitrogen                          |
| SOC              | Soil organic carbon               |
| SOMD             | Soil organic matter decomposition |
| WFPS             | Water filled pore space           |
| HB               | Hierarchical Bayesian             |
| CO <sub>2</sub>  | Carbon dioxide                    |
| N <sub>2</sub> O | Nitrous oxide                     |
| NO               | Nitrogen monoxide                 |
| CH <sub>4</sub>  | Methane                           |
| GHG              | Greenhouse gas                    |
| CE               | Carbon sequestration efficiency   |
| NBP              | Net biome productivity            |
| NPP              | Net primary productivity          |
| Rh               | Heterotrophic respiration         |

# 1. General introduction

Global climate change is becoming a hot issue in contemporary sciences as well as politics. A scientific consensus is forming that the emissions of greenhouse gases (GHGs), including carbon dioxide (CO<sub>2</sub>), nitrous oxide (N<sub>2</sub>O) and methane (CH<sub>4</sub>), from anthropogenic activities may play a key role in elevating the global temperatures. The carbon (C) balance in terrestrial ecosystems has large implications on the variation in atmospheric CO<sub>2</sub> emission. Agriculture profoundly affects global C, water and nutrient cycles, as well as the planetary surface energy balance ([Bondeau et al., 2007](#)). Soils are the main source of N<sub>2</sub>O emission and nitrogen monoxide (NO) emissions via microbial processes of nitrification and denitrification ([Wrage et al., 2001](#)). N<sub>2</sub>O emissions currently increasing at a rate of 0.2–0.3% per year at agricultural field due to greater use of nitrogen (N) fertilizers which have enhanced these two processes ([Abdalla et al., 2010](#)). Quantifying soil GHGs emissions is an essential task for understanding the atmospheric impacts of anthropogenic activities in terrestrial agro-ecosystems.

CO<sub>2</sub> is released mainly from microbial decay or burning of plant litter and soil organic matter (SOM), which showed less spatial-temporal variable than N<sub>2</sub>O emission ([Wang and Chen, 2012](#)). N<sub>2</sub>O is primarily produced by the microbially-mediated nitrification and denitrification processes in soils ([Davidson et al., 1991](#)). Modeling is a useful tool for tracing detailed processes, estimating regional GHGs fluxes, and also predicting changes in the fluxes that will be caused by climate change ([Del Grosso et al., 2005](#)). In general, these estimations have been performed using detailed process-based models ([Potter et al., 1996](#)) or simple data-oriented models ([Bond-Lamberty and Thomson, 2010](#)), and these two approaches compensate

for the disadvantages of each. The process-models are developed for tracing detailed processes. Whereas simpler models cannot trace such detailed processes, they are essential for incorporation into other models and require fewer inputs and are easier to handle (e.g., a simple model by [Hashimoto et al., 2011](#)).

Soil GHGs are influenced by a suite of climate and soil variables, interacting soil and plant N transformations (either competing or supplying substrates) as well as land management practices ([Li et al., 2007](#)). Computer simulation models, which can integrate all of these variables, are required for the complex task of providing quantitative determinations of N<sub>2</sub>O emissions. Numerous process-based models have been developed to predict CO<sub>2</sub> and N<sub>2</sub>O production ([Chen et al., 2008](#)), such as, NEMIS ([Hénault et al., 2005](#)), CERES-EGC ([Gabrielle et al., 2006a](#)) and DNDC ([Li et al., 2005](#)), however, they often require a large amount of input data that is not available at regional scale, which making regional and global emission estimates difficult to achieve ([Bell et al., 2012](#)). ECOSSE is a process-based model designed to simulate soil C and N stocks and gaseous emissions from using only data which is commonly available at a regional scale ([Bell et al., 2012](#)). Another limitation to the wide-spread use of these models lies in the fact that their predictions are highly dependent on parameter settings, and carry a large uncertainty due to uncertainties in parameter values, driving variables and model structure ([Gabrielle et al., 2006a](#)). Even though model parameterization and uncertainty analysis are widely developed in the literature on agro-ecosystem models, they are rarely considered simultaneously ([Monod et al., 2006](#); [Makowski et al., 2006](#)).

The advantage of Bayesian statistics is that it can simultaneously take into account the uncertainty analysis and parameterization through calibrating unknown model parameters in terms of probability density functions (pdfs) with 95% confidence interval (CI) ([Gallagher and Doherty, 2007](#); [Gabrielle et al., 2006a](#); [Xu et al., 2006](#)); and also it can reduce the uncertainty associated with the parameters ([Yeluripati et al.,](#)

2009). Different from nonhierarchical Bayesian model, the hierarchical model represents a modeling structure with capacity to exploit diverse sources of information, and yields subunit-specific parameter estimates, but shares commonality in values across systems. The nonhierarchical Bayesian model assumes that there is a “true” parameter value that is incrementally approached with increasing sample size. However, Hierarchical Bayesian (HB) assumes that parameter has distribution of its own; therefore hierarchical model assigns two hyper parameters to yield the posterior distribution of each subunit-specific parameter. It be beneficial to identify such “hyper parameters” to explain variability of parameter. Thus, HB models have been developed in recent years for a number of environmental applications (Borsuk et al., 2001; Agarwal et al., 2005; Cable et al., 2009; Patrick et al., 2009). In general, the current challenge is how to scale up the relatively more robust field-scale model to catchment, regional and national scales, meanwhile, the uncertainty analysis and parameterization should be taken into account simultaneously.

Assessment of soil C stock changes over time is typically based on application of two methods, namely (i) repeated soil inventory and (ii) determination of the net biome productivity (NBP) by continuous measurement of CO<sub>2</sub> exchange in combination with quantification of other C imports and exports (Leifeld et al., 2011). However, soil C inventory has some limitation, such as not providing an annual C budget, not necessarily taking into account dead organic matter C, and placing limitations on extrapolation due to high spatial variability. The NBP is the term applied to the total rate of organic C accumulation (or loss) from ecosystems (Chapin III et al., 2006; Schulze and Heimann, 1998; Buchmann and Schulze, 1999). The main advantages of using NBP to calculate C budget arise from their: (i) spatial explicitness, (ii) flexibility over a range of crops, (iii) reflection of local varieties and field management practices used in the study area and (iv) allowing a simple estimation of annual plant C inputs.

In principal, an indication for the uncertainty in NBP should be provided and thus a direct quantitative evaluation of methods is available. Meanwhile, the NBP value for an agricultural system should be directly comparable with the C stock change measured by repeated sampling of soil, but up to now, there has been few field study that directly compared the two approaches at an agricultural system at the regional scale.

The specific objectives are:

1. To design and produce the model to simulate CO<sub>2</sub> from soils (CO<sub>2</sub>-HB) based on simple model theory using soil temperature, soil water and soil information and to quantify uncertainty by developing a suitable calibration method, and to up-scale the CO<sub>2</sub>-HB model at regional scale and incorporate it into other model as sub-model.
2. To design and produce the model to simulate N<sub>2</sub>O and NO emissions from soils (N-HB model) and to quantify the uncertainty of model simulations by developing a suitable calibration method, and to investigate the model extrapolation and the parameters' variability using soil information.
3. To explore trends and interannual variability of NBP at regional scale, focusing on the spatial and temporal patterns of NPP, crop residue inputs at main land use: upland, paddy and grass from 1959 to 2011 by using relationship-based estimation of plant C inputs and CO<sub>2</sub>-HB modeling, and to verify the C stocks change at main land uses from 2005 to 2011 by comparing two methods: (i) repeated soil inventory and (ii) C flux budget (NBP).

There are a total of 8 chapters in this thesis. This introduction (Chapter 1) is followed by a literature review (Chapter 2), where studies on simulating the greenhouse gases (GHGs) emissions in agricultural soils and the agro-ecosystem global warming potential and net biome productivity (NBP) during the last century are reviewed. Chapter 3 describes a general introduction of Ikushubetsu watershed,

introduction of monitoring data of GHG gas, introduction and application of Bayesian method to the monitoring data, and application of CO<sub>2</sub>-HB model to estimate C change at regional scale. Chapter 4 presents modeling soil CO<sub>2</sub> flux from cropland using soil texture (CO<sub>2</sub>-HB model). Chapter 5 presents modeling soil N<sub>2</sub>O and NO fluxes from cropland (N-HB model). Based on the estimation done in Chapter 4 and Chapter 5, applying CO<sub>2</sub>-HB model to estimate the NBP at regional scale during the last four decades was presented in Chapter 6. Finally, all results are discussed in general and together with outline of further research needs in Chapter 7.

## **2. Literature Review**

### **2.1 Greenhouse gas (GHG) emissions in agricultural soils**

Agricultural lands occupy 37% of the earth's land surface. Agriculture accounts for 52% and 84% of global anthropogenic CH<sub>4</sub> and N<sub>2</sub>O emissions ([Smith et al., 2007b](#)). Agricultural soils may also act as a sink or source for CO<sub>2</sub>. Agriculture releases to the atmosphere significant amounts of CO<sub>2</sub>, CH<sub>4</sub> and N<sub>2</sub>O ([Cole et al., 1997](#); [Haines, 2003](#); [Paustian et al., 2004](#)). CO<sub>2</sub> is released largely from microbial decay or burning of plant litter and soil organic matter ([Janzen, 2004](#); [Smith et al., 2004](#)). CH<sub>4</sub> is produced when organic materials decompose in oxygen-deprived conditions, notably from fermentative digestion by ruminant livestock, stored manures and rice grown under flooded conditions ([Mosier et al., 1998](#)). N<sub>2</sub>O is generated by the microbial transformation of N in soils and manures, and is often enhanced where available N exceeds plant requirements, especially under wet conditions ([Smith and Conen, 2004](#); [Oenema et al., 2005](#)).

#### **2.1.1 Mechanism of carbon and nitrogen dynamics in upland agricultural soils**

Upland soils constitute the majority of soils in agricultural areas throughout the world. Because these soils tend to be better aerated than wetland soils, oxygen presence plays a key role in the process dynamics and management responses of these systems, and generally promotes higher decomposition rates of organic materials compared to wetland soils. Periodic wet and dry cycles on a seasonal or more frequent basis cause temporary shifts in oxygen (O<sub>2</sub>) availability that in turn affect process rates and directions. The landscape position of agriculture upland soils promotes drainage and movement of nutrients and soil particles to lower lying areas, and aspect

exposure can have significant effects on temperature and water retention regimes. Location of the soils on the Earth relative to latitude and elevation also plays an important role in the accumulation of soil organic matter (SOM) and associated C/N dynamics ([Povirk et al., 2000](#)). Particularly in far, upland soils have experienced dramatic changes since the introduction of agriculture ([Dregne, 1982](#)). Losses of SOM in the surface horizons from erosion and accelerated decomposition rates have been pronounced worldwide, and continue to occur especially in areas converted from the native condition within the past 50 to 100 years ([Miller et al., 1985](#)).

### **2.1.2 Carbon cycling in upland agricultural soils**

Organic C in upland soil occurs as SOM, dead and living plant material (tops and roots), micro-flora biomass (dead and living), and soil micro-, and macro-fauna (dead and living). Fractionation of C into various designated pools for purposes of analysis by empirical methods and simulation modeling has been attempted for many years. C pools used in the simulation models are mostly conceptual ([Ma and Shaffer, 2001](#); [McGechan et al., 2001](#)) and are only approximately correlated with the physical/chemical/biomass pools described above. Soil organic C (SOC) in soils is a continuous (time and space) product of microbial processes, and fractionation into pools probably should be entirely microbial based. In general, the physical C pools are described based on size and include litter or easily recognizable residues (>2 mm in size), a light fraction that can be floated off using dense liquids (0.25 to 2 mm in size), and particulate organic matter that is separated using dispersion and physical separation techniques (0.05 to 2 mm in size) ([Jenkinson et al., 1991](#)). Soil microbial biomass C is determined using the chloroform fumigation-incubation (CFI) method ([Jenkinson et al., 1991](#)); and more resistant forms of SOM, including humic acid, fulvic acid, and humin, are fractionated using chemical techniques such as the HCl and NaOH methods ([Ping et al., 2001](#)). As an approximation, most model-based pools

can be compared to the physical/chemical/microbial pools as follows. The fast SOM model pools are similar to the light and/ or particulate pools, the microbial biomass pools are similar to each other, and the slow SOM model pool is similar to the resistant SOM pool. In some cases, the slow residue model pool may be similar to the light SOM pool. The model pools are highly dynamic and initialization depends on the design of the model, the rate coefficients, and the relationships of model C/N components to other parts of the model.

The relative contributions of above- and below-ground higher plant parts to SOC vary depending on the ecosystem involved. Agricultural system receives the majority of its SOC from above-ground plant parts, while grassland and tundra systems receive SOM primarily from root decay ([Povirk et al., 2000](#)). [Sobecki et al. \(2001\)](#) present a comparison of standing organic C residues for various ecosystems such as forests, grasslands, tundra/desert, and croplands. Forests have the most above- and below-ground biomass C, with  $177 \text{ Mg C ha}^{-1}$ , followed by grasslands with  $19.8 \text{ Mg C ha}^{-1}$ , croplands with  $16.4 \text{ Mg C ha}^{-1}$ , and tundra/desert with  $4.2 \text{ Mg C ha}^{-1}$ . Living microorganisms mediate the vast majority of the C/N cycling processes in soils, although these organisms constitute only about 0.3 to 5% of the SOM C. Microbial activity in soils is highly dependent on the presence of C substrates, which is why most activity and associated microbial biomass occurs near the soil surface and immediately after introduction of residues.

Soil inorganic C in the form of  $\text{CO}_2$ , bicarbonate, and carbonic acid, and soil and rock carbonates constitute most of the remaining C ([Monger and Martinez-Rios, 2000](#)). Given a long enough time period, C cycles among all of these pools. Cycling times vary from a few hours for  $\text{CO}_2$  and plant materials, to a few weeks for plant material and fresh SOM, to several decades for labile SOM, to thousands of years for stable SOM, and to millions of years for carbonate rocks. Of most concern to agricultural manager and modelers is SOM with short turnover times up to several

decades. This material supplies nutrients to the crops and can be managed and replaced, while the older material needs to be protected but is less easily managed. Cycling of C is closely tied to cycles involving other soil nutrients, such as N, phosphorus, sulfur, potassium, and trace constituents (McGill and Cole, 1981).

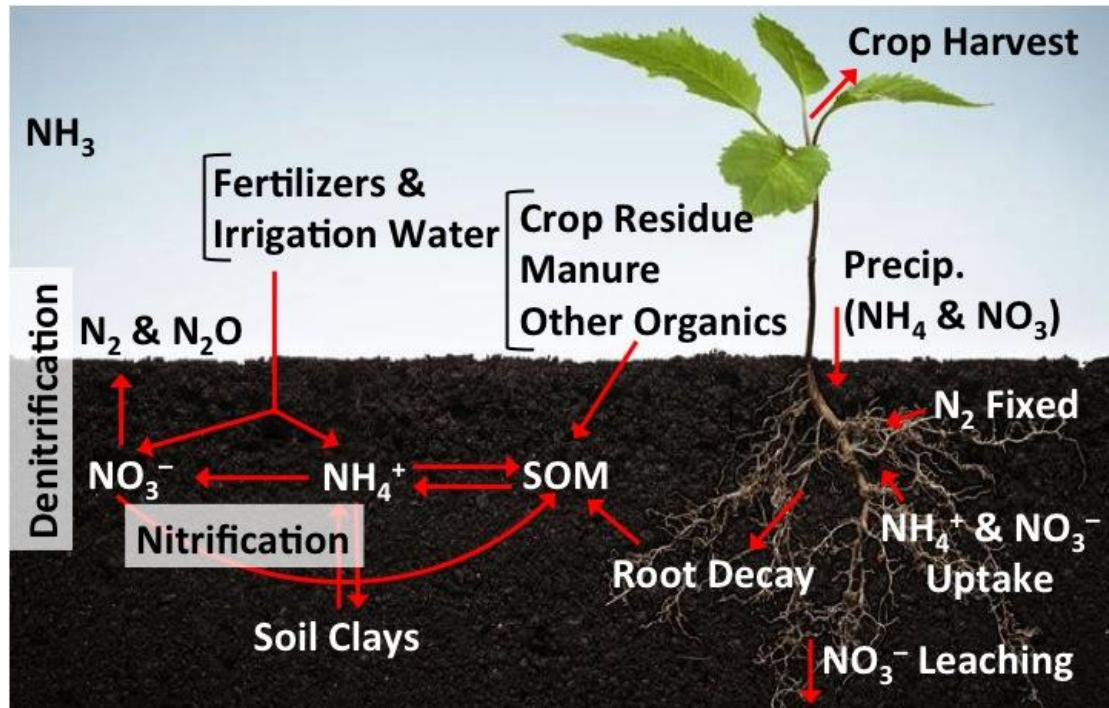
Upland agricultural soils have been studied extensively over the years under a range of management and climate regimes. For example, long-term plots such as the High Plains Agricultural Laboratory site at Sidney, Nebraska (Lyon et al., 1996), and the Morrow Plots at Urbana, Illinois (Darmody and Peck, 1996), provide evidence of the effects of long-term agricultural management on soil C, fertility, and crop productivity. The decrease in soil C in these plots relative to the native state is quite evident and ranges from 40 to 80%. Disturbances resulting from cultivation (biological oxidation), removal of crop residues, and soil erosion are factor in these losses (Darmody and Peck, 1996). In the case of biological oxidation, disturbance of the soil from tillage has been shown to release significant amounts of CO<sub>2</sub> gas (Reicosky et al., 1995). Buyanovsky et al. (1996) have demonstrated that decomposition of crop residues such as corn, wheat, and soybean returned to the soil makes only a minimal contribution to the more stable (long-term) soil C pool. Most of the C cycling from crop residues takes place in the faster, less stable pools. However, the return of crop residues to the land, rather than removal, has produced significant increase in organic C levels (Buyanovsky et al., 1996).

The introduction of reduced tillage and no-till has had significant impacts on C/N cycling. This is due primarily to decreased mixing of residues in the plow layer and a decrease in aeration plus an increase in soil water content. Soil organic C levels are significantly higher under no-till, especially near the surface (Peterson and Westfall, 1996).

### 2.1.3 Nitrogen cycling in upland agricultural soils

Considerable work has been published over the past several decades on C/N dynamics in soils ([Campbell et al., 1995](#); [Nakane et al., 1997](#); [Janzen et al., 1997](#)). The N and C cycles are closely linked and cannot be effectively studied or modeled separately ([McGill and Cole, 1981](#)). This is especially true with upland agricultural soils where good aeration coupled with periodic wet-dry and temperature cycles direct the microbial and plant biological processes and significantly influences the physical processes. In fact, most models simulate N cycling from C cycling. N cycle occurs along with C in all of crop residue and SOM pools and also occurs as inorganic  $\text{NO}_3^-$  and  $\text{NH}_4^+$ , urea, and as  $\text{N}_2$ ,  $\text{N}_2\text{O}$ ,  $\text{NO}_x$ , and  $\text{NH}_3$  gases. The relative amounts of N found in the soil generally are  $\text{SOM-N} > \text{residue-N} > \text{NH}_4^+\text{-N} > \text{gaseous-N}$  forms. From the standpoints of mobility and negative effects on the environment,  $\text{NO}_3^-$ -N and the gaseous-N forms ( $\text{N}_2\text{O}$ ,  $\text{NO}_x$ , and  $\text{NH}_3$ ) are of most concern.

The N cycle in upland soils is shown in [Figure 2.1](#). N enters the soil symbiotic plants (e.g., legumes) fix N, from animal manures, and from the addition of commercial fertilizer and other organic materials such as sewage sludges and compost. Soil losses of N include removal in crops, nitrate ( $\text{NO}_3^-$ ) leaching, denitrification and gaseous losses as  $\text{NH}_3$ , and losses in surface runoff and erosion ([Römkens et al., 1973](#)). The relative N loss amounts are highly variable and any of these major loss components can dominate given the right conditions. These may occur rapidly and major soil N changes can occur within a few hours or days ([Shaffer et al., 1994](#)).



**Figure 2. 1** The nitrogen cycle in soils.

Figure 2.1 also depicts N cycling or turnover within the soil where, under aerobic conditions, the microbial processes of mineralization (or ammonification) decompose residues and SOM to  $\text{NH}_4^+$  and more stable forms of SOM.  $\text{CO}_2$  is the primary by-product, although temporary or localized anaerobic conditions in upland soils can also result in ammonification with the by-product  $\text{CH}_4$  being produced instead of  $\text{CO}_2$ .

The heterotrophic microorganisms (primarily soil fungi along with lesser biomass quantities for bacteria and actinomyces) utilize C and N from the decomposing residues and N from the soil  $\text{NO}_3^-$  and  $\text{NH}_4^+$  pools to produce microbial biomass. This biomass generally ranges from about 250 to 900 kg C ha<sup>-1</sup> for a range of agricultural soils (Doran, 1987). Rangeland biomass levels in the top 30 cm range from 65 g m<sup>-2</sup> to 635 g m<sup>-2</sup>, depending on the type of prairie ecosystem (Reeder et al., 2000). With C-rich residues such as wheat and barley straw C/N is higher than 80, insufficient N is

available in the residues to supply the demand of the biomass growth ( $C/N=6$ ), resulting in temporary net uptake or immobilization of mineral soil  $NO_3^-$  and  $NH_4^+$ .  $NH_4^+$  then released from microbial biomass when the microbes die. However, crops will not have access to this N source while it is immobilized. In general, decay of residues with C/N ratios greater than about 25 or 30 will cause temporary net immobilization, while lower C/N ratios result in net mineralization. Systems decomposing residues with C/N ratios greater than 30 may become deficient in mineral N and become self-limiting in their ability to decompose these residues. Soil temperature and moisture content are important state variables in the mineralization process and control the microbial rates of growth and death ([Melillo et al., 1989](#)).

N has the capacity to cycle fairly rapidly between the inorganic and organic forms within the soil and a few weeks can see the complete turnover of some inorganic/organic N forms. Conversely, some forms of organic N, such as soil humus, may be very stable and have an age of several thousand years. Studies to identify the relative ages for SOM pools have been performed using C isotope ratios ([Follett et al., 2015](#)).

Conversion of  $NH_4^+$  to  $NO_3^-$  is called nitrification and is mediated by specific genera of aerobic autotrophic microorganisms, namely *Nitrosomonas* and *Nitrobacter* ([Alexander, 1977](#)). These organisms use  $CO_2$  as a C source, with *Nitrosomonas* oxidizing  $NH_4^+$  to nitrite ( $NO_2^-$ ) and *Nitrobacter* converting  $NO_2^-$  to  $NO_3^-$ . Nitrification state variables in upland soil include temperature and water content with a strong dependency on pH. Nitrification rates in uplands soils are generally medium relative to other C/N cycling processes, and 2 to 4 weeks are usually needed in the warmer months to nitrify and application of commercial ammonia-based fertilizer. The nitrification process is not 100% efficient and some conversion of  $NO_3^-$  to  $N_2O$  and  $NO_x$  greenhouse gases can occur ([Xu et al., 1998](#)). Nitrification is sensitive to soil pH, with significant reduction in process rates below pH 6.0 and above pH 8.0.

Nitrification inhibitors such as nitrapyrin have been developed that slow the process by enzyme inhibition of *Nitrosomonas* (Peoples et al., 1995).

Denitrification involves the conversion of  $\text{NO}_3^-$  and  $\text{NO}_2$  to  $\text{N}_2$ ,  $\text{N}_2\text{O}$  and  $\text{NO}_x$ . The process is mediated primarily by facultative anaerobic bacteria that oxidize organic C and reduces N oxides in the absence of  $\text{O}_2$ . The key to understanding and simulating denitrification in upland agricultural soils is the transient and localized nature of the anaerobic conditions. Complete reduction of N oxides to  $\text{N}_2$  is an anaerobic process, while partial or transient anaerobiosis results in the production of  $\text{N}_2\text{O}$  and  $\text{NO}_x$ . Denitrification tends to be a very rapid pulse process with major losses of soil N possible in a single day given the right conditions (Xu et al., 1998). Ideal pulse conditions involve the occurrence of significant amounts of soil  $\text{NO}_3^-$ , a fresh C source such as manure or other residue SOM, warm temperature, a precipitation or irrigation event, or temporary flooding (Tiedje, 1988). These conditions are common in the early spring or summer in upland soils and apply to production of the greenhouse gases and  $\text{N}_2$  (Tiedje, 1988).

Gaseous loss of  $\text{NH}_3$  from upland agricultural soils is primarily a soil surface process. In addition, it is one of the few soil N processes that is abiotic and not directly mediated by microorganism, although they play a key role in  $\text{NH}_4^+$  production.  $\text{NH}_3$  gas exists in chemical equilibrium with the  $\text{NH}_4^+$  ion in soil water, and the reaction is highly dependent on soil pH. Applications of ammonia fertilizer and manure to the soil surface set the stage for major N losses as  $\text{NH}_3$  volatilization. The process is enhanced by high pH levels (>8.5) and by wind and high temperatures (Smith et al., 1996). Incorporation of fertilizers and manure into the soil can significantly reduce or eliminate  $\text{NH}_3$  volatilization.

Nitrate leaching below the crop root zone of upland soils is a primary mechanism for N loss from these soils and contributes to pollution of underlying shallow aquifers. Nitrate leaching amounts from upland soils vary greatly, but values from less than 25

to greater than  $300 \text{ kg ha}^{-1} \text{ yr}^{-1}$  are common depending on management, soil and climate. Leaching of  $\text{NO}_3^-$  is a pulse process keyed to precipitation and irrigation events, but tied closely to previous N and water management, crop N uptake, and soil texture (Shaffer et al., 1994).  $\text{NO}_3^-$  is highly soluble in water and move quickly along with the water transport because they are not usually adsorbed by soil particles. Once leached below the root zone, recovery or reduction of  $\text{NO}_3^-$  is difficult and further downward movement over time can result in contamination of the ground water (Shaffer et al., 1995). Application of a  $\text{NO}_3^-$  leaching index for annual mass of  $\text{NO}_3^-$  leached below the crop root zone can be used to help identify potential “hotspot” regions in aquifers (Shaffer et al., 1995). Leaching of  $\text{NO}_3^-$  can be controlled by applying fertilizers and manure in smaller increments as needed by the crop to reduce the potential leaching risk from precipitation and irrigation, and by managing water applications where appropriate to reduce leaching (Shaffer et al., 1994; Follett et al., 2015). Other mitigation techniques such as planting deep-rooted cover crops can be beneficial.

Plant uptake of  $\text{NO}_3^-$  and  $\text{NH}_4^+$  represents an important sink process in the N cycle and proper accounting is essential for simulation of C/N cycling and  $\text{NO}_3^-$  leaching in soils (Follett et al., 2015). For agricultural crops on upland soils, typical crop uptake of N is from amount 50 to over  $400 \text{ kg N ha}^{-1} \text{ yr}^{-1}$  (Follett et al., 2015). Producers are tempted to pre-apply large doses of commercial fertilizers or manure to help ensure that the crop will not become nutrient deficient. However, this practice runs the risk of losing significant amounts of N to the major sinks such as  $\text{NO}_3^-$  leaching, denitrification, and  $\text{NH}_3$  volatilization. Nitrifier populations have decreased by 16 to 56% in reduced and no-till plots relative to conventional tillage. While denitrifier populations have increased (Lyon et al., 1996). Microbial biomass levels of no-till soils averaged 54% higher in the surface layer compared to plowed soils (Doran, 1987).

## **2.2 Methods for simulating greenhouse gas (GHG) emissions from soil**

A significant number of models for predicting GHG emissions from agricultural lands have been developed. Each of them has been developed for a specific purpose, with their own view and interpretation of the processes and controlling variables for GHG emissions, with its unique strengths, limitations and for different scales, ranged from laboratory, field, regional to global scales. Increased emphasis on up-scaling processes at various scales has been evident in the more recent literature.

### **2.2.1 Laboratory scale to field scale models**

The laboratory-scale models simulate microbial growth, substrate dynamics, solute and gas transport through the soil profile and aggregates, and mostly are used to test the researchers' hypothesis of mineralization, nitrification, denitrification and associated mechanisms of C and N trace gas emissions from soils. The major factors considered at this level are soil water content, soil pH, soil organic C content, ammonium and  $\text{NO}_3^-$  concentrations and soil temperature. The laboratory models explicitly simulate the denitrification reaction, but only for singular incubation experiments with limited applications outside of these strict boundaries. In addition, the  $\text{N}_2\text{O}$  contribution from soil nitrification is not simulated. Because of the complexity across natural and agricultural ecosystems, the application of laboratory-scale models is very limited. However, the laboratory-scale models serve as the theoretical basis for more complex field-scale models (e.g. DNDC, DAYCENT, ECOSSEs and WNMM) which incorporate soil water dynamics, plant growth, C and N cycling and the impacts of site-specific soil properties, climate and agricultural management practices.

## 2.2.2 Field to regional models

Field-scale models have received the most attention in last two decades due to the need to simulate ‘real world’ conditions by integrating generic processes in plant-soil C/N and water cycling and anthropogenic influences (i.e. land use change and management practices). A field-scale model can also be used to develop a decision support system for mitigation ([Chen et al., 2005](#)). Review from [Langeveld and Leffelaar \(1996\)](#) outlined several common features within the process-oriented N<sub>2</sub>O emission simulation models: soil-air atmosphere and climate interactions, plant growth, C and N cycling, and land use management. In the N cycling component of each model, the contributions of N<sub>2</sub>O from both denitrification and nitrification are estimated. These models reviewed in this paper include NGAS-DAYCENT ([Mosier et al., 1983](#); [Mosier and Parton, 1985](#); [Parton et al., 1988b](#); [Parton et al., 1988a](#); [Parton et al., 1996](#); [Parton et al., 2001](#); [Del Grosso et al., 2000](#)), DNDC ([Li, 2000](#); [Li et al., 1992](#)), NLOSS ([Riley and Matson, 2000](#)), Expert-N ([Engel and Priesack, 1993](#)), WNMM ([Li et al., 2005](#)), FASSET ([Chatskikh et al., 2005](#)) and CERES-NOE ([Hénault et al., 2005](#); [Gabrielle et al., 2006b](#)).

Field-scale models such as DNDC, DAYCENT, and WNMM have also been coupled with GIS or have the built-in spatial capability for application at regional scales, to estimate the spatial and temporal variability of GHGs emissions in different landscapes if the detailed spatial information (specifically climate and soil) required by these models is available. With spatially explicit input data, it is possible to explore inter-daily, inter-seasonal, and inter-annual variation of GHG emissions in direct response to soil, climate and sub-regional management practices. Whilst the use of very simplistic approaches such as the IPCC methodology for identifying, climate or annual differences across a region is not possible, regression models such as those developed by [Hargreaves et al. \(1994\)](#) and [Sozanska et al. \(2002\)](#) may work.

If users are only interested in the spatial pattern of annual GHGs emissions from agricultural soils, e.g. for regional or national inventories, it may not be essential to use a detailed field-scale models to simulate specific management interactions in fine detail because of the intensive data requirements. A calibrated regional-scale models may be adequate for such a task whereby a select series of pre-determined simulations are run using the field-scale approach but then articulated as simpler GHGs responses based on regressions. The land use, soil type, topography and climate are generally recognized as the major environmental controlling factors to contribute to the spatial and temporal variations of GHGs emissions from landscapes, and, thus such information is often used for constructing regional-scale models.

### **2.2.3 Regional scale to global scale models**

The regional/global-scale models can produce the monthly, seasonal or annual pattern of GHG emissions for large landscapes or globally by using a few parameters through regression models, scaling approaches, empirical models, or in rare cases, simplistic mechanistic or processed-oriented models such as NASA CASA. In contrast to field and regional scales models, there are few published modelling approaches at the global level: the monthly version of the NASA CASA model ([Potter et al., 1996](#)), Bouwman's scaling model ([Bouwman et al., 2002](#)), the IPCC scaling model ([UNEP, 1995](#); [Gómez et al., 2006](#)) and FAO/IFA model ([FAO/IFA 2001](#)). The total amount of global annual N<sub>2</sub>O emissions from soils estimated by Bouwman's model is 6.9 Tg N yr<sup>-1</sup>, while NASA CASA predicted 6.1 Tg N yr<sup>-1</sup> N<sub>2</sub>O emissions globally. In terms of global estimates of N<sub>2</sub>O emissions from agricultural lands, the prediction by FAO/IFA model (2.9 Tg N yr<sup>-1</sup>) FAO/IFA (2001) is higher than that by the NASA CASA model (2.1 Tg N yr<sup>-1</sup>) ([Potter et al., 1996](#)). The FAO/IFA estimation was developed using higher resolution land use and management data than the other approaches.

Some field and regional models have the potential for upscaling to provide global annual N<sub>2</sub>O emissions, but the underlying uncertainty is potentially large due to the fact that field and regional models were normally calibrated for localized areas, e.g. several to thousands hectares. Even though many of the processes underpinning the soil C, N and water cycles are generic, when applying some models to different climatic zones or latitude regions in which they were developed, the originally boundary conditions in these models may be exceeded. For example, the findings by [Sabey et al. \(1959\)](#) and [Malhi and McGill \(1982\)](#) indicated that the optimal temperature for soil nitrification process tends to decrease from tropical to cool temperate regions. The DNDC and DAYCENT models are probably the two most prolific models in use today across a variety of scales and environments and continue to be used by a diverse group of users around the globe.

## **2.3 Existing studies on parameterization and uncertainty in modeling greenhouse gas emissions from soil**

Several studies on model comparisons and testing via experimental data indicate that on one hand, in-depth studies via lab and field experiments on the physical, chemical, and biological mechanisms for each process are still needed; on the other hand, significant knowledge gaps exist in the development of reasonable models and the application of appropriate models: (a) limited temporal and spatial experimental data is available for model calibration and verification; (b) multiple processes and complex model structure engender great challenges in model parameterization; and (c) a lack of information on uncertainties from different sources brings difficulty in model selections and applications ([Chen et al., 2005](#); [Wu and McGechan, 1998](#)).

### 2.3.1 Parameterization

Process-oriented models have led to a better understanding of C and N transformation processes, and resulted in complexity and difficulty in model parameterization. There are three categories of model parameters controlling C and N processes: (a) experimentally measurable parameters (e.g., weather data, topographic and soil data, management practices); (b) internal parameters that cannot be directly measured (e.g., nitrification/denitrification rate constant); and (c) the parameters that depend on other processes in an ecosystem (e.g. soil water movement and heat transfer, may be measured at limited sites within a very small region) ([Ma and Shaffer, 2001](#)). However, it is neither economical nor practical to conduct continuous field observation in a large area because of the temporal and spatial variability. For these reasons, the response functions of soil water and temperature were used in models to modify the transformation rates ([Li et al., 1992](#)).

Consequently, one of the main tasks for parameterization is associated with the second category of parameters. Fortunately, some model developers have prepared a database for the parameters corresponding to specific conditions, especially topography, land cover, and soils. For instant, DNDC provides a graphical user interface (GUI) with geographical information system (GIS) for users to select the study area, where the corresponding county-level database is used to parameterize and initialize the model ([Li, 2007](#)). [Wu and MCGechan \(1988\)](#) selected the major parameter values for SOILN model based on a combination of field experiments and literature sources. Some parameters were estimated from short-term experiments, thus it is difficult to achieve good simulation results at any specific site. This means that model calibration is still essential.

Due to the complexity of process-based model, the subjective optimization method ([McCuen, 2003](#)) was usually used to manually adjust parameter values based on the

modeler's subjective knowledge. The subjective optimization method requires modelers to have a good understanding of both parameters and input data. A limited number of parameters are selected for model calibration, and usually one parameter is adjusted at each model run. Undoubtedly, it is a great challenge for users to apply the model to their own studies.

### 2.3.2 Uncertainty

The efficacy of mathematical modeling as a tool for estimating GHG emissions from soil depends on the uncertainty. Studies on systematic evaluation of various sources of uncertainties in GHG models are still limited. Most studies currently focus on uncertainty from individual sources, e.g., parameter or input. In addition, the methods are confined to simple sensitivity analysis and Monte Carlo simulations. The sensitivity analysis of PnET-N-DNDC model to changes in environmental factors indicated that the simulated N-trace gas emission varied with measured ranges ([Stange et al., 2000](#)). The environmental factors include temperature, precipitation and some model input variables (litter mass, SOC, pH, soil texture, etc.). The sensitivity analysis was conducted by changing one factor and keeping all others constant. [Abdalla et al. \(2010\)](#) and [Thorsen et al. \(2001\)](#) used the Monte Carlo method to analyze the propagation of uncertainty from input data to model output, and found that the magnitude of uncertainty was significantly associated with the investigated temporal and spatial scale, ie., smaller output uncertainty on catchment scale than on gird level. [Reth et al. \(2005\)](#) used the Monte Carlo technique to assesse the uncertainty of model output, where a Gaussian distribution within  $\pm$  one standard error was used for parameter sampling. [Reth et al. \(2005\)](#) concluded that the uncertainty of DenNit output was about 32% for unlimited nutrient availability and the optimum values of soil temperature, water and pH values. In the comparison of C and N dynamics under conditions of conventional and diversified rotations, 64

parameter combinations were identified to test their impacts on model outcomes (Tonitto et al., 2007).

DNDC has provided an uncertainty analysis tool for SOC, clay, bulk density and pH value. This tool allows for the selection of either Monte Carlo or Most Sensitive Factor (MSF) method (Li, 2007). The MSF method involves running the model twice for each spatial unit with the maximum and minimum parameter values. These two runs generate two gas fluxes to form an interval that theoretically covers the real gas fluxes with a high probability (Li, 2007). Using this uncertainty model, several highly sensitive factors influencing DNDC model were identified. N<sub>2</sub>O emission was found to be sensitive to soil clay content, SOC and mean annual temperature; while CO<sub>2</sub> emission was significantly affected by SOC, clay fraction, mean annual temperature and annual precipitation (Li et al., 1992).

The Monte Carlo analysis was also adapted to assess uncertainties in soil N<sub>2</sub>O simulations from model input and structure of DAYCENT (Del Grosso et al., 2005). Probability distribution functions (pdfs) of major model inputs (weather, soil texture, and N applications) were assigned to quantify the uncertainty due to model inputs. The structural uncertainty was a synthesis of parametric uncertainty and model residual errors derived by an empirically-based linear mixed effect model (Ogle et al., 2007). Based on the range of confidence intervals of simulated N<sub>2</sub>O, they concluded that the total uncertainty was majorly attributed to model structure (80–85%) rather than the model input (Del Grosso et al., 2010).

The Bayesian inference based on Markov Chain Monte Carlo (MCMC) has been used to calibrate parameters and quantify parametric uncertainty in the N<sub>2</sub>O submodel of CERES-EGC (Lehuger et al., 2009). The uniform probability distributions were assigned as a priori for 11 global parameters. The uncertainty in N<sub>2</sub>O simulations was significantly reduced by the site-specific calibration.

HB models have been developed in recent years for a number of environmental applications ([Agarwal et al., 2005](#); [Cable et al., 2009](#); [Yeluripati et al., 2009](#)). This approach allows model inferences to be shared across sites (or other subunits, such as species) and yields subunit-specific parameter estimates. While HB model is clearly not the only way to address uncertainty, it stands out as an approach that can accommodate complex systems in a fully consistent framework. ([Malve and Qian, 2006](#)) indicated that a hierarchical modeling approach can be used to pool data from different sources to reduce the model uncertainty and improve the parameter accuracy; additionally, a hierarchical model can be used to form a realistic model without over-fitting the data by obtaining sufficient data from the hierarchical probability distribution.

## **2.4 Assessing greenhouse gases (GHGs) and net biome productivity (NBP) at regional scale**

The NBP is the C remaining in the ecosystem when all other fluxes have been accounted for ([Schulze and Heimann, 1998](#); [Chapin III et al., 2006](#)). In croplands, due to the removal each year of the crop material, the NBP is estimated by measuring the long-term change in SOC.

For soil C, long-term C cycling is often studied by measuring changes in total SOC over long periods (years to decades; [Smith et al., 1997](#)). In many sites, while SOC concentration has been measured over many years, calculation of total SOC concentration has been hindered by the absence of data on soil bulk density and by discrepancies in sampling techniques (e.g. no standardization of soil depth and of soil layers). In the last decade, individual long-term experiments have been brought together into networks such as the Soil Organic Matter Network (SOMNET ([Smith et al., 1997](#)), EuroSOMNET ([Smith et al., 1997](#)) and LTSE ([Richter Jr, 2014](#))). Such

networks allow the impacts of management practices on SOC stocks to be determined and for regional projections of the impact of different management strategies to be explored (e.g. [Ogle et al., 2005](#)).

In addition to measurement of changes in bulk SOC, other techniques are now being used to better understand SOC turnover. Various fractionation techniques are being used to isolate different components of SOC (e.g. [Six et al., 2011](#); [Del Galdo et al., 2003](#)) to better understand SOC turnover, and to identify sensitive indicators of SOC change. Mathematical methods to test the relationship between measured fractions and model pools are being developed (e.g. [Smith et al., 2002](#); [Zimmermann et al., 2007](#)), in order that this information can be incorporated into process-based models.

The main method for interpreting flux (and other) results, and for extrapolating temporally and spatially the data in agro-ecosystem (and other systems), is the use of process-based models ([Wattenbach et al., 2010](#)). Process-based models are continually being improved, with the most significant advance in the last decade being the development, and testing of models that simulate all biogenic GHGs. The main hurdle to applying such models at the regional level is data limitation. In recent years, high-resolution, spatially-explicit datasets have become more readily available. National, regional and global databases have been improved and it is now possible to run models for entire sub-continental regions (e.g. Europe, USA) at fine spatial scale such as a 10' by 10' grid ([Gervois et al., 2008](#); [Wattenbach et al., 2010](#)), at US county level ([Parton et al., 2005](#)) or even at 1 km<sup>2</sup> grid scale. Historical climate data have been interpolated to higher spatial resolution and future climate scenarios from global climate models have been downscaled to the same spatial resolution (e.g. [Mitchell et al., 2004](#)). Soil data are now available at high spatial resolution (e.g. at 1km<sup>2</sup> for Europe, [Jones et al., 2005](#)) and historical land-use data and future land use scenarios

are beginning to be constructed at high resolution (e.g. [Rounsevell et al., 2006](#)). There are many areas in which these datasets require further improvement, but significant advances have been made in some regions in recent years, including in Europe. In some other regions, however, especially in the developing world, such datasets are poor or non-existent. The development of airborne (satellite data) and ground flux measurements can provide sufficient information to estimate the C balance at large scale, which is a valuable tool to validate regional models (e.g. [Gioli et al., 2004](#); [Miglietta et al., 2007](#)).

Improvements in remote sensing capability and products have greatly improved datasets on land use and land cover and enabled improvements in modeling the consequences of recent land use change. All land based sectors use process based models and remote sensing products. Remote sensing data and land information systems for C accounting have been particularly successful when land is converted from forest to other land use ([Nobre and Harriss, 2002](#)).

## **2.5 Research needs in Agro-ecosystem GHG modeling**

Significant progress has been made in the simulation modeling of N<sub>2</sub>O at all scales, from the laboratory to the globe. N<sub>2</sub>O simulation models at the field scale are the most widely used models, not only because they bridge the knowledge gaps between the laboratory level and regional/global level, but also they simulate the entire agro-ecosystems, including water dynamics, C and N cycling and agricultural management, therefore it can be used to develop N<sub>2</sub>O mitigation strategies which align closely as the best management practices within the particular industry. These approaches still has many uncertainties, and significant knowledge gaps still exist in the construction of suitable models and need to be addressed: (a) limited temporal resolution of experimental data, particularly N<sub>2</sub>O emissions as a function of the

quantity, quality and timing of N applied; (b) limited unequivocal data, particularly using isotopes, to separate the N<sub>2</sub>O contribution between nitrification and denitrification; (c) the need for a detailed examination of N<sub>2</sub>O leakage in the nitrification process; (d) limited data for partitioning N<sub>2</sub>O and N<sub>2</sub> in denitrification; (e) a need for development of N<sub>2</sub>O emissions from chemo-denitrification and nitrifier denitrification; and (f) detailed analysis of gaseous diffusion of N<sub>2</sub>O from depth and its assimilation in the soil profile.

The challenging task is how to scale up the relatively more robust-scale models to catchment, regional and national scales, especially the interaction of biophysical processes between fields. Upscaling is an essential requirement, not only for more accurate regional and national inventories, but also for development of site-specific mitigation practices with increased interest in full GHGs accounting and emissions trading in the agricultural sector.

### 3. Materials and Methods

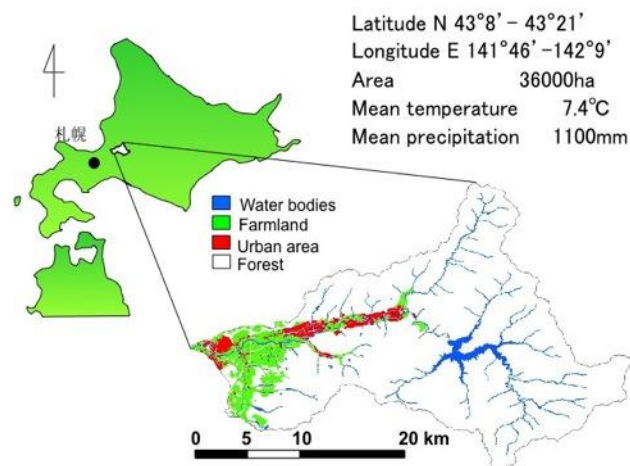
#### 3.1 Study site

The study site is the Ikushunbetsu River watershed located in central Hokkaido, Japan, latitude 43°14'N, longitude 141°57' E, which covers an area of 35,887 ha (Fig. 3.1) (Mu et al., 2008). The 30-year average temperature is 7.4°C, and the annual precipitation is 1154 mm (Japan Meteorological Agency, 2014). The main agricultural land uses are paddy rice (*Oryza sativa* L.), growing onion (*Allium cep* L.) and winter wheat (*Triticum aestivum*). Vegetable such as soybean (*Glycine max* L.) is the minor crop.

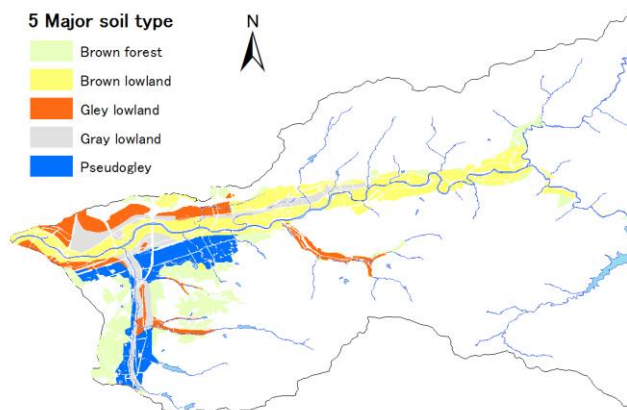
The altitudinal range of the Ikushunbetsu River Basin was 20 to 1054m (Digital Map 50m Grid, Geographical Survey Institute, 2001). At the regional scale, there are total 15 soil types, 6 soil textures and 5 major soil types including information of C content (TC) (g kg<sup>-1</sup>), total N content (TN) (g kg<sup>-1</sup>), clay content (%), silt content (%), clay + silt content (%) depended on different soils (Table 3.1). The 5 major soil types were according to a basic survey on soil fertility (Hokkaido Central Agricultural Experiment Station, 1971). Brown lowland soils were found along the main stream of the Ikushunbetsu River, surrounded by gray and gley lowland soils. Pseudogleys were distributed on the left side of the Ikushunbetsu River (Fig. 3.2). Other parts have not been identified, but they are thought to be brown forest soils. In each major soil type, the sub-soil type was defined. Grey lowland soils included soils of B-2, Hk-2, A-2, H-2 and forest (for); Brown lowland soils included soils of Ik-2, M-3, Sg-3, To-3 and Tu-3; Gley lowland soils included soils of Ks-3, Mi-2 and Kb-2; Pseudogleys included soils of Ni-3 and Kn-2 (Hokkaido Central Agriculture Experiment Station, 1971) (Fig. 3.3). The type of soil textures across the whole region around 6, they are clay loam (CL), light clay (LiC), silty clay (SiC), silty clay loam (SiCL), sandy loam

(SL) and heavy clay (HC). The main 4 soil textures are classified in this study, included CL, LiC, SiC and SiCL (Fig. 3.4). LiC soils were found along the main stream of the Ikushunbetsu River, surrounded CL, SiC and SiCL.

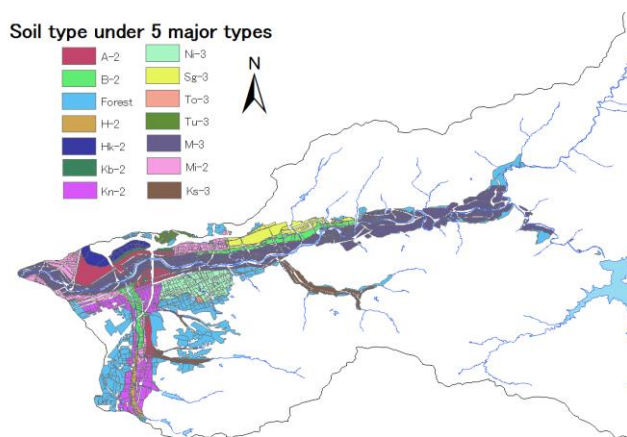
Land use history was analyzed using 1:25,000 maps from the Geographical Survey Institute (1959, 1966, 1976, 1988, 1994). Fallow land was defined as an area with previous artificial land use, but no cultivation or construction in the ground survey years. Bush land was defined as the fallow land was abandoned more than two years. Ground survey were conducted in 2002, 2005, 2007 and 2011 to locate the land use areas, and the land use distribution was mapped digitally using ArcView 10.0. According to a ground survey conducted in July 2011, the total upland area was 723 ha, paddy field area was 430 ha, grassland area was 320 ha, and bush/fallow area was 673 ha (Fig. 3.5). Among upland field, the main crops are soybean (33 ha), vegetable (19 ha), onion (279 ha) and wheat (392 ha). Cultural conditions and plant biomass components for major crops in Ikushunbetsu river watershed was shown in Table 3.2.



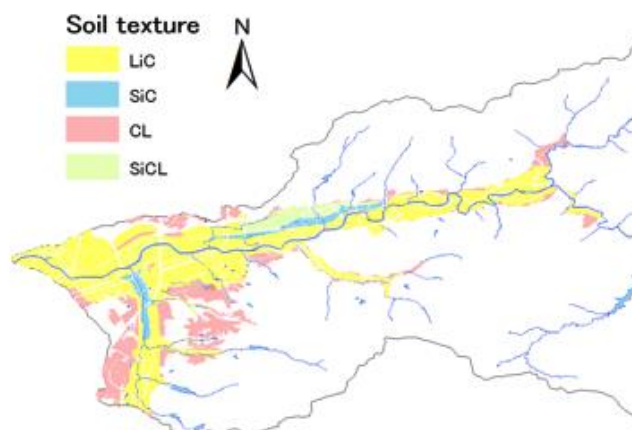
**Figure 3. 1** Location and characteristics of the study site.



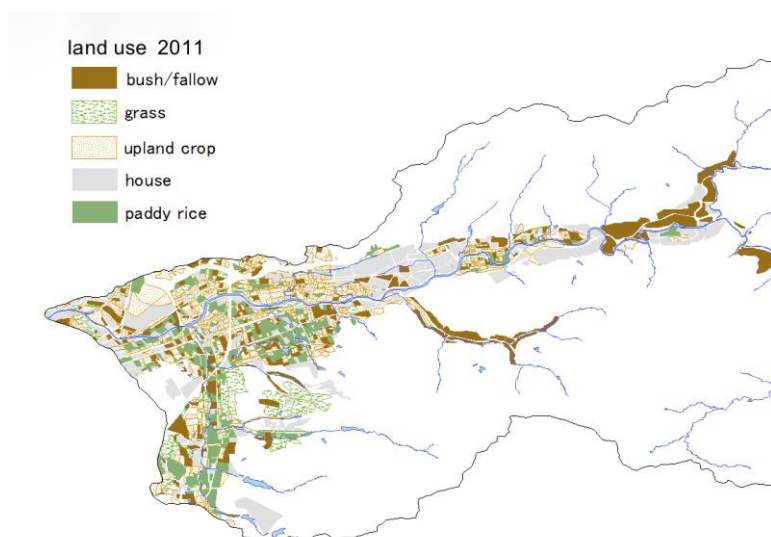
**Figure 3. 2** Distribution of 5 main soil types in Ikushunbetsu watershed.



**Figure 3. 3** Distribution of sub-soil types under the 5 main soil types in Ikushunbetsu watershed.



**Figure 3. 4** Distribution of soil texture in Ikushunbetsu watershed (LiC: Light Clay; SiC: Silty Clay; CL: Clay Loam; SiCL: Silty Clay Loam.)



**Figure 3. 5** Distribution of major land uses conducted in 2012 in Ikushunbetsu watershed.

**Table 3. 1** The general information of soil type at the regional scale.

| Sub-soil<br>type <sup>a</sup> | Sand | Silt | Clay | Texture | TC                 | TN                 | pH  | Soil type     |
|-------------------------------|------|------|------|---------|--------------------|--------------------|-----|---------------|
|                               | %    | %    | %    |         | g kg <sup>-1</sup> | g kg <sup>-1</sup> |     |               |
| B-2                           | 33.8 | 30.8 | 35.3 | LiC~SiC | 16.0               | 1.4                | 6.0 | Grey lowland  |
| Hk-2                          | 30.1 | 33.7 | 36.2 | LiC     | 53.5               | 3.8                | 5.7 | Grey lowland  |
| Ik-2                          | 28.5 | 40.9 | 30.5 | SiC~CL  | 30.9               | 1.8                | 6.8 | Brown lowland |
| Ks-3                          | 31.8 | 32.4 | 35.8 | LiC     | 62.0               | 4.6                | 5.5 | Gley lowland  |
| M-3                           | 34.5 | 30.6 | 34.9 | LiC     | 28.7               | 2.5                | 5.4 | Brown lowland |
| Mi-2                          | 21.9 | 38.5 | 39.5 | LiC     | 28.0               | 2.3                | 5.4 | Gley lowland  |
| Ni-3                          | 27.6 | 35.9 | 36.5 | LiC     | 34.0               | 3.0                | 5.5 | Pseudogley    |
| Sg-3                          | 40.8 | 30.3 | 28.9 | SL~SiCL | 21.3               | 2.0                | 5.8 | Brown lowland |
| Kb-2                          | 17.4 | 44.5 | 38.1 | CL~LiC  | 55.0               | 4.0                | 5.8 | Gley lowland  |
| Kn-2                          | 20.2 | 35.6 | 44.3 | LiC     | 33.1               | 2.2                | 5.5 | Pseudogley    |
| To-3                          | 46.6 | 28.7 | 24.7 | CL      | 23.4               | 1.6                | 6.5 | Brown lowland |
| Tu-3                          | 31.1 | 39.7 | 29.2 | LiC     | 27.0               | 7.2                | 5.2 | Brown lowland |
| H-2                           | 36.9 | 31.0 | 32.0 | LiC     | 22.0               | 2.0                | 4.9 | Grey lowland  |
| A-2                           | 21.6 | 42.1 | 36.3 | HC~LiC  | 64.0               | 4.9                | 5.2 | Grey lowland  |
| for                           | 32.6 | 36.4 | 31.0 | CL      | -                  | -                  | -   | Grey lowland  |

<sup>a</sup> Hokkaido Central Agriculture Experiment Station, 1971.

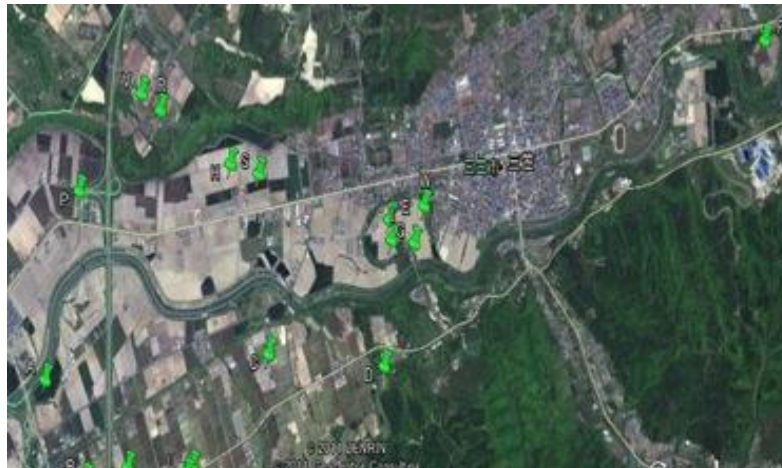
HC: Heavy Clay; LiC: Light Clay; SiC: Silty Clay; CL: Clay Loam; SL: Sandy Loam; SiCL: Silty Clay Loam.

**Table 3. 2** Cultural conditions and plant biomass components for major crops in the Ikushunbetsu watershed of central Hokkaido, Japan.

| Crop       | Sowing                          | Harvesting                | Harvested biomass | Plant biomass component                         |                                                        |                                                     |
|------------|---------------------------------|---------------------------|-------------------|-------------------------------------------------|--------------------------------------------------------|-----------------------------------------------------|
|            |                                 |                           |                   | Non-harvest biomass<br>(removed from the field) | Above-ground residue biomass<br>(returned to the soil) | Below-ground residue biomass (returned to the soil) |
| Soybean    | Mid May to late May             | Late September            | Grain             |                                                 | Leaves, stalks, pods                                   | Stubble and roots                                   |
| Potato     | Mid May to late May             | Late September            | Tubers            |                                                 | Leaves and stems                                       | Roots                                               |
| Buckwheat  | Mid June to late August         | Late September            | Grain             |                                                 | Stems                                                  | Stubble and roots                                   |
| Vegetable  | Mid May to late May             | Late September            | Head and Heart    |                                                 | Leaves                                                 | Roots                                               |
| Onion      | Late April to early May         | Late September            | Bulb              |                                                 | Leaves                                                 | Roots                                               |
| Maize      | Mid May to late May             | Late September            | Ears              |                                                 | Leaves and stalks                                      | Stubble and roots                                   |
| Greenhouse | Mid May to late May             |                           | Head and Heart    |                                                 | Leaves                                                 | Roots                                               |
| Wheat      | Mid September to late September | Late July to early August | Grain             | Straw                                           | Stubble and husks                                      | Stubble and roots                                   |
| Grass      | Early May                       | Late September            | Grass             |                                                 | Stubble                                                | Stubble and roots                                   |
| Paddy      | Early May                       | Late September            | Rice              |                                                 | Leaves and rice hulls                                  | Stubble and roots                                   |

## 3.2 Data sets

All data were obtained from upland agricultural field sites at the Ikushunbetsu River watershed in central Hokkaido, Japan, latitude 43°14'N, longitude 141°57'E, which covers an area of 35,887 ha (Kimura et al., 2010; Mu et al., 2008). Samples were measured in 15 fields comprising 11 land use types over a period of 9 years from 2003 to 2011 (Fig. 3.6) (Table 3.3). The data set includes information on study site location, dates of study, climate, precipitation, soil type, soil texture, soil temperature, soil water, soil pH, soil  $\text{NO}_3^-$  and  $\text{NH}_4^+$  contents, soil organic C and N contents,  $\text{CO}_2$ ,  $\text{N}_2\text{O}$  and NO emission.



**Figure 3. 6** Sampling sites of greenhouse gas in Ikushunbetsu watershed from 2003–2012.

**Table 3. 3** General information of 15 experimental sites.

| Site_No. | Site | Soil texture | TC<br>mg/g | TN<br>mg/g | C/N ratio | pH  | clay<br>% | silt<br>% | sand<br>% |
|----------|------|--------------|------------|------------|-----------|-----|-----------|-----------|-----------|
| 1        | B    | LiC          | 19.8       | 1.8        | 10.9      | 5.1 | 34.7      | 37.9      | 27.4      |
| 2        | BL   | LiC          | 21.7       | 1.9        | 11.3      | 5.9 | 36.6      | 57.4      | 6.0       |
| 3        | C    | CL           | 24.1       | 2.2        | 11.0      | 5.8 | 20.4      | 32.6      | 47.0      |
| 4        | D    | CL           | 16.2       | 1.3        | 12.1      | 5.8 | 20.4      | 32.6      | 47.0      |
| 5        | E    | CL           | 23.3       | 1.8        | 12.8      | 5.3 | 36.6      | 57.4      | 6.0       |
| 6        | F    | CL           | 26.2       | 2.2        | 12.2      | 5.9 | 18.6      | 38.1      | 43.3      |
| 7        | G    | CL           | 16.0       | 1.5        | 10.4      | 5.7 | 23.7      | 40.1      | 36.2      |
| 8        | GL   | SiC          | 32.1       | 2.8        | 11.5      | 5.5 | 37.3      | 51.1      | 11.7      |
| 9        | P    | SiC          | 27.0       | 2.1        | 13.0      | 6.0 | 33.9      | 47.7      | 18.4      |
| 10       | R    | SiCL         | 35.3       | 2.5        | 14.0      | 5.2 | 24.5      | 47.6      | 27.9      |
| 11       | S    | LiC          | 38.7       | 3.1        | 12.3      | 5.8 | 33.1      | 42.1      | 24.7      |
| 12       | T    | LiC          | 20.6       | 1.8        | 11.4      | 5.8 | 31.4      | 36.3      | 26.2      |
| 13       | U    | LiC          | 12.3       | 2.7        | 4.6       | 5.7 | 19.0      | 40.1      | 31.0      |
| 14       | V    | CL           | 31.5       | 2.6        | 12.1      | 5.4 | 17.9      | 29.1      | 53.1      |
| 15       | W    | CL           | 9.3        | 1.0        | 9.2       | 5.7 | 36.6      | 57.4      | 6.0       |

TC: the total carbon content. TN: the total nitrogen content. CL: Clay Loam. LiC: Light Clay. SiC: Silty Clay. SiCL: Silty Clay Loam.

### 3.2.1 Soil properties

TC and TN are the soil total C and total N concentration at 0–20 cm depth, respectively (Kimura et al., 2007). Soil temperature at a depth of 5 cm was recorded using a digital thermometer (CT-220; Custom Corporation, Tokyo, Japan). The content of soil  $\text{NO}_3^-$  was analyzed by using a Dionex ion chromatograph equipped with a conductivity detector, the content of  $\text{NH}_4^+$  was determined by using the indophenol blue colorimetric method (Mu et al., 2008b). In  $\text{CO}_2$ -HB model, soil water content was expressed as the percentage of water-filled pore space (WFPS) in the top layer from 0 to 5 cm depth, using the measured soil bulk density ( $\text{g}/\text{cm}^3$ ) (average of three measuring dates in May, July, and September of each year) and assuming a particle density of  $2.65 \text{ g}/\text{cm}^3$  (Mu et al., 2008b). In N-HB model, soil water content was expressed as the amount of water (in mm of water depth) present in a layer of soil

using depth of soil layer (mm) and soil water content by volume (%). Soil water content by volume (%) was calculated by soil water content by mass (g/g) and bulk density ( $\text{g/cm}^3$ ) (Mu et al., 2008b). Soil water saturation ( $\text{mm layer}^{-1}$ ), field capacity ( $\text{mm layer}^{-1}$ ) and permanent wilting point ( $\text{mm layer}^{-1}$ ) were estimated based on soil texture and organic matter (Saxton and Rawls, 2006). The WFPS was also simulated by using HYDRUS-1D for future regional model up-scaled, as it will be more precisely mentioned. The soil temperature at a depth of 5 cm ranged from 6.73°C to 30.02°C. The measured WFPS (WFPS\_measured) ranged from 0.24 to 0.83 with a median of 0.39 (mean: 0.44) and skewness of 1.38. The simulated WFPS (WFPS) ranged from 0.37 to 0.87 with a median of 0.25 (mean: 0.49) and skewness of 0.70 (Table 3.4).

**Table 3. 4** Statistics of measured data used in this study. CI indicates confidence interval.

|                           | Median | Mean  | SD    | 95% CI        | Skewness | Kurtosis |
|---------------------------|--------|-------|-------|---------------|----------|----------|
| soil temperature(°C)      | 21.45  | 20.47 | 6.52  | 6.73 ~ 30.02  | -0.46    | -0.71    |
| WFPS_measured             | 0.39   | 0.44  | 0.66  | 0.24 ~ 0.83   | 1.38     | 1.28     |
| WFPS                      | 0.25   | 0.49  | 0.70  | 0.37 ~ 0.87   | 0.70     | -0.34    |
| TC ( $\text{g kg}^{-1}$ ) | 17.00  | 18.64 | 11.13 | 0.90 ~ 38.70  | 0.15     | -1.17    |
| TN ( $\text{g kg}^{-1}$ ) | 1.67   | 1.48  | 0.78  | 0.10 ~ 3.14   | 0.07     | -1.05    |
| C/N ratio                 | 12.17  | 12.38 | 14.27 | 9.20 ~ 20.78  | 2.10     | 7.92     |
| silt(%)                   | 40.60  | 42.70 | 8.17  | 24.80 ~ 57.40 | -0.20    | -0.36    |
| clay(%)                   | 25.30  | 27.47 | 6.28  | 16.8 ~ 36.70  | 0.07     | -1.31    |

WPFPP\_measured is the measured value of water filled pore space. WFPS is the simulated value.

### 3.2.2 Greenhouse gas (GHG) emission

The GHG measurements were carried out on 15 experimental sites weekly using the closed chamber method throughout the non-snow period (Middle April to Early November) across 9 years from 2003 to 2011(for details, see Kusa et al., 2002; Toma et al., 2007; Mu et al., 2008a,b). GHG fluxes from heterotrophic respiration ( $R_h$ ) were measured from the bare soils where the soils were not treated with chemical and

organic fertilizers or residues, and weeds were removed from the monitoring plots. For use in the CO<sub>2</sub> calibration, the CO<sub>2</sub> emission from heterotrophic respiration (Rh) was used. And in order to decrease the effects of daily weather or temporal variations at the field scale, and to decrease the uncertainty in emissions, which is particularly large during periods of high emissions (Chatskikh et al., 2005; Chatskikh and Olesen, 2007; Chatskikh et al., 2008), the measured CO<sub>2</sub> flux data were aggregated on a monthly basis. Cumulated monthly CO<sub>2</sub> emissions (kg C ha<sup>-1</sup> month<sup>-1</sup>) were estimated by linear interpolation between measurements on the dates of the corresponding daily fluxes and then divided by the number of days of one month to obtain the daily flux (kg C ha<sup>-1</sup> day<sup>-1</sup>) on a monthly basis, with number points  $N = 154$ . For use in the N<sub>2</sub>O and NO calibration, N<sub>2</sub>O and NO emission from both ctrl and fop treatment were used at daily step directly, with number points  $N = 607$ .

### 3.2.3 Land management

An inquiry was carried out to investigate the actual amount of applied N fertilizer and yield in each land use category. Farmers were asked about their management methods for each crop. In addition to these inquiries, unpublished data were obtained from Iwamizawa Agriculture Cooperation, Mikasa Branch and Agriculture Improving Center of Central Sorachi. The investigated farm numbers for each type of land use were 12 for paddy rice, 22 for wheat, 10 for onion, 6 for vegetables and 17 for grasslands. Among 15 experiments sites, for some sites, different treatments were conducted with various N-fertilizer amounts supplied to the crop (Table 3.5). Chemical fertilizers or residues were not applied on the ctrl treatments and weeds were removed from the monitoring plots without any crop cultivation. The fop (Fertilizer, Organic matter, Plant) treatments were applied with chemical fertilizer (F), organic matter (O) and crop cultivation (Plant). For some sites, there were not only control treatments but also conducted with fop treatment. There were a total of 26

site/treatment combinations ([Table 3.5](#)). Bare soil means no chemical application; no organic fertilizer application and no plant application (for details, see [Naser et al., 2007](#); [Mu et al., 2008a,b](#)).

**Table 3. 5** Information of land management in 15 experimental sites and 26 site/treatment combinations.

| Site | Site_No. | ID           | ID_No. | Year            | Crop type | Treatment | N fertilizer<br>kg N ha <sup>-1</sup> yr <sup>-1</sup> | Crop Residue<br>kg N ha <sup>-1</sup> yr <sup>-1</sup> |
|------|----------|--------------|--------|-----------------|-----------|-----------|--------------------------------------------------------|--------------------------------------------------------|
| B    | 1        | B_ctrl       | 1      | 2003            | None      | ctrl      | 0                                                      | 0                                                      |
|      |          | B_fop        | 2      | 2003            | Wheat     | fop       | 140                                                    | 104                                                    |
| BL   | 2        | BL_ctrl      | 3      | 2006, 2007      | Onion     | ctrl      | 0                                                      | 0                                                      |
|      |          | BL_fop       | 4      | 2006, 2007      | Onion     | fop       | 180                                                    | 57                                                     |
| C    | 3        | C_ctrl       | 5      | 2003            | None      | ctrl      | 0                                                      | 0                                                      |
|      |          | C_fop        | 6      | 2003            | Maize     | fop       | 110                                                    | 14                                                     |
| D    | 4        | D_ctrl       | 7      | 2003, 2005      | None      | ctrl      | 0                                                      | 0                                                      |
|      |          | D_fop        | 8      | 2003            | Wheat     | fop       | 140                                                    | 104                                                    |
| E    | 5        | E_ctrl       | 9      | 2003            | None      | ctrl      | 0.0                                                    | 0.0                                                    |
|      |          | E_fop**      |        | 2008            | Onion     | fop       | 165                                                    | 42                                                     |
| F    | 6        | F_ctrl       | 10     | 2003            | None      | ctrl      | 0                                                      | 0                                                      |
|      |          | F_fop        | 11     | 2003            | Wheat     | fop       | 112                                                    | 104                                                    |
| G    | 7        | G_ctrl       | 12     | 2003            | Soybean   | ctrl      | 0                                                      | 0                                                      |
| GL   | 8        | GL_ctrl      | 13     | 2006–2009       | None      | ctrl      | 0                                                      | 0                                                      |
|      |          | GL_fop       | 14     | 2006–2009       | Onion     | fop       | 237                                                    | 45                                                     |
|      |          | Verification |        | 2010–2011*      | Onion     | fop       | 237                                                    | 45                                                     |
| P    | 9        | P_ctrl       | 15     | 2006–2007       | None      | ctrl      | 0                                                      | 0                                                      |
|      |          | P_fop        | 16     | 2007            | Onion     | fop       | 200                                                    | 70                                                     |
| R    | 10       | R_ctrl       | 17     | 2006–2007, 2009 | None      | ctrl      | 0                                                      | 0                                                      |
|      |          | R_fop        | 18     | 2005            | Potato    | fop       | 94                                                     | 22                                                     |
|      |          |              |        | 2007            | Potato    | fop       | 32                                                     | 22                                                     |
|      |          |              |        | 2009            | Potato    | fop       | 196                                                    | 122                                                    |
|      |          | Verification |        | 2010, 2011*     | Potato    | fop       | 196                                                    | 122                                                    |
| S    | 11       | S_ctrl       | 19     | 2006            | None      | ctrl      | 0                                                      | 0                                                      |
| T    | 12       | T_ctrl       | 20     | 2007, 2008      | None      | ctrl      | 0                                                      | 0                                                      |
|      |          | T_fop        | 21     | 2007, 2009      | Buckwheat | fop       | 106                                                    | 16                                                     |
| U    | 13       | U_ctrl       | 22     | 2007            | None      | ctrl      | 0                                                      | 0                                                      |
|      |          | U_fop        | 23     | 2007            | Maize     | fop       | 146                                                    | 235                                                    |
| V    | 14       | V_ctrl       | 24     | 2009            | None      | ctrl      | 0                                                      | 0                                                      |
|      |          | V_fop        | 25     | 2007            | Soybean   | fop       | 57                                                     | 57                                                     |
|      |          |              |        | 2009            | Maize     | fop       | 79                                                     | 14                                                     |
|      |          | Verification |        | 2010, 2011*     | Maize     | fop       | 79                                                     | 14                                                     |
| W    | 15       | W_ctrl       | 26     | 2009            | None      | ctrl      | 0                                                      | 0                                                      |
|      |          | Verification |        | 2010, 2011*     | Onion     | fop       | 342                                                    | 45                                                     |

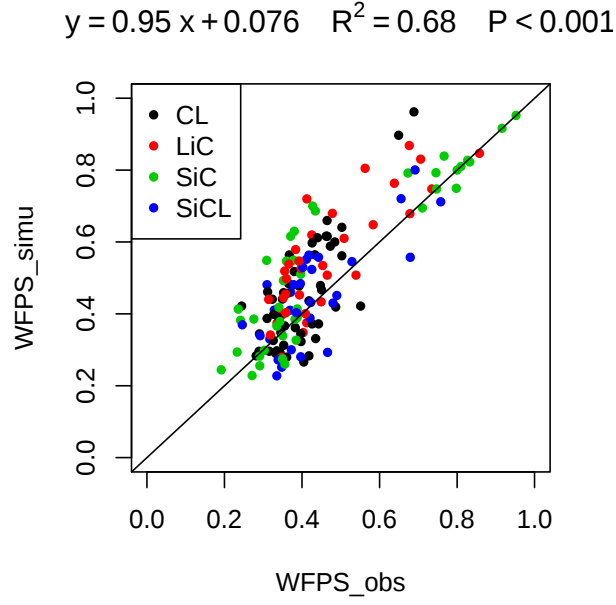
ctrl: bare soil without any fertilizer, organic matter and plant residue treatment. fop: Planted soil with fertilizer, organic matter and plant residue treatment.

\* Data for verification

\*\*No detailed data of NO flux, therefore didn't included in the database.

### 3.2.4 WFPS simulation

It is difficult to calculate WFPS at the regional scale, therefore the daily WFPS was simulated in order to make the CO<sub>2</sub>-HB model future up-scaled possible. WFPS was calculated from the simulated daily soil water content and measured soil bulk density (Mu et al., 2008b). HYDRUS-1D was calibrated using 9 years (2003–2011) of daily soil water content data in the 0–5 cm soil layer at 15 sites. The HYDRUS-1D model required input of the potential evaporation (PE) to perform surface flux simulation. PE was calculated from the average daily values of air temperature (°C), humidity (%), wind speed (km d<sup>-1</sup>), and solar radiation (hr) using the Penman-Monteith Combination Equation (Jensen et al., 1990). Daily meteorological data were obtained from the Japan Meteorological Agency (<http://www.jma.go.jp/jma/>). Water flow conditions were chosen to allow the surface water layer to increase from precipitation and decrease from infiltration and evaporation for the upper boundary. Free drainage was selected for the lower boundary. The most important factor for successful application of unsaturated flow theory to actual field problems is obtaining the parameters for the governing transfer equation (Dixon, 1999). The hydraulic parameters used in this study for hydraulic conductivity function were predicted using textural characteristics by Van Genuchten et al. 1992. WFPS calculated by HYDRUS was used for HB calibration after values obtained by HYDRUS simulation were found to be significantly correlated with the measured values of WFPS ( $R^2 = 0.68$ ,  $P < 0.001$ , Fig. 3.7).



**Figure 3. 7** Comparison between predicted and measured water-filled pore space (WFPS).

### 3.3 Bayesian calibration theory

To estimate the soil gas flux, a Bayesian approach was developed to calibrate the parameters. Bayesian methods are used to estimate model parameters by combining two sources of information: prior information about parameter values and observations on output variables. The prior information is based on expert knowledge, literature review or by measuring parameters directly in the field or laboratory. In our case, the observations on output variables are field measurements. Here Bayesian theory is briefly describe,

$$p(\theta|y) = \frac{f(y|\theta)\pi(\theta)}{g(y)} \quad (3.1)$$

where  $\theta$  is the parameter that we are estimating and  $y$  represents the observed data. Both  $\theta$  and  $y$  are considered to be random variables.  $p(\theta|y)$  is the posterior distribution which represents the probability of the model parameter ( $\theta$ ) values given the observed data ( $x$ ),  $g(y)$  is the unconditional probability of the observed data,  $\pi(\theta)$  is the prior distribution, and  $f(y|\theta)$  is the conditional probability of the observations on  $\theta$ , termed the likelihood function.

The likelihood function for all observation can be expressed as:

$$f(y|\theta) = \prod_{i=1}^N \frac{1}{\sqrt{2\pi\sigma_y^2}} e^{-\frac{(y_i - (\mu_y)_i)^2}{2\sigma_y^2}} \quad (3.2)$$

where,  $y_i$  is the  $i$ -th observed data and  $(\mu_y)_i$  is the predicted values,  $N$  is the number of data points.  $\sigma_y$  is the standard deviation that corresponds to observed data.

Different from nonhierarchical Bayesian model (Bayesian pooled model), the hierarchical model assigns two hyper parameters  $\alpha$  and  $\beta$  to yield the posterior distribution of parameter ( $\theta$ ), which is different from Eq. 3.1:

$$p(\theta, \alpha, \beta | y) = \frac{\prod_{j=1}^n f(y_j | \theta_j) \pi(\theta_j | \alpha, \beta) u(\alpha) v(\beta)}{g(\theta | \alpha, \beta)} \quad (3.3)$$

where  $j$  is the class number,  $\theta_j$  indicates that each individual class can have a different parameter, but all are linked through hyper parameter.  $u(\alpha)$  and  $v(\beta)$  are the prior distribution of hyper parameters.

To generate a representative sample of parameters from the posterior distribution, the Markov Chain Monte Carlo (MCMC) method was used (Congdon, 2007). For calibration, three parallel Markov chains were started from three different starting points: the default parameter value and its lower ( $\theta_{mix}$ ) and upper bounds ( $\theta_{max}$ ). Convergence was checked with the diagnostic method proposed by Gelman and Rubin (1992), which is based on the comparison of within-chain and between-chain variances and is similar to a classical analysis of variance. Convergence is reached when the variance between chains no longer exceeds the variance within each individual chain.

Total 10,000 iterations of sampling from the prior distribution within each chain was conducted to obtain the posterior probability distributions, discarding the first 2,000 iterations as non-representative “burn-in” of chains to avoid the influence of the initial values and using the remaining 8,000 iterations to evaluate the posterior distribution of parameters (Van Oijen et al., 2005).

### 3.4 CO<sub>2</sub>-HB model

The CO<sub>2</sub>-HB runs on a daily weighed time step, which has been developed, based on Rh to simulate soil CO<sub>2</sub> emission with data that can drive the model on a range of spatial scales and as a sub-model incorporated into other models.

#### 3.4.1 CO<sub>2</sub>-HB model structure

Simple greenhouse gas (SG) models were used to estimate GHG fluxes ([Hashimoto et al., 2011](#)). The model structure developed for CO<sub>2</sub> flux (kg C ha<sup>-1</sup> day<sup>-1</sup>) in this study is based on the SG model, which can be generally described using response functions of  $h(T)$  and  $g(WFPS)$  as follows:

$$CO_2 = \exp(\beta_1)h(T)g(WFPS) \quad (3.4)$$

where  $\beta_1$  is a constant, and  $T$  is the soil temperature at a depth of 5 cm (°C).

$h(T)$  is the response function of soil temperature and can be described as an exponential function as follows:

$$h(T) = \exp(\beta_2 T) \quad (3.5)$$

where  $\beta_2$  is the parameter.

$g(WFPS)$  is the response function of WFPS in the top soil layer at a depth of 0–5 cm. The following function was adopted from the DAYCENT ([Parton et al., 1996](#)) and SG models ([Hashimoto et al., 2011](#)):

$$g(WFPS) = \left(\frac{WFPS - \beta_3}{\beta_4 - \beta_3}\right)^{\beta_6} \left(\frac{WFPS - \beta_5}{\beta_4 - \beta_5}\right)^{\frac{-\beta_6(\beta_4 - \beta_5)}{(\beta_4 - \beta_3)}} \quad (3.6)$$

where  $\beta_3$ ,  $\beta_4$  and  $\beta_5$  are the parameters which are the minimum, optimum, and maximum values of WFPS, respectively (i.e.,  $\beta_3 < \beta_4 < \beta_5$ ), and  $\beta_6$  is the parameter controlling the curvature of the function.

#### 3.4.2 Hierarchical model

This study mainly focused on using the HB model to predict CO<sub>2</sub> flux across

various soil textures. The HB model is summarized as follows:

$$CO_{2ij} \sim N(\mu_{yij}, \sigma_y^2) \quad (3.7)$$

$$\mu_{yij} = \exp(\beta_{1,j}) \exp(\beta_{2,j} T_{ij}) \left( \frac{WFPS_{ij} - \beta_{3,j}}{\beta_{4,j} - \beta_{3,j}} \right)^{\beta_{6,j}} \left( \frac{WFPS_{ij} - \beta_{5,j}}{\beta_{4,j} - \beta_{5,j}} \right)^{\frac{-\beta_{6,j}(\beta_{4,j} - \beta_{5,j})}{(\beta_{4,j} - \beta_{3,j})}} \quad (3.8)$$

$$\beta_{k,j} \sim N(\mu_{\beta k}, \sigma_{\beta k}^2) \quad (3.9)$$

where  $CO_{2ij}$  is the  $i$ -th observation of  $CO_2$  flux for the  $j$ -th texture class and  $i$ -th data,  $i$  is the data point number ranging from 1 to  $N$ , and  $j$  is the texture class number ( $j=1$ , CL;  $j=2$ , LiC;  $j=3$ , SiC;  $j=4$ , SiCL).  $N$  is the total number of data points.  $k$  is the  $k$ -th number of the parameter,  $k=1, \dots, 6$ , denoted as  $\beta_{1,j}, \dots, \beta_{6,j}$ , respectively.  $\beta_{k,j}$  is the texture-specific model parameter which consists of the constant ( $\beta_{1,j}$ ), the parameter ( $\beta_{2,j}$ ) for  $h(T)$ , and the parameters ( $\beta_{3,j}, \beta_{4,j}, \beta_{5,j}, \beta_{6,j}$ ) for  $g(WFPS)$ .  $\sigma_y^2$  is the variance of the model error.  $\mu_{\beta k}$  and  $\sigma_{\beta k}^2$  are the mean and variance for  $\beta_{k,j}$ .  $\mu_{\beta k}$  and  $\sigma_{\beta k}^2$  are defined as hyper parameters. Note that the hierarchical notation in [Equations 3.7–3.9](#) indicates conditional distributions, *i.e.*,  $CO_{2ij}$  is normally distributed conditional on  $\mu_{yij}$  and  $\sigma_y^2$ , and  $\beta_{k,j}$  is normally distributed conditional on  $\mu_{\beta k}$  and  $\sigma_{\beta k}^2$ . In the HB method, all of the hyper parameters also need the prior information along with the other parameters (*e.g.*,  $\sigma_y$ ). The non-informative or vague prior information of  $\mu_{\beta k}$ ,  $\sigma_{\beta k}$ , and  $\sigma_y$  in [Equations 3.7–3.9](#) are as follows:

$$\mu_{\beta k} \sim N(0, 10\,000) \quad (3.10)$$

$$\sigma_{\beta k}, \sigma_y \sim Unif(0, 100) \quad (3.11)$$

where  $N(0, 10\,000)$  is the normal distribution of  $\mu_{\beta k}$  with mean 0 and variance 10,000 and  $Unif(0, 100)$  is the uniform distribution of  $\sigma_{\beta k}$  and  $\sigma_y$  with lower (0) and upper (100) limits.

### 3.4.3 Nonhierarchical Bayesian model (Bayesian pooled model)

To evaluate the goodness-of-fit of hierarchical Bayesian (HB) models, we also applied the Bayesian pooled model across all soils. Rather than [Equations 3.7–3.11](#),

the Bayesian pooled model can be described as:

$$CO_{2i} \sim N(\mu_{yi}, \sigma_y^2) \quad (3.12)$$

$$\mu_{yi} = \exp(\beta_1) \exp(\beta_2 T_i) \left( \frac{WFPS_i - \beta_3}{\beta_4 - \beta_3} \right)^{\beta_6} \left( \frac{WFPS_i - \beta_5}{\beta_4 - \beta_5} \right)^{\frac{-\beta_6(\beta_4 - \beta_5)}{(\beta_4 - \beta_3)}} \quad (3.13)$$

$CO_{2i}$  is the  $i$ -th observation of  $CO_2$  flux,  $i$  is the data number ranging from 1 to  $N$ , and  $N$  is the total data number.  $\beta_k$  ( $k = 1, \dots, 6$ ) are the model parameters, which consist of the constant ( $\beta_1$ ); parameter ( $\beta_2$ ) for  $h(T)$ , and parameters ( $\beta_3$ ,  $\beta_4$ ,  $\beta_5$ , and  $\beta_6$ ) for  $g(WFPS)$ .  $CO_{2i}$  is normally distributed conditional on  $\mu_{yi}$  and  $\sigma_y^2$ .  $\sigma_y^2$  is the variance of the model error. The vague prior distributions of  $\beta_k$  and  $\sigma_y$  are as follows:

$$\beta_k \sim N(0, 10\,000) \quad (3.14)$$

$$\sigma_y \sim Unif(0, 100) \quad (3.15)$$

where  $N(0, 10\,000)$  is the normal distribution of  $\beta_k$  with mean 0 and variance 10,000, and  $Unif(0, 100)$  is the uniform distribution of  $\sigma_y$  with lower (0) and upper (100) limits.

### 3.4.4 Model evaluation and comparison

The goodness of fit of the HB models and the Bayesian pooled version were compared. The HB models and the Bayesian pooled version were evaluated by comparing the prediction of  $CO_2$  flux to the observed values using the root mean square error (RMSE) to quantify the mismatch between the predictions and the mean values of the measurements. In addition, we used an evaluation method developed specifically for evaluating both HB and Bayesian pooled models, the deviance information criterion (DIC) ([Spiegelhalter et al., 2002](#)).

Some authors suggest using the posterior mean deviance  $\bar{D} = E[D(\theta)]$  as a measure of model fit, where  $D(\theta)$  is the deviance defined as:

$$D(\theta) = -2 * \text{likelihood} = -2 \log p(x|\theta) \quad (3.16)$$

However, more complex models will fit the data better and thus will have a smaller  $\bar{D}$ ; therefore, a measurement of model complexity was introduced to counterbalance

$\bar{D}$ .

Model complexity was measured by estimating the effective number of parameters,  $pD$ .

$$pD = E[-2\log p(x|\theta)] - \left(-2\log p\left(x|\bar{\theta}(x)\right)\right) = \bar{D} - D(\bar{\theta}) \quad (3.17)$$

where  $\bar{\theta} = E[x|\theta]$ . In this case  $pD$  can be described as:  $pD$ =[mean value evaluated at the posterior distribution of deviance] – [deviance evaluated at the posterior mean of the parameters].

Therefore, DIC is defined as:

$$DIC = D(\bar{\theta}) + 2PD = \bar{D} + pD \quad (3.18)$$

Both RMSE and  $\bar{D}$  decrease as the model complexity (number of parameters) increases. In contrast, the DIC considers both the goodness of fit ( $\bar{D}$ ) and a penalty for model complexity ( $pD$ ), and it is specifically designed to overcome the difficulty in determining the effective number of parameters and degrees of freedom to assign to hierarchical models. A small DIC is estimated to be the model that would predict a replicate dataset that has the same structure as the currently observed data.

### 3.4.5 Calculations and statistics

HB calibration was applied to the CO<sub>2</sub>-HB model by using data of total 15 experimental sites. Bayesian calibration was performed with the statistical package R (R Development Core Team, 2005), particularly its R2jags package (Plummer, 2003). Convergence diagnostic analysis and model evaluation and comparison were performed with the R ‘boa’ package (Smith et al., 2007b). Simple linear regression analysis was applied between the mean values of estimated parameters and soil properties. Akaike’s information criterion (AIC) (Akaike, 1987) for the different simple linear regressions was compared to choose the best variables (soil properties) for the estimated parameters. A smaller AIC value indicates a better predictor variable. Regression analysis was applied between the estimated parameters and the best

variables. In HB statistics, a significant difference at the 10% level among parameters was defined when the 90% CIs of the posterior distribution of the parameters failed to overlap each other (Scheibehenne and Pachur, 2015; Kraft et al., 2010; Lu et al., 2012). The goodness of fit of the effect of soil temperature and WFPS on daily CO<sub>2</sub> flux was tested by comparing the model performance with that obtained with the HB model structure including only the response function of soil temperature  $CO_2 = \exp(\beta_1)h(T)$  and including only the response function of soil WFPS  $CO_2 = \exp(\beta_1)g(WFPS)$ .

### 3.5 N-HB model

The N-HB model runs on a daily time step, which has been developed, based on process theory of nitrification and denitrification to simulate soil N gaseous emission with data that can drive the model on a range of spatial scales.

#### 3.5.1 Nitrification process

Nitrification in N-HB is simulated according to the amount of ammonium (NH<sub>4</sub><sup>+</sup>) in the soil layer, and is modified according to the temperature, soil water content and soil pH. The amount of N nitrified,  $N_n$  (in kg N ha<sup>-1</sup>), is calculated using the expression for nitrification developed by Bradbury et al. (1993), and modified by Bell et al. (2012) *i.e.*

$$N_n = N_{NH_4} \left( 1 - e^{-Nitri_{rate} \cdot m_t \cdot m_w \cdot m_{pH}} \right) \left( 1 - \frac{N_{NH_4}}{C_{max} + N_{NH_4} + N_{FERT}} \right) \quad (3.19)$$

where  $Nitri_{rate}$  is the nitrification rate,  $N_{NH_4}$  is the amount of NH<sub>4</sub><sup>+</sup> in the soil (kg N ha<sup>-1</sup>),  $m_t$  is a rate modifier due to soil temperature,  $m_w$  is a rate modifier due to soil water content, and  $m_{pH}$  is a rate modifier due to soil pH,  $N_{FERT}$  is N in NH<sub>4</sub><sup>+</sup> and urea in the added fertilizer (kg N ha<sup>-1</sup>),  $C_{max}$  is a set for a range of soil types, but can be calibrated using data showing the maximum flux rate of N<sub>2</sub>O as an indication of the

maximum rate of nitrification at high  $\text{NH}_4^+$  levels (Bell et al., 2012).

Conversion of  $\text{NH}_4^+$  to  $\text{NO}_3^-$  by nitrification is accompanied by gaseous losses of N due to partial and complete nitrification. The gaseous losses as NO and  $\text{N}_2\text{O}$  are calculated using a linear relationship.

The equations of the response functions of nitrification with the associated unitless response function ( $m_t$ ,  $m_w$ ,  $m_{pH}$ ) as follows:

$$m_t = \frac{T_1}{\left(1 + \exp\left(\frac{T_2}{T_{air}} + T_3\right)\right)} \quad (3.20)$$

where  $m_t$  is the temperature rate modifier for nitrification.  $m_t$  is taken from Bradbury et al. (1993).  $T_1$ ,  $T_2$  and  $T_3$  are parameters, and  $T_{air}$  is the daily air temperature ( $^{\circ}\text{C}$ ).

$$m_{pH} = pH_{cons} + \frac{\tan^{-1}(3.14 \times pH_{modif}(pH - pH_{Tr}))}{3.14} \quad (3.21)$$

where  $m_{pH}$  is the pH rate modifier for nitrification.  $m_{pH}$  is taken from Parton et al. (1996).  $pH_{cons}$  is the constant,  $pH_{modif}$  controls the modifier shape and  $pH_{Tr}$  are pH threshold for pH rate change.

$$m_w = 1 - \frac{(1 - m_{w0})(\theta_f - \theta_c - \theta_i)}{\theta_f - \theta_i} \quad (3.22)$$

$$m_w = 1 - \frac{(1 - m_{w0})(\theta_c - \theta_f)}{\theta_s - \theta_f} \quad (3.23)$$

where  $m_w$  is the water rate modifier for nitrification.  $m_w$  is calculated by the equation presented by Bradbury et al. (1993).  $m_{w0}$  is the soil water rate modifier for decomposition at permanent wilting point and saturation.  $\theta_c$  is the amount of water held in a particular soil layer above the permanent wilting point ( $\text{mm layer}^{-1}$ ),  $\theta_i$  is the amount of water held between field capacity and  $-100$  kPa ( $\text{mm layer}^{-1}$ ), and  $\theta_f$  is the amount of water held between field capacity and the permanent wilting point ( $\text{mm layer}^{-1}$ ).  $\theta_s$  is the water content between saturation and permanent wilting point. Below field capacity, the rate modifier is assumed to follow a linear increase (Eq. 3.22). When above field capacity, the rate modifier is assumed to follow a linear decline to the minimum rate of  $m_{w0}$  (Eq. 3.23).

The amount of gas emitted as N<sub>2</sub>O during nitrification,  $N_{n,N_2O}$  (kg N ha<sup>-1</sup>), is given by

$$N_{n,N_2O} = \left( \left( n_f \times \frac{\theta_c}{\theta_f} \right) + \left( n_{gas} (1 - n_{no}) \right) \right) N_n \quad (3.24)$$

where  $n_f$  is the proportion of N<sub>2</sub>O, which is produced due to partial nitrification at soil water field capacity,  $\theta_c$  is the amount of water in a particular soil layer above the permanent wilting point (mm layer<sup>-1</sup>), and  $\theta_f$  is the amount of water held between field capacity (mm layer<sup>-1</sup>) and the permanent wilting point. N<sub>2</sub>O produced from partial nitrification increases with ratio of  $\theta_c$  and  $\theta_f$ . The proportion of full nitrification gaseous loss to N<sub>2</sub>O and NO is  $n_{gas}$ , and  $n_{no}$  is the proportion of NO loss due to full nitrification. Similarly, the amount of gas emitted as NO during nitrification,  $N_{n,NO}$  is given (kg N ha<sup>-1</sup>) by

$$N_{n,NO} = n_{gas} \times n_{NO} \times N_n \quad (3.25)$$

### 3.5.2 Denitrification process

Total denitrification in N-HB is simulated as a proportion of the NO<sub>3</sub><sup>-</sup> content of the layer, modified according to water content and biological activity of the soil (as described by CO<sub>2</sub> release during decomposition). The denitrified N is then divided into N<sub>2</sub>, N<sub>2</sub>O and NO according to the soil water content and NO<sub>3</sub><sup>-</sup> content of the soil. The total loss of N due to denitrification is given by:

$$N_d = D_p \times m'_{NO_3} \times m'_w \times m'_b. \quad (3.26)$$

where  $N_d$  is the amount of N emitted from the soil during denitrification (kg N ha<sup>-1</sup>);  $m'_{NO_3}$  is the effect of soil NO<sub>3</sub><sup>-</sup> content on the denitrification,  $m'_w$  is the effect of soil water content on the denitrification, and  $m'_b$  is the effect of biological activity on denitrification.  $D_p$  is the potential denitrification rate.  $D_p$  varies as a function of soil texture and soil biological activity, and is considered as site-specific parameter (Hénault et al., 2005).

The equations of the response functions of denitrification with the associated unitless response function ( $m'_{NO_3}$ ,  $m'_w$ ,  $m'_b$ ) as follows:

$$m'_{NO_3} = \frac{N_{NO_3}}{N_{d50} + N_{NO_3}} \quad (3.27)$$

where  $m'_{NO_3}$  is the  $NO_3^-$  modifier for denitrification.  $m'_{NO_3}$  is based on the work of [Hénault and Germon \(2000\)](#).  $N_{d50}$  is soil  $NO_3^-$  content at which denitrification is 50% of its full potential.  $N_{NO_3}$  is the amount of  $NO_3^-$  in the soil ( $kg\ N\ ha^{-1}$ ).

$$m'_w = 0, \frac{\theta_c}{\theta_f} < w_1 \quad (3.28)$$

$$m'_w = \left[ \frac{\frac{\theta_c}{\theta_f} - w_1}{1 - w_1} \right]^{w_2}, \frac{\theta_c}{\theta_f} \geq w_1 \quad (3.29)$$

where  $m'_w$  is the water modifier for denitrification.  $m'_w$  is calculated by the equation presented by [Bradbury et al. \(1993\)](#).  $\theta_c$  is the amount of water held in a particular soil layer above the permanent wilting point ( $mm\ layer^{-1}$ ), and  $\theta_f$  is the amount of water held between field capacity and the permanent wilting point ( $mm\ layer^{-1}$ ).  $w_1$  is the soil water threshold for denitrification.  $w_2$  is the exponent of power function for denitrification.

$$m'_b = BioAct \times CO_2 \quad (3.30)$$

where  $m'_b$  is the biological activity modifier.  $m'_b$  is based on the relationship developed by [Bradbury et al. \(1993\)](#).  $BioAct$  is the rate for soil biological activity.  $CO_2$  is the amount of  $CO_2$  produced during mineralization ( $kg\ C\ ha^{-1}\ timestep^{-1}$ ). This acts as a surrogate measure of the soil biological activity.

The N lost by denitrification,  $N_d$ , is partitioned into  $N_2$  and  $N_2O$  using simple linear relationships. The amount of  $N_2$  gas lost by denitrification,  $N_{d,N_2}$  ( $kg\ N\ ha^{-1}$ ), is given by:

$$N_{d,N_2} = P_w \times P_{NO_3} \times N_d \quad (3.31)$$

where  $N_{d,N_2}$  is amount of  $N_2$  gas lost by denitrification ( $kg\ N\ ha^{-1}$ ),  $P_w$  is the proportion of denitrification into  $N_2$  according to the soil water content,  $P_{NO_3}$  is the proportion of denitrification into  $N_2$  according to the soil  $NO_3^-$  content.

The amount of N<sub>2</sub>O gas lost by denitrification,  $N_{d,N_2O}$  (kg N ha<sup>-1</sup>), is similarly calculated by:

$$N_{d,N_2O} = N_d(1 - (P_w \times P_{NO_3})) \quad (3.32)$$

$$P_w = P_{N_2,f} \times \frac{\theta_c}{\theta_f} \quad (3.33)$$

$$P_{NO_3} = 1 - \left( \frac{N_{NO_3}}{P_{NO_3,f} + N_{NO_3}} \right) \quad (3.34)$$

$P_{N_2,f}$  is the proportion of denitrification into N<sub>2</sub> according to soil water content.  $P_{NO_3,f}$  is NO<sub>3</sub><sup>-</sup> content of the soil at which N is released in equal of N<sub>2</sub> and N<sub>2</sub>O in denitrification process.  $N_{NO_3}$  is the amount of NO<sub>3</sub><sup>-</sup> in the soil (kg N ha<sup>-1</sup>).

For a full description of ECOSSE model refer to [Smith et al. \(2010c\)](#).

### 3.5.3 N-HB model structure

The modules simulate the production of N<sub>2</sub>O in soils through both nitrification ( $N_{n,N_2O}$ ) and denitrification ( $N_{d,N_2O}$ ) pathways. N<sub>2</sub>O was calculated according to

$$N_{2O} = N_{n,N_2O} + N_{d,N_2O} \quad (3.35)$$

$N_{n,N_2O}$  can be further described by [Eqs. \(3.24\)](#) and [\(3.25\)](#).  $N_{d,N_2O}$  can be described by [Eqs. \(3.32\)](#). Therefore, the equation can be further written as follows:

$$N_{2O} = \left( \left( \frac{n_f \theta_c}{\theta_f} \right) + (n_{gas}(1 - n_{NO})) \right) \left( \frac{N_{n,NO}}{n_{gas} \cdot n_{NO}} \right) + (1 - (P_w \cdot P_{NO_3})) N_d \quad (3.36)$$

The module simulates the production of NO in soils only through nitrification, and was calculated using [Eqs. \(3.19\)](#) and [\(3.25\)](#).

Therefore, the equation can be further written as follows:

$$NO = n_{gas} \cdot n_{NO} \cdot N_{NH_4} \left( 1 - e^{-Nitri_{rate} \cdot m_t \cdot m_w \cdot m_{pH}} \right) \left( 1 - \frac{N_{NH_4}}{c_{max} + N_{NH_4} + N_{FERT}} \right) \quad (3.37)$$

Parameter of  $n_{gas}$  and  $n_{NO}$  used here are regarded as the mean value of posterior distribution from the result of HB calibration of N<sub>2</sub>O flux module ([Eqs. \(3.36\)](#)).

The N<sub>2</sub>O and NO sub-models in this study involves a total set of 19 parameters [ $\theta_1, \dots, \theta_{19}$ ]. Prior information was gathered on all parameters from reviewing

literature, which was assigned uniform distributions within their likely range derived from the literature data (Table 5.1). A total of 15 parameters  $[\theta_1, \dots, \theta_6]$  and  $[\theta_{11}, \dots, \theta_{19}]$  were calibrated as site-specific parameters, and other 4 parameters  $[\theta_7, \dots, \theta_{10}]$  were calibrated as global parameters for all sites (Table 5.1).

The hierarchical model structure for the N-HB model is given by as follows:

$$N_2O_{ij} \sim N(\mu_{N_2O,ij}, \sigma_{N_2O}), \quad (3.38)$$

$$NO_{ij} \sim N(\mu_{NO,ij}, \sigma_{NO}), \quad (3.39)$$

where  $N_2O_{ij}$  and  $NO_{ij}$  are the  $i$ -th observation of  $N_2O$  and  $NO$  flux at  $j$ -th class and  $i$ -th data,  $i$  is the data number ranging from 1 to  $N$ ,  $j$  is the sites class number,  $N$  is the total data number. After the HB calibration on  $N_2O$  module, the average value of posterior distribution of  $\theta_9$  and  $\theta_{10}$  was set as a constant to put in  $NO$  flux module.

$$\theta_{k,j} \sim N(\mu_{\theta k}, \sigma_{\theta k}) \quad (3.40)$$

where  $\theta_{k,j}$  is the class-specific model parameter for  $N_2O$  and  $NO$ ,  $k$  is the  $k$ -th number of parameter,  $k=1, \dots, 6$  for  $N_2O$  and  $k=11, \dots, 19$  for  $NO$ , respectively.  $\theta_7, \dots, \theta_{10}$  are the parameters for  $N_2O$  module considered as global-parameters,  $\sigma_{N_2O}$  and  $\sigma_{NO}$  are variance of the model error for  $N_2O$  and  $NO$ . The hyper parameters  $\alpha$  and  $\beta$  ( $\mu_{\theta k}$  and  $\sigma_{\theta k}$  in Eq. (3.41) and Eq. (3.42) described the density of parameter  $\theta_{k,j}$ ,  $\mu_{\theta k}$  and  $\sigma_{\theta k}$  are mean and variance for  $\theta_{k,j}$ . There are two hyper parameters plus 15 site-specific parameters. In HB method, all the hyper parameters also need a prior distribution along with the other parameters (e.g.  $\sigma_{N_2O}$  and  $\sigma_{NO}$ ). The vague prior distribution of hyper parameters  $\mu_{\theta k}$  and  $\sigma_{\theta k}$ ;  $\sigma_{N_2O}$  and  $\sigma_{NO}$  are as shown:

$$\mu_{\theta k} \sim N(0, 10\ 000) \quad (3.41)$$

$$\sigma_{\theta k}, \sigma_{N_2O}, \sigma_{NO} \sim Unif(0, 100) \quad (3.42)$$

where  $N(0, 10\ 000)$  is the normal distribution of  $\mu_{\theta k}$  with mean 0 and variance 10 000 and  $Unif(0, 100)$  is the uniform distribution of  $\sigma_{\theta k}$ ,  $\sigma_{N_2O}$  and  $\sigma_{NO}$  with lower (0) and upper (100) limits. Equations 3.36 & 3.37 were fit to the observed data to estimate model parameters ( $\theta_{k,j}$ ) and the hyper parameters using the HB approach

**Table 3. 6** Description of 19 parameters of N<sub>2</sub>O and NO flux module. The prior probability distribution is defined as uniform between bounds  $\theta_{min}$  and  $\theta_{max}$  which were extracted from literature reviews.

| Gas module                   | Parameter vector $\theta=[\theta_1,...,\theta_{19}]$ |               |                |                                                                                                            | Default value                             | Prior probability distribution |                   |            |                                                                                                                                                                                               |
|------------------------------|------------------------------------------------------|---------------|----------------|------------------------------------------------------------------------------------------------------------|-------------------------------------------|--------------------------------|-------------------|------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|                              | Parameter                                            | Symbol        | Description    | Unit                                                                                                       |                                           | $\theta_{min}(i)$              | $\theta_{max}(i)$ | References |                                                                                                                                                                                               |
| N <sub>2</sub> O flux module | Site-specific                                        | $\theta_1$    | $N_{d50}$      | Soil nitrate content at which denitrification is 50% of its full potential                                 | kg N ha <sup>-1</sup> layer <sup>-1</sup> | 16.5                           | 5                 | 20         | (Stanford et al., 1995), (Maag and Vinther, 1999), (Gabrielle, 2006), (Lehuger et al., 2009), (Bell et al., 2012)                                                                             |
|                              |                                                      | $\theta_2$    | $w_1$          | soil water threshold for denitrification                                                                   | %                                         | 0.62                           | 0.5               | 1          | (Gabrielle, 2006), (Hénault and Germon, 2000), (Johnsson et al., 1991), (Lehuger et al., 2009), (Bell et al., 2012), (Parton et al., 2001), (Frolking et al., 1998)                           |
|                              |                                                      | $\theta_3$    | $w_2$          | Exponent of the power function for denitrification                                                         | uniteless                                 | 1.74                           | 1.3               | 2.5        | (Stanford et al., 1975), (Smith et al., 1998), (Johnsson et al., 1991), (Maag and Vinther, 1996), (Maag and Vinther, 1999), (Skopp et al., 1990), (Lehuger et al., 2009), (Bell et al., 2012) |
|                              | flux                                                 | $\theta_4$    | $BioAct$       | Rate for soil biological activity                                                                          | uniteless                                 | 0.005                          | 0                 | 0.01       | (Bradbury et al., 1993), (Bell et al., 2012)                                                                                                                                                  |
|                              |                                                      | $\theta_5$    | $P_{NO3,f}$    | NO <sub>3</sub> content of the soil at which N is released in equal of N <sub>2</sub> and N <sub>2</sub> O | uniteless                                 | 200                            | 150               | 250        | (Frolking et al., 1998), (Bell et al., 2012)                                                                                                                                                  |
|                              |                                                      | $\theta_6$    | $D_P$          | Potential denitrification rate                                                                             | kg N ha <sup>-1</sup> layer <sup>-1</sup> | Site-specific                  | 0                 | 1          | (Parton et al., 1996), (Parton et al., 2001), (Bell et al., 2012)                                                                                                                             |
|                              | global                                               | $\theta_7$    | $nf$           | Proportion of N <sub>2</sub> O produced due to partial nitrification at filed capacity                     | uniteless                                 | 0.02                           | 0.01              | 0.4        | (Bell et al., 2012)                                                                                                                                                                           |
|                              |                                                      | $\theta_8$    | $P_{N2,f}$     | Denitrification proportioned into N <sub>2</sub> according to water content                                | uniteless                                 | 0.5                            | 0                 | 1          | (Frolking et al., 1998), (Bell et al., 2012)                                                                                                                                                  |
|                              |                                                      | $\theta_9$    | $n_{gas}$      | Proportion of full nitrification lost as gas                                                               | uniteless                                 | 0.02                           | 0.01              | 0.09       | (Bell et al., 2012)                                                                                                                                                                           |
|                              |                                                      | $\theta_{10}$ | $n_{no}$       | Proportion of full nitrification gaseous loss that is NO                                                   | uniteless                                 | 0.4                            | 0.1               | 1          | (Frolking et al., 1998), (Bell et al., 2012)                                                                                                                                                  |
| NO flux module               | Site-specific                                        | $\theta_{11}$ | $Nitri_{rate}$ | Nitrification rate                                                                                         | kg N ha <sup>-1</sup> layer <sup>-1</sup> | 0.6                            | 0                 | 1          | None information                                                                                                                                                                              |
|                              |                                                      | $\theta_{12}$ | $T_1$          | Parameter for air temperature                                                                              | uniteless                                 | 47.9                           | 45                | 55         | (Bradbury et al., 1993)                                                                                                                                                                       |
|                              |                                                      | $\theta_{13}$ | $T_2$          | Parameter for air temperature                                                                              | uniteless                                 | 106                            | 90                | 110        | (Bradbury et al., 1993)                                                                                                                                                                       |
|                              |                                                      | $\theta_{14}$ | $T_3$          | Parameter for air temperature                                                                              | uniteless                                 | 18.3                           | 15                | 25         | (Bradbury et al., 1993)                                                                                                                                                                       |
|                              |                                                      | $\theta_{15}$ | $pH_{cons}$    | Constant for pH modifier                                                                                   | uniteless                                 | 0.56                           | 0.2               | 0.7        | (Parton et al., 1996)                                                                                                                                                                         |
|                              |                                                      | $\theta_{16}$ | $pH_{modif}$   | Shape of pH modifier                                                                                       | uniteless                                 | 0.45                           | 0.2               | 0.7        | (Parton et al., 1996)                                                                                                                                                                         |
|                              |                                                      | $\theta_{17}$ | $pH_{Tr}$      | pH threshold for pH rate change                                                                            | uniteless                                 | 5                              | 4                 | 6          | (Parton et al., 1996), (Mortland, 1970), (Gilmour, 1984)                                                                                                                                      |
|                              |                                                      | $\theta_{18}$ | $m_{w0}$       | Soil water rate modifier for decomposition at permanent wilting point                                      | %                                         | 0.2                            | 0.1               | 0.3        | (Bell et al., 2012)                                                                                                                                                                           |
|                              |                                                      | $\theta_{19}$ | $Cmax$         | Maximum rate of nitrification possible                                                                     | uniteless                                 | 50                             | 40                | 60         | (Parton et al., 1996)                                                                                                                                                                         |

### 3.5.4 Calculations and statistics

HB calibration was applied to the N-HB model by using data of total 15 experimental sites. Bayesian calibration was performed with the statistical package R ([R Development Core Team, 2005](#)), particularly its R2jags package ([Plummer, 2003](#)). Convergence diagnostic analysis and model evaluation and comparison were performed with the R ‘boa’ package ([Smith et al., 2007b](#)). Simple linear regression analysis was applied between the mean values of estimated parameters and soil properties. Analysis of association was used to reveal how well the trends in the measured values were simulated, and indicate whether the model was showing the correct response to changes in conditions; this was calculated using the coefficient of determination ( $R^2$ ) and correlation coefficient ( $r$ ), and the significance of the correlation was quantified using an  $F$  test ([Smith et al., 1997](#)). The degree of coincidence was calculated as the root mean squared error ( $RMSE$ ) and the significance was quantified where standard errors were available by comparing to the calculated value for  $RMSE$  at the 95% confidence interval of the measurements around the mean ([Smith et al., 1997](#)). Bias in the model was analyzed by calculating the mean difference ( $M$ ) and then undertaking a  $t$  test to check for significance in  $M$ . Also bias was analyzed by calculating relative error ( $E$ ) and compare to the  $E$  value at the 95% confidence interval of the measurements.

## 3.6 C budget calculation

### 3.6.1 Measurements of the net biome productivity

NBP is the total rate of organic C accumulation in (or loss from) ecosystems ([Chapin III et al., 2006](#); [Schulze and Heimann, 1998](#); [Buchmann and Schulze, 1999](#)), Based on studies by [Ciais et al. \(2010\)](#), NBP is quantified as

$$NBP = NPP - Rh - CH_4 - H + I \quad (3.43)$$

NPP is the net primary production (NPP) using crop-level yield statistics and crop-specific

allometric relationships developed by [Koga et al. \(2011\)](#).  $R_h$  is the soil heterotrophic respiration ( $R_h$ ), which is calculated based on soil temperature ( $T$ , 5 cm depth) and water-filled pore space (WFPS, 5 cm depth), and soil texture classes ([Li et al., 2015](#)).  $CH_4$  losses from croplands are expected to be a significant component in paddy rice, but in other cropland systems on well aerated soils it is negligible or even a net sink (i.e. methane oxidation outweighs methane production) ([Smith et al., 2010](#)), thus,  $CH_4$  is the  $CH_4$  emission from paddy field in this study.  $CH_4$  flux in a paddy rice field showed a high correlation with the applied amount of straw and was calculated by a function of the amount of straw residues ([Naser et al., 2007](#)).  $H$  is the harvested component of NPP ( $TC_h$ ).  $I$  is the C input into the soil as residue C, which is plant residue C include above-ground residue biomass ( $TC_a$ ) and below-ground biomass ( $TC_b$ ), and C input from manure, which was only considered in grassland ( $2.41 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$ , [Kimura et al., 2010](#)). The ratio of NBP/NPP is defined as the C sequestration efficiency (CE) ([Ciais et al., 2010](#)).

We consider the loss of dissolved C to be of minor importance of the NBP determination in this study. C lost in fires was considered to be low/negligible in northern Japan. Part of the organic material produced during NPP is lost via emission of volatile organic compounds (VOC), we consider VOC as being negligible here because VOC losses in croplands are relatively small compared to losses from forest ([Smith et al., 2010](#)). We consider surface runoff and erosion as being negligible here given the non-hill slopes, permanent soil coverage and level surface at our site ([Leifeld et al., 2011](#)).

### **3.6.2 Estimation of net primary production, carbon harvest and residue carbon inputs**

For each crop, crop-level NPP and plant C inputs from plant residues to the soil were calculated using crop yield ([Table 3.8](#)) and crop-dependent plant parameters ([Table 3.7](#)), which were developed by ([Koga et al., 2011](#)). Crop yield production ( $\text{kg ha}^{-1} \text{ yr}^{-1}$ ) in 1994, 2002, 2005, 2007, 2009 and 2012 were from the total yield production (t) per year and

planted area (ha) in Iwamizawa city ([Ministry of Agriculture, Forestry and Fisheries, Japan](#)). Crop yield production ( $\text{kg ha}^{-1} \text{ yr}^{-1}$ ) in 1959, 1966, 1976 and 1988 were estimated by the total yield production (t) per year and planted area (ha) in Hokkaido ([Ministry of Agriculture, Forestry and Fisheries, Japan](#)).

$$\text{NPP} = TC_h + TC_r + TC_a + TC_b \quad (3.44)$$

$$\text{Plant C input} = TC_a + TC_b \quad (3.45)$$

where  $TC_h$ ,  $TC_r$ ,  $TC_a$  and  $TC_b$  were the quantities of C ( $\text{Mg C ha}^{-1} \text{ yr}^{-1}$ ) found in harvest biomass, non-harvested biomass removed from the field (wheat straw in this study), above-ground residue biomass and below-ground residue biomass, respectively. These, in turn, were calculated as follows:

$$TC_h = Y \times \frac{D_h}{100} \times \frac{C_h}{100} \quad (3.46)$$

$$TC_r = Y \times \frac{D_h}{100} \times R_r \times \frac{C_h}{100} \quad (3.47)$$

$$TC_a = Y \times \frac{D_h}{100} \times R_a \times \frac{C_a}{100} \quad (3.48)$$

$$TC_b = Y \times \frac{D_h}{100} \times R_b \times \frac{C_b}{100} \quad (3.49)$$

where  $Y$  was the crop yield on a fresh weight basis ( $\text{Mg ha}^{-1} \text{ yr}^{-1}$ ) obtained from crop yield statistics ([Table 3.8](#)),  $D_h$  was the dry matter content in harvested biomass (%),  $R_r$ ,  $R_a$  and  $R_b$  were the dry weight ratios of non-harvested biomass removed from the field, above-ground residue biomass and below-ground residue biomass to harvested biomass, respectively, and  $C_h$ ,  $C_r$ ,  $C_a$  and  $C_b$  were the dry weight-based C contents (%) of harvested biomass, non-harvested biomass removed from the field, above-ground residue biomass and below-ground residue biomass, respectively.

Crops such as fruits, melon and pumpkin which are lack of details of crop-dependent plant parameters ([Table 3.7](#)), their NPP ( $\text{Mg C ha}^{-1} \text{ yr}^{-1}$ ) and C in harvest ( $\text{Mg C ha}^{-1} \text{ yr}^{-1}$ ) were estimated from dry weight of total plant ( $\text{Mg C ha}^{-1} \text{ yr}^{-1}$ ) and dry weight of main plant using the empirical linear regression ([Matsumoto, 2000](#)). Dry weight of total plant ( $\text{Mg C ha}^{-1} \text{ yr}^{-1}$ ) and dry weight of main product ( $\text{Mg C ha}^{-1} \text{ yr}^{-1}$ ) were estimated from total crop production ( $\text{kg ha}^{-1} \text{ yr}^{-1}$ ), water content of main product (%) and the ratio of by product to main product

(Eq. 3.50 and 3.51). We used the water content of plant (%) and ratio of main product and by product were developed (Table 3.7).

$$\text{NPP (Mg C ha}^{-1} \text{ yr}^{-1}) = (\text{Crop production of each land use type (kg C ha}^{-1} \text{ yr}^{-1}) \times (100 - \text{Water content of each main product (\%))} / 100 \times (1 + \text{Ratio of by product to main product}) \times 0.446 - 0.00067) \times 0.001 \quad (3.50)$$

$$\text{C in harvest (Mg C ha}^{-1} \text{ yr}^{-1}) = (\text{Crop production of each land use type (kg C ha}^{-1} \text{ yr}^{-1}) \times (100 - \text{Water content of each main product (\%))} / 100 \times 0.446 - 0.00067) \times 0.001 \quad (3.51)$$

The crop residue was defined as that part of the crop not harvested as product, including root. The amount of total crop residue for a given land use type was calculated using the ratio of the by product to the main product (Eq. 3.44).

$$\text{C in residue (kg C ha}^{-1} \text{ yr}^{-1}) = (\text{C in harvest (kg C ha}^{-1} \text{ yr}^{-1})) \times \text{Ratio of by product to main product} \times 0.001 \quad (3.52)$$

**Table 3. 7** Crop-specific allometric relationships and C contents used to estimate crop NPP, C harvest and plant C inputs.

| Crop        | Dry biomass content in harvested biomass (%) | Ratio of plant biomass to harvested biomass in dry weight |                                                     |                                                     | C content (%)               |                                                |                                                     |                                                     |       | main product water content <sup>d</sup> | by prod/main prod <sup>d</sup> |
|-------------|----------------------------------------------|-----------------------------------------------------------|-----------------------------------------------------|-----------------------------------------------------|-----------------------------|------------------------------------------------|-----------------------------------------------------|-----------------------------------------------------|-------|-----------------------------------------|--------------------------------|
|             |                                              | Non-harvested biomass (removed from the field)            | Above-ground residue biomass (returned to the soil) | Below-ground residue biomass (returned to the soil) | Harvested biomass ( $C_h$ ) | Non-harvested biomass (removed from the field) | Above-ground residue biomass (returned to the soil) | Below-ground residue biomass (returned to the soil) |       |                                         |                                |
|             |                                              |                                                           |                                                     |                                                     |                             |                                                |                                                     |                                                     |       |                                         |                                |
|             | $D_h$                                        | $R_r$                                                     | $R_a$                                               | $R_b$                                               | $C_h$                       | $C_r$                                          | $C_a$                                               | $C_b$                                               | %     | % (DW base)                             |                                |
| Soybean     | 85 <sup>a</sup>                              | -                                                         | 1.14(27) <sup>a</sup>                               | 0.298(27) <sup>a</sup>                              | 56(2.1) <sup>a</sup>        | -                                              | 43.5(3.7) <sup>a</sup>                              | 37.9(10) <sup>a</sup>                               | -     | -                                       |                                |
| Potato      | 22.1(4.5) <sup>a</sup>                       | -                                                         | 0.0845(33) <sup>a</sup>                             | 0.0827(23) <sup>a</sup>                             | 43.4(1.4) <sup>a</sup>      | -                                              | 33.3(12) <sup>a</sup>                               | 37(11) <sup>a</sup>                                 | -     | -                                       |                                |
| Buckwheat   | 86.5 <sup>d</sup>                            | -                                                         | 1.2 <sup>b</sup>                                    | 0.17 <sup>b</sup>                                   | 45 <sup>c</sup>             | -                                              | 45.8 <sup>b</sup>                                   | 45.8 <sup>b</sup>                                   | -     | -                                       |                                |
| Vegetable   | 28 <sup>d</sup>                              | -                                                         | 0.7 <sup>b</sup>                                    | 0.04 <sup>b</sup>                                   | 45 <sup>c</sup>             | -                                              | 33.2 <sup>b</sup>                                   | 39.4 <sup>b</sup>                                   | -     | -                                       |                                |
| Onion       | 16 <sup>d</sup>                              | -                                                         | 0.12 <sup>b</sup>                                   | 0.005 <sup>b</sup>                                  | 45 <sup>c</sup>             | -                                              | 39.3 <sup>b</sup>                                   | 40.4 <sup>b</sup>                                   | -     | -                                       |                                |
| Maize       | 19.1(14) <sup>a</sup>                        | -                                                         | 1.47(13) <sup>a</sup>                               | 0.422(67) <sup>a</sup>                              | 47.5(1.3) <sup>a</sup>      | -                                              | 45.2(2.4) <sup>a</sup>                              | 26.4(23) <sup>a</sup>                               | -     | -                                       |                                |
| Greenhouse  | 28 <sup>d</sup>                              | -                                                         | 0.7 <sup>b</sup>                                    | 0.04 <sup>b</sup>                                   | 45 <sup>c</sup>             | -                                              | 33.2 <sup>b</sup>                                   | 39.4 <sup>b</sup>                                   | -     | -                                       |                                |
| Fruits      | -                                            | -                                                         | -                                                   | -                                                   | -                           | -                                              | -                                                   | -                                                   | 89.70 | 0.44                                    |                                |
| Melon       | -                                            | -                                                         | -                                                   | -                                                   | -                           | -                                              | -                                                   | -                                                   | 74.70 | 1.50                                    |                                |
| Pumpkin     | -                                            | -                                                         | -                                                   | -                                                   | -                           | -                                              | -                                                   | -                                                   | 94.70 | 0.53                                    |                                |
| Wheat       | 86.5 <sup>a</sup>                            | 0.986(16) <sup>a</sup>                                    | 0.831(18) <sup>a</sup>                              | 1.1(37) <sup>a</sup>                                | 44 <sup>a</sup>             | 43.5(2.1) <sup>a</sup>                         | 45.2(2.4) <sup>a</sup>                              | 25.3(26) <sup>a</sup>                               | -     | -                                       |                                |
| Grass       | 28 <sup>d</sup>                              | -                                                         | 0.1 <sup>b</sup>                                    | 0.55 <sup>b</sup>                                   | 45 <sup>c</sup>             | -                                              | 43.4 <sup>b</sup>                                   | 43.8 <sup>b</sup>                                   | -     | -                                       |                                |
| Paddy       | 95 <sup>d</sup>                              | 1.2 <sup>b,e</sup>                                        | 1.42 <sup>b</sup>                                   | 0.27 <sup>b</sup>                                   | 45 <sup>c</sup>             | 38.1 <sup>e</sup>                              | 38 <sup>b</sup>                                     | 38 <sup>b</sup>                                     | -     | -                                       |                                |
| Bush Fallow | -                                            | -                                                         | -                                                   | -                                                   | -                           | -                                              | -                                                   | -                                                   | -     | -                                       |                                |

<sup>a</sup> Data from [Koga et al. \(2011\)](#)<sup>b</sup> Data from [Ogawa \(1988\)](#)<sup>c</sup> The C content of crop dry matter was assumed to be 45% from [Matsumoto \(2000\)](#) when there is no detailed data of C content in harvested biomass, above-ground residue biomass and below-ground residue biomass.<sup>d</sup> Guidelines for cultivation of green manure crops in Hokkaido, Hokkaido Government of Agriculture, Hokkaido Agricultural Development and Extension Association.<sup>e</sup> Data from [Naser \(2006\)](#)

**Table 3. 8** Crop yield (Mg C ha<sup>-1</sup> yr<sup>-1</sup>) data in the Ikushunbetsu watershed from 1959 to 2011.

| Year          | 1959 <sup>a</sup> | 1966 <sup>a</sup> | 1976 <sup>a</sup> | 1988 <sup>a</sup> | 1994 <sup>b</sup> | 2002 <sup>b</sup> | 2005 <sup>b</sup> | 2007 <sup>b</sup> | 2009 <sup>b</sup> | 2012 <sup>b</sup> |
|---------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|
| Soybean       | 1.5               | 0.7               | 1.8               | 1.9               | 2.4               | 2.1               | 2.3               | 2.7               | 2.2               | 2.7               |
| Potato        |                   |                   |                   |                   | 24.2              | 28.6              | 28.6              | 31.4              | 26.9              | 25.8              |
| Buckwheat     |                   |                   |                   |                   | 0.7               | 0.9               | 0.8               | 0.7               | 0.7               | 0.9               |
| Vegetable     | 22.6              | 27.0              | 51.2              | 53.5              | 55.2              | 61.5              | 62.2              | 64.5              | 56.6              | 63.4              |
| Onion         | 65.5              | 46.9              | 56.2              | 50.2              | 42.2              | 53.1              | 51.0              | 37.4              | 37.4              | 50.0              |
| Maize         |                   |                   |                   |                   | 10.2              | 11.3              | 10.8              | 10.4              | 10.4              | 11.2              |
| Greenhouse    |                   |                   |                   |                   | 55.2              | 61.5              | 62.2              | 64.5              | 56.6              | 63.4              |
| Fruits        |                   |                   |                   |                   | 8.9               | 7.3               | 8.5               | 8.5               | 8.5               | 8.5               |
| Melon         |                   |                   |                   |                   | 18.4              | 18.4              | 20.2              | 21.1              | 21.1              | 22.3              |
| Pumpkin       |                   |                   |                   |                   | 19.8              | 15.3              | 14.6              | 10.8              | 11.2              | 12.8              |
| Wheat         | 2.0               | 1.2               | 3.1               | 4.1               | 3.9               | 4.5               | 4.7               | 5.0               | 3.4               | 4.9               |
| Grass         | 21.3              | 21.5              | 30.9              | 42.2              | 34.8              | 33.9              | 34.4              | 33.5              | 32.8              | 32.9              |
| Paddy         | 3.1               | 3.9               | 4.5               | 4.9               | 5.3               | 5.4               | 6.0               | 5.4               | 4.9               | 5.7               |
| Bush / Fallow | 38.4              | 38.4              | 38.4              | 38.4              | 38.4              | 38.4              | 38.4              | 38.4              | 38.4              | 38.4              |

<sup>a</sup> Crop yield were estimated from the total yield production (t) per year and planted area (ha) in Hokkaido (Ministry of Agriculture, Forestry and Fisheries, Japan).

<sup>b</sup> Crop yield were estimated from the total yield production (t) per year and planted area (ha) in Iwamizawa city (Ministry of Agriculture, Forestry and Fisheries, Japan)

### 3.6.3 Soil heterotrophic respiration

Soil heterotrophic respiration ( $R_h$ ) was from decomposition of soil organic matter decomposition (SOMD) in uplands, which was simulated based on soil temperature ( $T$ , 5 cm depth), water-filled pore space (WFPS, 5 cm depth) and soil texture (Li et al., 2015). Soil temperature was calculated by air temperature based on the empirical equation (Kimura et al., 2010). We converted the gravimetric soil water content data simulated by HYDRUS-1D to WFPS after making the assumption, based on local soil textural data, that bulk density of the clay loam (CL), light clay (LiC), silty caly (SiC) and silty caly loam (SiCL) was 1.22 ( $\pm 0.15$ ) g/cm, 1.15 ( $\pm 0.12$ ) g/cm, 1.12 ( $\pm 0.11$ ) g/cm and 1.09 ( $\pm 0.00$ ) g/cm, respectively. Gravimetric soil water content in each soil texture was simulated by HYDRUS-1D in the 0–5 cm soil layer (Li et al., 2015).

### 3.6.4 Uncertainty in net biome productivity

Uncertainty classes were assigned to individual budget terms depending on the accuracy of the data source using a similar classification scheme as proposed by (Vogt et al., 2013). The overall uncertainty of the NBP ( $E_{\Delta NBP/\Delta t}$ ) was calculated as the square root of the sum of the error ( $E$ ) squares.

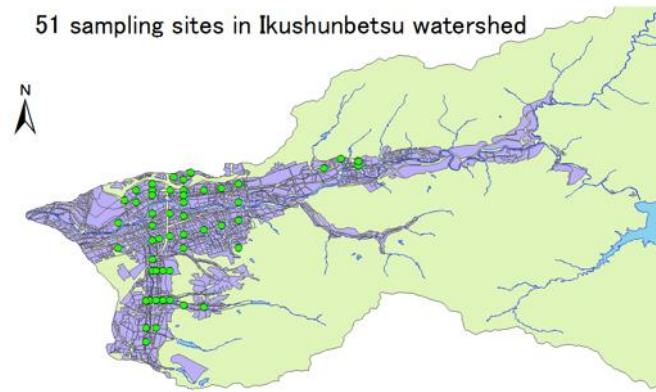
$$E_{\Delta NECB/\Delta t} = \text{sqrt}[(E_{NPP})^2 + (E_{Rh})^2 + (E_{CH4})^2 + (E_H)^2 + (E_I)^2] \quad (3.53)$$

The uncertainty associated with the NPP ( $E_{NPP}$ ) is estimated based on standard deviations for  $TC_h$ ,  $TC_r$ ,  $TC_a$  and  $TC_b$ . Uncertainty of  $TC_h$ ,  $TC_r$ ,  $TC_a$  and  $TC_b$  were calculated based on standard deviations of crop-specific plant parameters (Table 3.7). The uncertainty of C harvest and plant C inputs was based on standard deviation of crop-specific plant parameters (Table 3.7). The uncertainty of manure C inputs is estimated to be low (10%) (Kimura et al., 2011). The uncertainty of ( $E_{Rh}$ ) is considered to be the 95% confidence interval of the simulated value (Li et al., 2015). The uncertainty of  $CH_4$  emissions ( $E_{CH4}$ ) is estimated to be high (90%) due to straw application in paddy rice

field ([Naser et al., 2007](#)). The Temporal uncertainty of NPB was estimated as the inter-annual variation between 1959 and 2011.

### 3.6.5 Soil inventory

There are total 51 soil sampling sites across land use of upland, paddy and grass at Ikushunbetsu river watershed. Sampling points at regional scale were drawn on a map and the main soil type of was determined using ArcGIS. Soil properties sampling were conducted every two years from 2002 to 2011, with the number of sampling points  $N=51$  drawn on an ArcGIS map ([Fig. 3.8](#)). The land use change from paddy to upland occurs at only 3 soil-sampling sites from 2005–2011. There are 4 soil-sampling sites at grass, 15 at paddy, 29 at upland from 2005–2011. The first soil inventory took place on September 2005 and the second one on September 2011. For each soil inventory, in the soil depth (0–30 cm), each soil depth was divided into 2 or 3 layers, volumetric soil samples were taken by hand with steel cores ( $100\text{ cm}^3$ ) in each layers with 5 replications. Soil samples were sieved over 0.5 mm mesh to remove stones and coarse roots and dried as dry soil. Total C (TC) ( $\text{mg C kg}^{-1}$ ) was analyzed by TC analyzer ([NC-1000, Sumika Chemical Analysis Service, Ltd., Osaka, Japan](#)). Bulk Density (BD) ( $\text{Mg m}^{-3}$ ) was measured in 2007, 2009 and 2011. There was no data record of BD in 2005, therefore, the average value from 2007–2011 was used to calculate BD in 2005. The change of soil C stock at non land-use change at individual land use (upland, paddy, grass) from 2005–2011 was compared with the C budget change from NBP method.



**Figure 3. 8** Sampling sites for soil properties (N=51) in Ikushunbetsu watershed.

### 3.6.6 Calculations and statistics

Correlations between each weather variable and residue production ( $\text{Mg C ha}^{-1} \text{ hr}^{-1}$ ) were determined using the Pearson correlation. To determine which combination of weather variables could best predict the observed temporal pattern of residue C input rates (i.e., as an indicator of primary productivity), and growing season (Beginning of April until middle of September) weather data were used as independent variables in a suite of backward stepwise regression (in R).

## 4. Modeling soil carbon dioxide (CO<sub>2</sub>) flux from cropland (CO<sub>2</sub>-HB model)

### 4.1 Introduction

Soil emits CO<sub>2</sub> mainly through microbial decay of plant litter and soil organic matter (SOM) ([Wang and Chen, 2012](#)), and quantitative studies on soil CO<sub>2</sub> flux from SOM is basic and essential for understanding C and N cycle. CO<sub>2</sub> flux estimation have provided insights into the factors controlling soil CO<sub>2</sub> flux, which are mainly soil temperature and soil water, and shown that the importance of these factors varies depending on soil type ([Jenkinson et al., 1991](#); [Raich and Potter, 1995](#); [Hashimoto et al., 2011](#)). [Hashimoto et al. \(2011\)](#) developed a simple greenhouse gas (SG) model based on three functions, namely soil physico-chemical properties, soil temperature, and soil water, and calibration revealed that the physico-chemical properties of the soil were less sensitive than soil temperature or soil water upon simultaneous application of these functions. The SG model is a complete pooled model created as one single model across all soil textures and sites; therefore, it neglects the inherent variation among CO<sub>2</sub> fluxes. As data often arrive with a multilevel structure (e.g., soils with different textures, with sampling performed on-site), the effect of soil water on soil gas flux (CO<sub>2</sub>, N<sub>2</sub>O, and CH<sub>4</sub>) is considered to depend on soil texture or clay content ([Parton et al., 1996](#)). Because the effect of soil water and soil temperature on CO<sub>2</sub> flux varies across different soil textures, thus, this chapter simulates CO<sub>2</sub> flux from soil at a daily time resolution, addresses the uncertainties associated with CO<sub>2</sub> flux estimation by the HB method, and quantifies the response of CO<sub>2</sub> flux to environmental factors with soil texture-specific estimation using a hierarchical structure.

## 4.2 Results

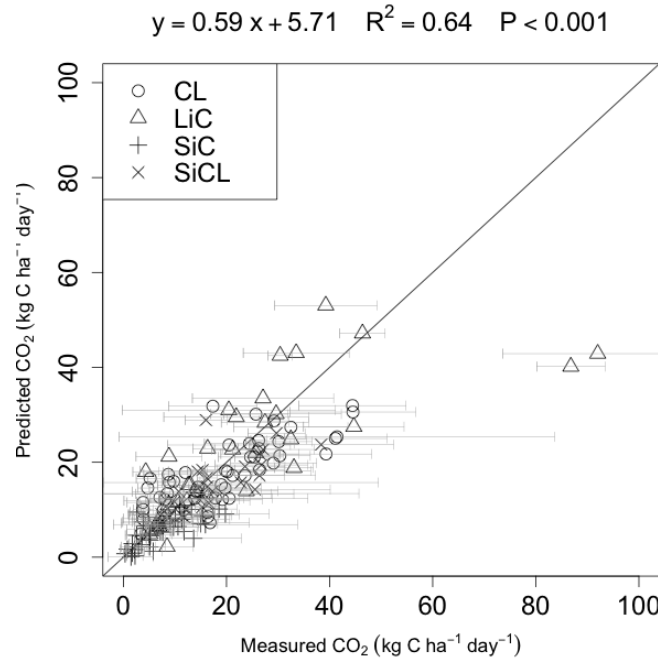
### 4.2.1 Hierarchical Bayesian calibration

The median, mean, and standard deviation values, in addition to the 95% confidence interval levels of the posterior probability distribution of the parameters ( $\beta_1$ ,  $\beta_2$ ,  $\beta_3$ ,  $\beta_5$ , and  $\beta_6$ ) estimated for the best fit of the HB model for each soil texture are summarized in Table 4.1. Daily CO<sub>2</sub> fluxes for each soil texture were predicted from the mean values, together with the soil temperature and WFPS. The HB model captured a large part of the measured variation in CO<sub>2</sub> fluxes (Fig. 4.1), with an  $R^2$  of 0.64 ( $P < 0.001$ ). The plots of the predicted against measured CO<sub>2</sub> fluxes for each soil texture were distributed around the 1:1 line (Fig. 4.1), indicating that the HB model could produce reliable predicted values for each soil texture. The value of  $R^2$  for CL, LiC, SiC, and SiCL were 0.58 ( $P < 0.001$ ),  $R^2 = 0.55$  ( $P < 0.001$ ),  $R^2 = 0.48$  ( $P < 0.001$ ), and  $R^2 = 0.57$  ( $P < 0.001$ ), respectively. The HB model accurately predicted the direction, timing, and magnitude of changes in CO<sub>2</sub> flux, and more than 90% of the predicted CO<sub>2</sub> flux values were distributed within the 95% confidence interval of the measured data (Fig. 4.2). The measured CO<sub>2</sub> flux showed clear seasonality, with high levels in summer and low levels in spring and autumn (no observation was conducted in winter), showed a good correspondence with the seasonality of soil temperature (Fig. 4.2). The resulting posterior area-specific export described by the 95% confidence interval can provide both point and interval estimations of CO<sub>2</sub> flux at different times. Taking the peak CO<sub>2</sub> flux at SiCL in the summer of 2008 as an example, the mean value was calculated as 28.9 kg C ha<sup>-1</sup> day<sup>-1</sup>, the median value was 23.2 kg C ha<sup>-1</sup> day<sup>-1</sup>, and the 95% confidence interval ranged from 10.2 to 69.7 kg C ha<sup>-1</sup> day<sup>-1</sup>.

**Table 4. 1** Characteristic values for posterior probability distributions of the parameters fit for hierarchical Bayesian (HB) CO<sub>2</sub> flux model for each soil texture. A uniform distribution was assumed for every prior distribution.

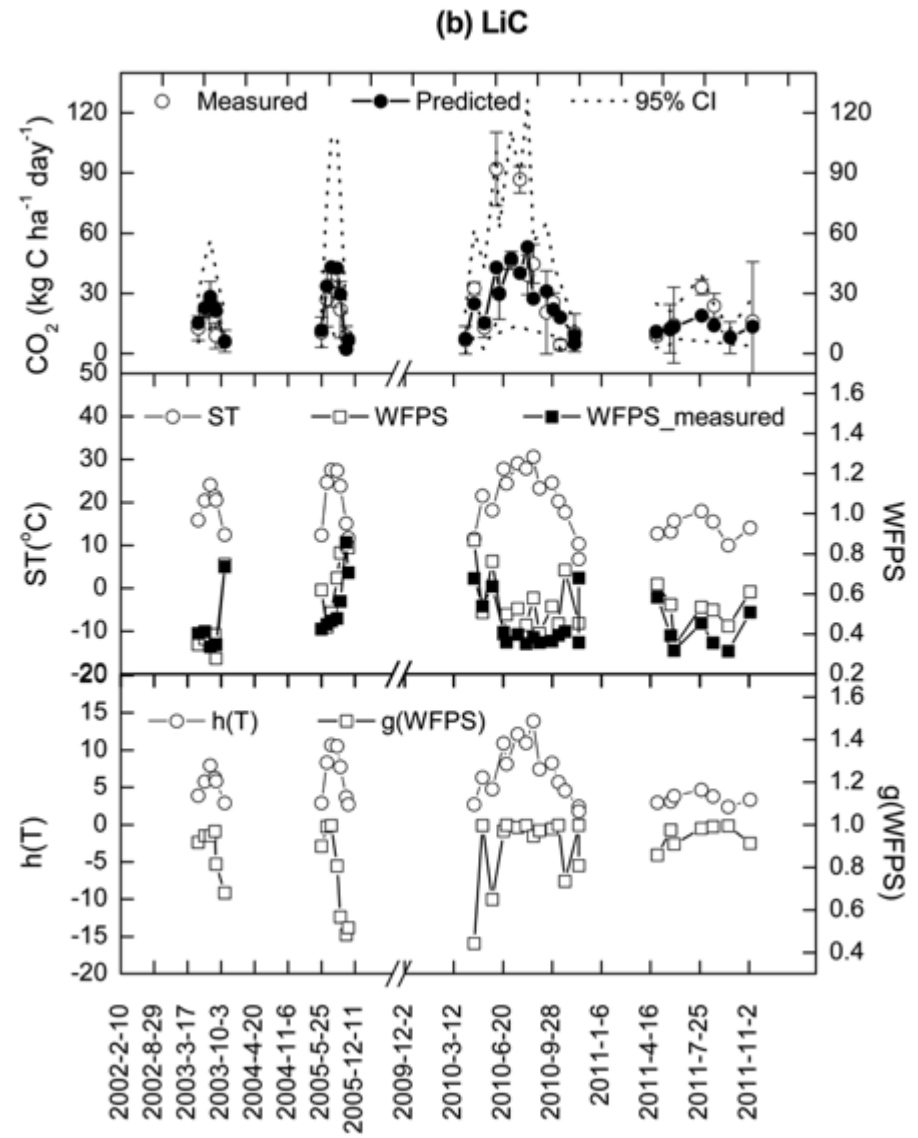
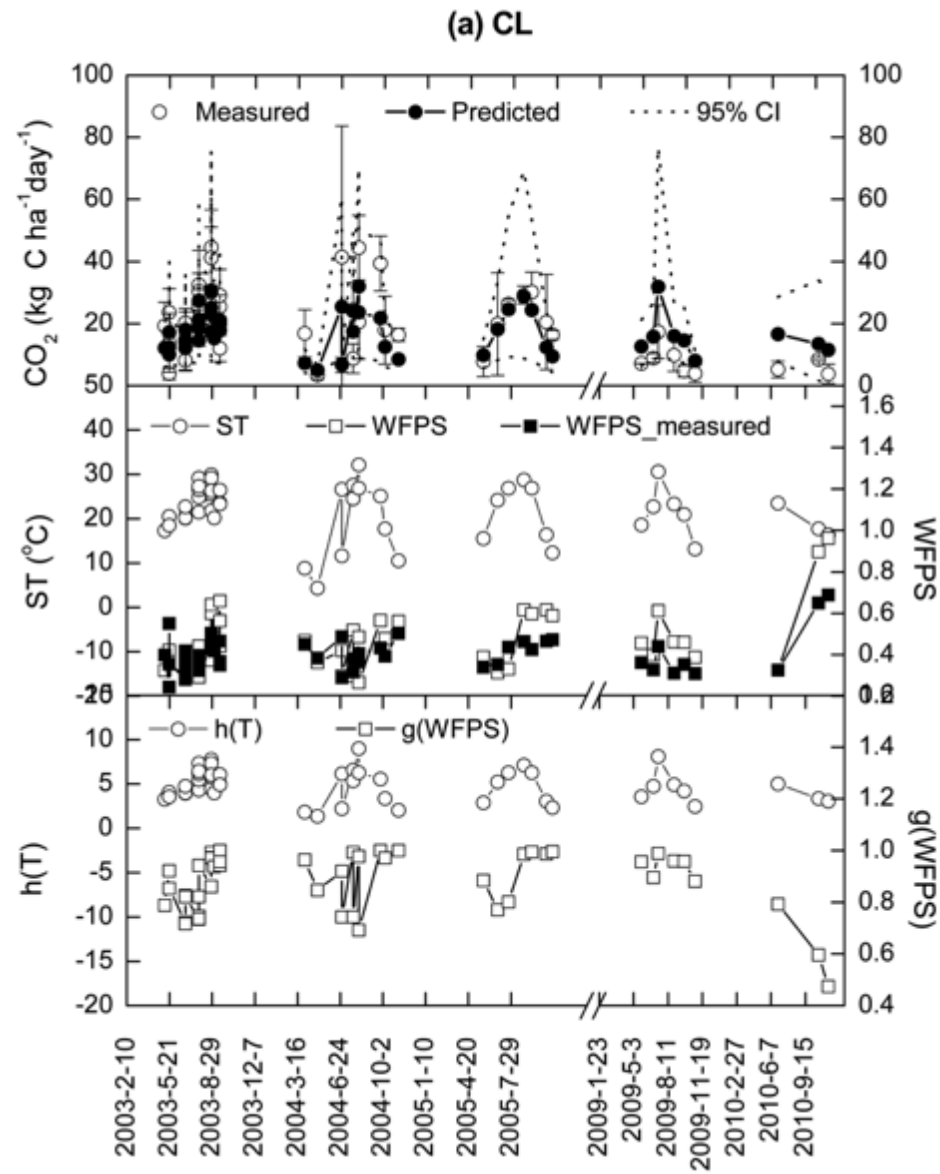
| Soil texture  | Function         | Parameter     | Median | Mean   | SD     | 2.50%  | 97.50% |
|---------------|------------------|---------------|--------|--------|--------|--------|--------|
| CL( $j=1$ )   |                  | $\beta_{k,i}$ |        |        |        |        |        |
|               | constant         | $\beta_{1,1}$ | 1.470  | 1.491  | 0.253  | 1.040  | 1.982  |
|               | $h(T)$           | $\beta_{2,1}$ | 0.067  | 0.065  | 0.011  | 0.046  | 0.087  |
|               | $g(\text{WFPS})$ | $\beta_{3,1}$ | -1.405 | -1.327 | 0.477  | -1.968 | -0.277 |
|               |                  | $\beta_{4,1}$ | 0.553  | 0.547  | 0.066  | 0.410  | 0.679  |
|               |                  | $\beta_{5,1}$ | 2.252  | 2.254  | 0.561  | 1.075  | 2.959  |
|               |                  | $\beta_{6,1}$ | 13.522 | 14.014 | 9.051  | 1.870  | 35.947 |
|               |                  |               |        |        |        |        |        |
| LiC( $j=2$ )  |                  |               |        |        |        |        |        |
|               | constant         | $\beta_{1,2}$ | 1.637  | 1.658  | 0.225  | 1.035  | 1.897  |
|               | $h(T)$           | $\beta_{2,2}$ | 0.074  | 0.073  | 0.011  | 0.063  | 0.104  |
|               | $g(\text{WFPS})$ | $\beta_{3,2}$ | -1.241 | -1.191 | 0.518  | -1.975 | -0.139 |
|               |                  | $\beta_{4,2}$ | 0.474  | 0.468  | 0.064  | 0.325  | 0.575  |
|               |                  | $\beta_{5,2}$ | 2.344  | 2.326  | 0.498  | 1.213  | 2.970  |
|               |                  | $\beta_{6,2}$ | 14.417 | 14.991 | 10.239 | 2.344  | 40.463 |
|               |                  |               |        |        |        |        |        |
| SiC( $j=3$ )  |                  |               |        |        |        |        |        |
|               | constant         | $\beta_{1,3}$ | 0.892  | 0.938  | 0.228  | 1.008  | 1.837  |
|               | $h(T)$           | $\beta_{2,3}$ | 0.059  | 0.057  | 0.012  | 0.019  | 0.065  |
|               | $g(\text{WFPS})$ | $\beta_{3,3}$ | -1.142 | -1.142 | 0.478  | -1.964 | -0.234 |
|               |                  | $\beta_{4,3}$ | 0.544  | 0.541  | 0.042  | 0.443  | 0.614  |
|               |                  | $\beta_{5,3}$ | 2.175  | 2.203  | 0.531  | 1.158  | 2.958  |
|               |                  | $\beta_{6,3}$ | 18.822 | 18.314 | 11.994 | 5.169  | 47.582 |
|               |                  |               |        |        |        |        |        |
| SiCL( $j=4$ ) |                  |               |        |        |        |        |        |
|               | constant         | $\beta_{1,4}$ | 1.658  | 1.670  | 0.188  | 1.264  | 1.997  |
|               | $h(T)$           | $\beta_{2,4}$ | 0.060  | 0.059  | 0.010  | 0.044  | 0.082  |
|               | $g(\text{WFPS})$ | $\beta_{3,4}$ | -1.401 | -1.320 | 0.504  | -1.973 | -0.182 |
|               |                  | $\beta_{4,4}$ | 0.610  | 0.602  | 0.045  | 0.537  | 0.697  |
|               |                  | $\beta_{5,4}$ | 2.325  | 2.308  | 0.546  | 1.087  | 2.961  |
|               |                  | $\beta_{6,4}$ | 13.723 | 14.194 | 7.290  | 2.105  | 29.207 |

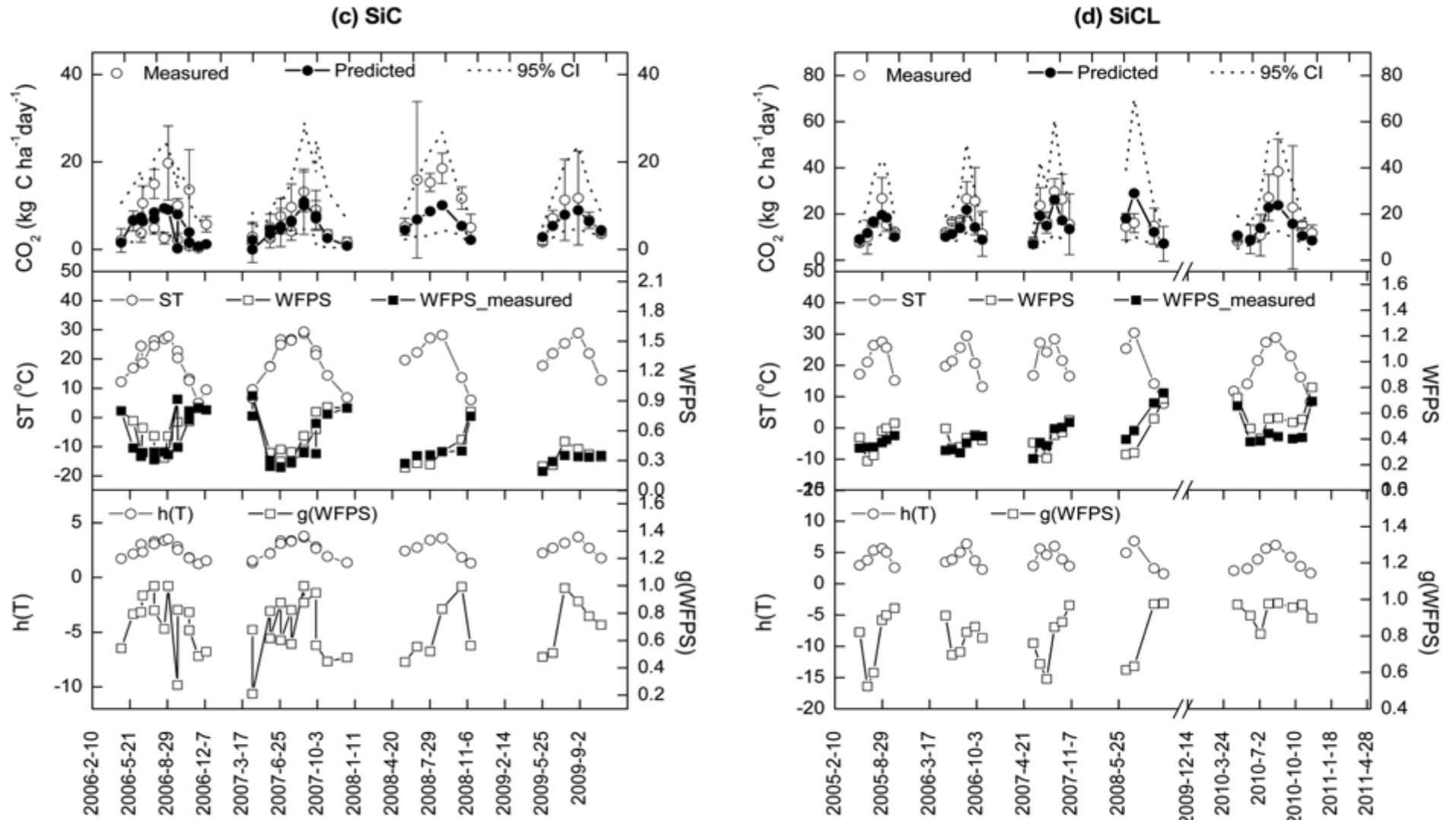
$\beta_{1,i}$  is the constant;  $\beta_{2,i}$  is the parameter for soil temperature function  $h(T)$ ;  $\beta_{3,i}$ ,  $\beta_{4,i}$  and  $\beta_{5,i}$  are minimum, optimum and maximum values of WFPS, respectively.  $\beta_{6,i}$  is the parameter controlling curvature of soil moisture function.



**Figure 4. 1** Comparison between CO<sub>2</sub> flux predicted by hierarchical Bayesian (HB) model and measured CO<sub>2</sub> flux. Bars indicate standard deviation for measured value.

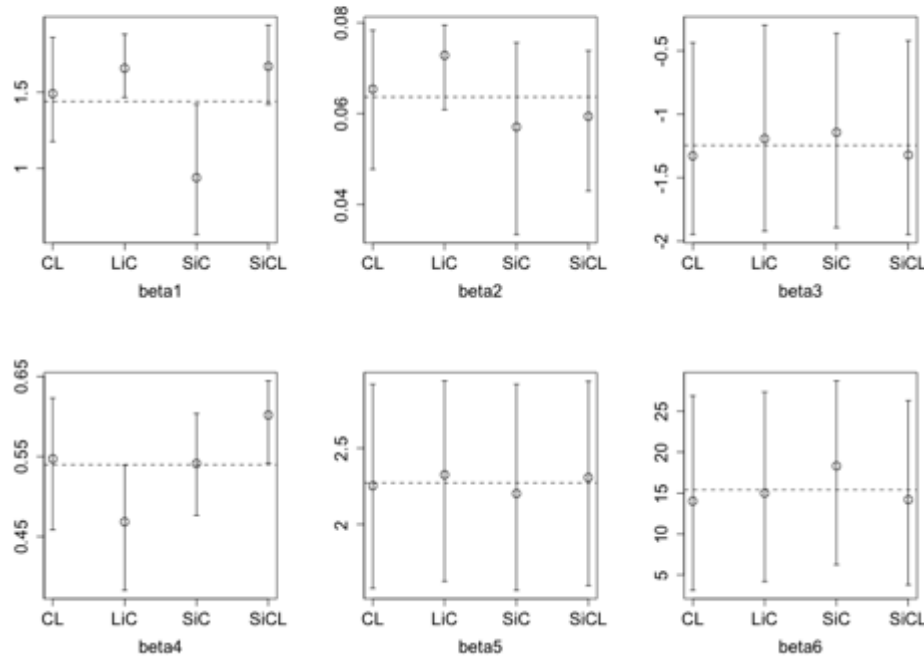
Daily CO<sub>2</sub> fluxes predicted by HB generally followed the pattern of the measured fluxes; however, some discrepancies were observed, especially regarding the high spike of CO<sub>2</sub> prediction, *e.g.*, in LiC measured in the summer of 2010 (Fig. 4.2). There were some further discrepancies between the measurements and predictions, particularly for SiC soils, where the model underestimated CO<sub>2</sub> flux in 2008 and failed to reproduce the wide fluctuations in 2006. High CO<sub>2</sub> peaks with high standard deviations explain the large discrepancies. The upper range of the 95% CI included high values, suggesting that the HB model exhibited high uncertainty for high CO<sub>2</sub> flux values (Wang et al., 2010). CO<sub>2</sub> flux had a larger confidence interval (95%) in the summer months of the study years (Fig. 4.2), indicating that the uncertainty of prediction increased with increased temperature.





**Figure 4. 2** Change in CO<sub>2</sub> flux, water-filled pore space (WFPS), measured value of WFPS (WFPS\_measured) and functions of soil temperature [h(T)] and WFPS [g(WFPS)] for each soil texture of (a) CL, (b) LiC, (c) SiC and (d) SiCL. Bars in measured CO<sub>2</sub> flux indicate standard deviation. Predicted CO<sub>2</sub> flux was estimated by the hierarchical Bayesian (HB) model. 95% CI of CO<sub>2</sub> flux was the range of quantile between 2.5% and 97.5% of the posterior distribution of the predicted CO<sub>2</sub> flux at each sampling time.

Figure 4.3 shows the posterior density intervals of the estimated parameters after calibration with texture-specific estimation. Such representation makes it possible to visualize differences between parameter pdfs across textures, whereas the shape of the intervals reveals the dispersion and symmetry of the marginal distribution. For the parameters  $\beta_3$ ,  $\beta_5$ , and  $\beta_6$ , the posterior density intervals overlapped, indicating a lack of credible differences among soil textures. A significant difference was found for SiC-LiC and SiC-SiCL in  $\beta_1$  and LiC-SiCL in  $\beta_4$ . For  $\beta_2$ , though the posterior density intervals did not all overlap, and there were no clear differences among soil textures.



**Figure 4. 3** Posterior density intervals of calibrated parameters ( $\beta_1$  to  $\beta_6$ ). Open circles indicate the mean posterior estimate for soil-specific estimation. Error bars are 90% posterior density intervals. Dashed line indicates the mean value over all soil textures.

Table 4.3 shows that the AIC for C:N ratio 2.60 was the smallest among predictor variables of  $\beta_1$  and also smaller than the AIC for no predictor variables. Therefore, the C:N ratio was the best predictor variable for  $\beta_1$ . In the same manner, the best predictor variables for  $\beta_2$ ,  $\beta_3$ ,  $\beta_4$ ,  $\beta_5$ , and  $\beta_6$ , were silt content, clay content, total C content, C:N ratio, and clay content, respectively. The regression analysis is shown in Figure 4.6, and a significant, positive correlation between clay content and parameter  $\beta_3$  was found.

## 4.2.2 Model evaluation and comparison

The HB model achieved better performance than the Bayesian pooled model (Table 4.2), which showed higher RMSE and DIC values than the HB model. In addition,  $R^2$ , which represented the fit of the model prediction to the measured values, was lower in the Bayesian pooled model (0.39) than in the HB model (0.64). However, the HB model required a higher effective number of parameters ( $pD$ ) (21.6) than the Bayesian pooled model (5.1). These findings indicate that the HB model provided better predictions but with increased model complexity. Table 4.2 also shows the goodness of fit of the effect of soil temperature and WFPS on daily CO<sub>2</sub> flux. The HB model with only the  $h(T)$  function explained 61% of the variability in the measured CO<sub>2</sub> flux, whereas 21% of the variability in the measured CO<sub>2</sub> flux was explained by the HB model with only the  $g(WFPS)$  function. DIC was also smaller in the full HB model (996) than in the HB model with only the  $h(T)$  function (1018) or only the  $g(WFPS)$  function (1131).

**Table 4. 2** Root mean square error (RMSE); deviance information criterion (DIC) of nonhierarchical Bayesian model (Bayesian pooled model) and hierarchical Bayesian (HB) model of CO<sub>2</sub> flux and determination coefficient ( $R^2$ ) of the correlation between measured and predicted values.  $exp(\beta_1)h(T)$  and  $exp(\beta_1)g(WFPS)$  represent HB model structure including only the response function for soil temperature and including only the response function for WFPS.

| Model                     | RMSE | DIC  |                |      | $R^2$ |
|---------------------------|------|------|----------------|------|-------|
|                           |      | $pD$ | $\overline{D}$ | DIC  |       |
| Bayesian Pooled           | 10.6 | 5.1  | 1168           | 1173 | 0.39  |
| Hierarchical Bayesian     |      |      |                |      |       |
| $exp(\beta_1)h(T)g(WFPS)$ | 8.37 | 21.6 | 974            | 996  | 0.64  |
| $exp(\beta_1)h(T)$        | 8.77 | 14.0 | 1004           | 1018 | 0.61  |
| $exp(\beta_1)g(WFPS)$     | 14.3 | 16.2 | 1115           | 1131 | 0.21  |

**Table 4. 3** The value of Akaike's Information Criterion (AIC) for selecting the best variables for estimated parameters. Smaller AIC value shows better predictor variable.

|           | silt   | clay   | silt+clay | TC     | TN     | C:N    | No predictor variables |
|-----------|--------|--------|-----------|--------|--------|--------|------------------------|
| $\beta_1$ | 5.70   | 5.34   | 4.85      | 7.66   | 7.65   | 2.60   | 5.66                   |
| $\beta_2$ | -28.08 | -23.38 | -24.96    | -26.42 | -26.88 | -23.31 | -25.28                 |
| $\beta_3$ | -3.55  | -14.24 | -6.01     | -3.22  | -2.92  | -8.24  | -4.81                  |
| $\beta_4$ | -8.08  | -7.69  | -7.04     | -12.43 | -11.21 | -8.19  | -9.00                  |
| $\beta_5$ | -7.93  | -7.46  | -7.88     | -6.91  | -6.91  | -9.62  | -8.91                  |
| $\beta_6$ | 19.01  | 14.99  | 15.68     | 21.75  | 21.70  | 15.96  | 19.76                  |

### 4.2.3 Behavior of response functions of CO<sub>2</sub> flux to soil temperature and soil water [ $h(T)$ and $g(WFPS)$ ]

Different soil textures showed different tendencies for the response function  $h(T)$  (Fig. 4.4). Light silt and clay soils showed the highest value for parameter  $\beta_2$  of the response function  $h(T)$  (Table 4.1) and also demonstrated the steepest increase of  $h(T)$  with increased soil temperature, followed by CL and SiCL, whereas SiC showed only a slight increase in  $h(T)$ . Parameter  $\beta_2$  was negatively correlated with the silt content, although the  $R^2$  of 0.7 was not significant (Fig. 4.6). The  $Q_{10}$  value calculated as  $Q_{10} = \exp(10\beta_2)$  was highest for LiC (2.08, with 1.87–2.83 of 95% confidence interval (CI)), followed by CL (1.92, with 1.58–2.40 of CI), SiCL (1.80, with 1.55–2.26 of CI), and finally SiC (1.77, with 1.21–1.92 of CI).

Different soil textures also showed different tendencies for the response function  $g(WFPS)$  (Fig. 4.5). Light clay soils showed the lowest optimal WFPS (0.468) for  $g(WFPS)$  (the value of parameter  $\beta_4$  in Table 4.1) and a steep decrease of  $g(WFPS)$  with increases in WFPS over the optimal value, which occurred rapidly in soils containing less clay and silt at above-optimal WFPS levels. In contrast, SiCL soils had the highest value of optimal WFPS (0.602) and a steep increase of  $g(WFPS)$  with increases in WFPS below the optimal values. The optimal WFPS for  $g(WFPS)$  of CL and SiC was 0.547 and 0.541, respectively. However, the change in  $g(WFPS)$  with WFPS was more gradual for CL than for SiC, possibly because CL had a lower value for parameter  $\beta_3$  (−1.327) than SiC (−1.142), thus indicating that insufficient parameter constraints resulted in the low sensitivity of  $g(WFPS)$  in CL.

## 4.3 Discussion

### 4.3.1 Suitability and benefits of Bayesian calibration

Evaluation of the performance of the HB model and the Bayesian pooled models

(Table 4.2), and comparison of the predicted and measured CO<sub>2</sub> flux (Fig. 4.2), show that the HB model provided much better predictions by providing texture-specific parameter estimates, except for the highest peaks with high experimental error which are underestimated in some cases. The HB model thus showed good performance in fitting the soil texture data and in providing reasonable prediction intervals. Prediction intervals are influenced by the combined effects of measurement error, variability in local climate, and soil conditions, and also from the uncertainty inherent in fitting models with finite data sets. When measurements are available across multiple soil types, the HB model provides a basis for pooling this information, thereby reducing the overall uncertainty while still maintaining soil-specific model estimates (Yang et al., 2011). Moreover, the HB model can be applied across different sites and different types of soils, as reflected in the lower RMSE and DIC values, although the model was of a higher complexity and required a higher effective number of parameters.

### 4.3.2 Effect of soil temperature

Both field and laboratory incubation studies have shown that the activity of soil microorganisms to decompose SOM generally increases with temperature and moisture (Drewnik, 2006; Kim et al., 2010); these effects can also be described by models (Xu and Qi, 2001). Additionally, several studies have shown that soil respiration increases exponentially with temperature when soil water or other factors are not limiting (Raich and Potter, 1995; Kätterer et al., 1998). Although soil temperature and moisture both significantly affect CO<sub>2</sub> flux, as the seasonality of soil temperature explains the high variation of CO<sub>2</sub> flux and CO<sub>2</sub> flux decreased when soils were both dry and wet (Fig. 4.2), the HB model with only the  $h(T)$  function explained 61% of the variability in the measured CO<sub>2</sub> flux (Table 4.2), indicating that soil CO<sub>2</sub> flux is primarily dependent soil temperature and that the control of soil water is weak, as previously indicated by another study (Hayakawa et al., 2014; Smith et al.,

2005).

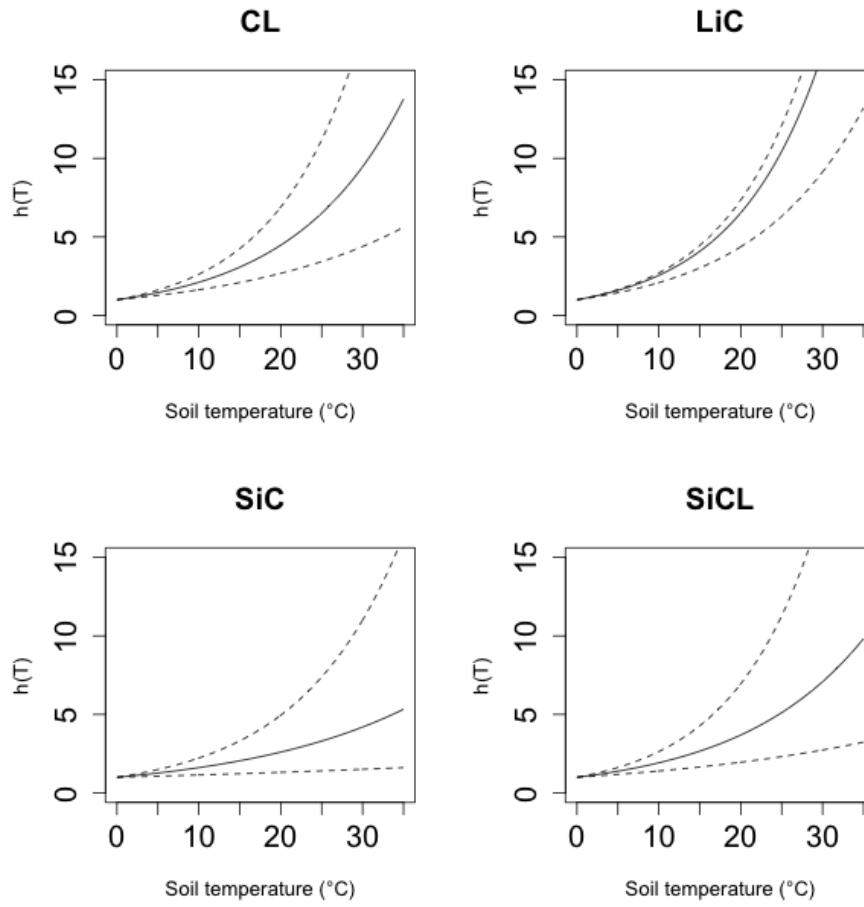
Although numerous investigations have evaluated the influence of texture on microbial activity and SOMD (Hayakawa et al., 2014), the influence of soil texture on soil CO<sub>2</sub> flux is seldom revealed by models. The calibration of the HB model in this study suggest that the effects of soil temperature and soil WFPS on CO<sub>2</sub> flux are complex and change with different soil conditions, and that their effects on CO<sub>2</sub> flux are confounded by each other.

The optimized function of soil temperature [ $h(T)$ ] was mildest in SiC soils among the four textures (Fig. 4.4). The  $Q_{10}$  values for each soil texture were in the range of previously reported values (Lenton and Huntingford, 2003, Hashimoto, 2005). Although parameter  $\beta_2$  for soil temperature did not show significant differences among soil textures (Fig. 4.3),  $\beta_2$  was found to decrease linearly with silt content (Fig. 4.6). The estimation of only four values representing the four soil textures means that the simple linear regression is restricted, and the  $R^2$  value of 0.7 obtained here is not significant (Fig. 4.6). However, our study with a small number of soils revealed that SOMD may be influenced by soil texture. Other studies have revealed that fine-textured soils can absorb organic matter and prevent it from being decomposed by microorganisms (Hassink, 1993; Chevallier et al., 2004), possibly through two mechanisms: (1) physically confining microorganisms in small pores, which makes them less active and protects them against grazing by the soil fauna; and (2) physically protecting nonliving soil organic matter from decomposition by surface adsorption. These may be reasons why temperature sensitivity is low in SiC soil, which had the highest total C and silt and clay content. However, the effect of soil texture on SOMD was undetectable (Hassink, 1993), perhaps because of the confounding effects of variability in substrate availability, microbial biomass (MBC), enzyme activity, and other biochemical characteristics among different soils. Trasar-Cepeda et al. (2007) showed that decomposition activity was highest in the soil

containing the highest amount of OM because the enzyme activity was highest in the soil with the highest OM. Although the amount of organic matter appears to be important, [Trassar-Cepeda et al. \(2007\)](#) indicated that because only a small number of soils was studied, no conclusions can be reached about which soil properties cause the variations of  $Q_{10}$  value.

Similar to most models of soil C dynamics, we simply assumed that SOM decomposition is nearly equally sensitive at different temperatures, but this assumption is contrary to kinetic theory ([Davidson et al., 2006](#); [Kirschbaum, 1995](#)). Some studies observed that temperature sensitivity is far greater at a low temperature than at high temperature ([Kirschbaum, 1995](#)); additionally, the decomposition rate of low-quality substrates has a stronger temperature dependence than that of high-quality substrates ([Bosatta and Ågren, 1999](#)). For simplicity, the temperature function used here adopts a simple exponential temperature response. This simplification may lead to errors in the estimation of soil CO<sub>2</sub> fluxes at low and high temperatures, although this limitation likely had a small effect on the study period because 95% of the measured soil temperature ranged from 6.73 to 30.02 °C ([Fig. 4.4](#)).

$h(T)$  exhibited high uncertainty, probably because the posterior distribution of CO<sub>2</sub> flux had a larger upper interval, particularly in the high-temperature range ([Fig. 4.4](#)). Indeed, occasional high CO<sub>2</sub> fluxes were observed in our study at high temperatures (*e.g.*, in October 2010 in LiC soils; [Fig. 4.2](#)), as also observed in recent studies ([Yang et al., 2011](#)). In addition, the estimation of  $Q_{10}$  from the exponential equation often showed high uncertainty; however, this type of uncertainty is ignored in traditional models.



**Figure 4. 4** Optimized functions of soil temperature [ $h(T)$ ] predicted by the hierarchical Bayesian (HB) model for each soil texture. Dashed line indicates 95% confidence interval.

### 4.3.3 Effect of soil water

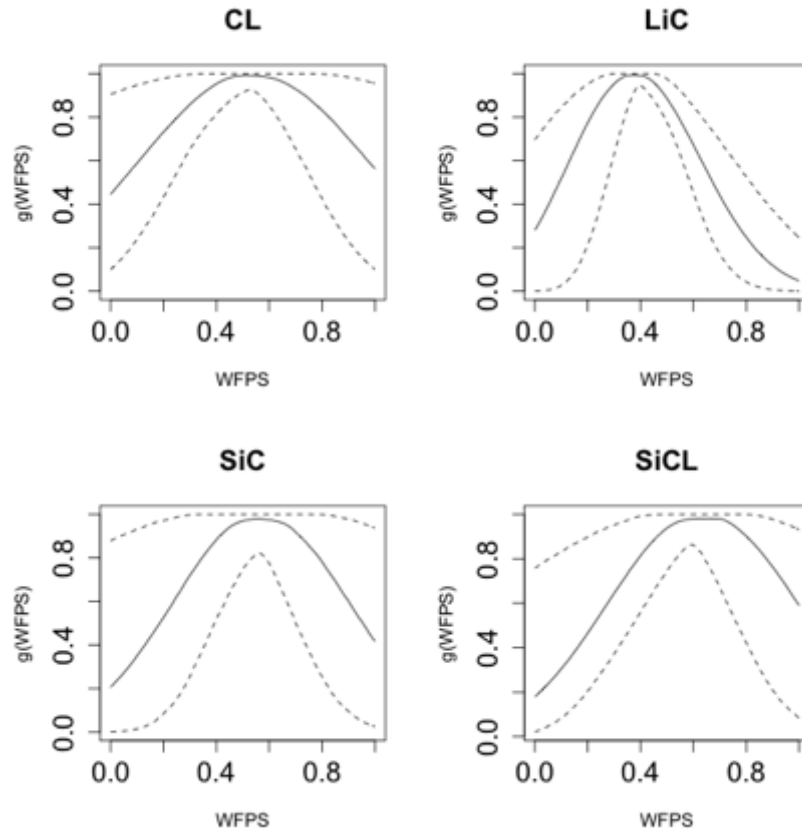
In general, three phases of the response of CO<sub>2</sub> flux to soil water can be identified in many experiments and models (Davidson et al., 2000; Howard and Howard, 1993; Abdalla et al., 2010; Linn and Doran, 1984; Skopp et al., 1990). (1) When soils are relatively dry, biological activities were limited through limitation of soluble organic C-substrates, and then increase strongly with water availability. (2) There is a range of near-optimum soil water content where CO<sub>2</sub> is maximally emitted because the macropore spaces are mostly air-filled, thus facilitating O<sub>2</sub> diffusion, and the micropore spaces are mostly water-filled, thus facilitating diffusion of soluble substrates. (3) Above the field capacity and approaching saturation, oxygen deficiency inhibits aerobic respiration. Therefore, the shape and curve of the response function of soil water for CO<sub>2</sub> become similar (Fig. 4.5), and this is a better way of expressing soil water content in relation to microbial activity (Rovira, 1953). According to the HB model, WFPS values in the range of 0.47 to 0.60 led to more optimal conditions for CO<sub>2</sub> flux for all textures in this study (Fig. 4.5), which was comparable to the optimum WFPS in other studies (0.34 to 0.56) (Howard and Howard, 1993; Hashimoto et al., 2011). However, some soil types showed different curvature in the relationship. Indeed, differences in the relationship between CO<sub>2</sub> flux and soil water for different types of soil have been found in several studies (Howard and Howard, 1993; Singh and Gupta, 1977).

Soil texture influences the effect of WFPS on SOMD and disturbance of the soil can impact the effect of WFPS on soil CO<sub>2</sub> flux (Fig. 4.5). No significant difference among soil textures was found in parameters of  $\beta_3$ ,  $\beta_5$ , and  $\beta_6$ , except for the significant difference of  $\beta_4$  between LiC and SiCL (Fig. 4.3). Del (2000) found that water is held more tightly with a higher clay and silt content; therefore, soil with a lower clay and silt content requires a lower water content to induce water stress on biological activity. The HB model revealed a higher minimum water content

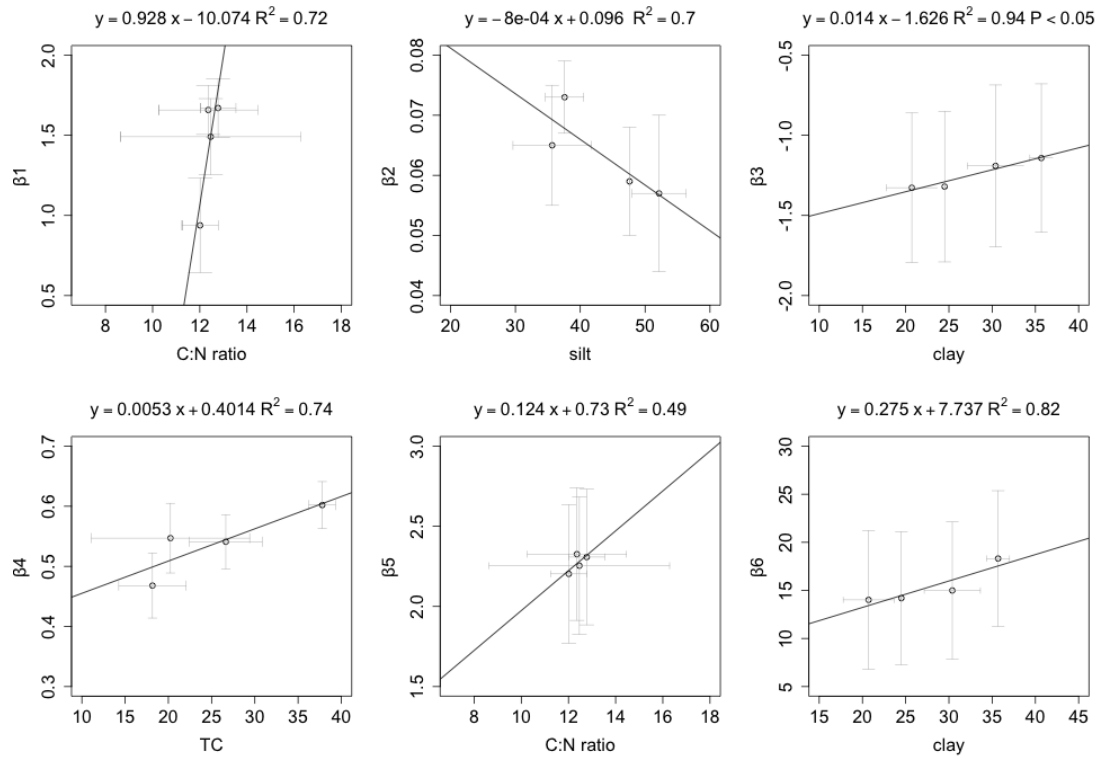
(parameter  $\beta_3$ ) in fine-texture soils with significant  $R^2 = 0.94$  (Fig. 4.6). Parameters  $\beta_4$ ,  $\beta_5$ , and  $\beta_6$  were positively associated with total C content, C:N ratio, and clay content, respectively, although the correlations were not statistically significant. Howard and Howard (1993) found that soil with a large organic matter content will have a lower degree of saturation than soil with a low organic matter content. However, there was no significant relationship between saturation (parameter  $\beta_5$ ) and total C content in this study.

LiC soil exhibited a sharper decrease of  $g(\text{WFPS})$  after the optimum WFPS (parameter  $\beta_4$ ) compared with other soils, which is unrealistic when only considering the effects of soil water on microbial activity because WFPS of approximately 0.47 is not sufficiently high to limit microbial activity or gas diffusion in soils. This phenomenon could be derived from the low  $\text{CO}_2$  flux from wet LiC soil when the snow melts in the end of April and early May, resulting in high soil water and low temperature. The soil water content has a lower effect on  $\text{CO}_2$  flux at a lower temperature than at a higher temperature (Douglas and Tedrow, 1959), and the spring soil respiration is controlled by temperature rather than moisture (Smith et al., 2003). Xu and Qi (2001) also found that the decrease in soil respiration rate at high soil water levels was mainly caused by the low temperature rather than by the moisture itself. This sharp decrease may indicate that correlations between soil water and  $\text{CO}_2$  flux can easily be confounded by other factors (Xu and Qi, 2001; Davidson et al., 1998), and that soil water is not necessarily the single most important factor.

The optimized function of the water-filled pore space [ $g(\text{WFPS})$ ] showed higher uncertainty, higher than that of  $h(T)$  (Fig. 4.4 and 4.5). When the best-fit functions were compared among soil textures, the range of  $g(\text{WFPS})$  in LiC was larger than that in other soils because LiC soils had the largest range of  $\text{CO}_2$  flux ( $4.3\text{--}92.0 \text{ kg C ha}^{-1} \text{ day}^{-1}$ ) among soils.



**Figure 4. 5** Optimized functions of soil water-filled pore space [ $g(\text{WFPS})$ ] predicted by hierarhical Bayesian (HB) model for each soil textures. Dashed line indicates 95% confidence interval.



**Figure 4. 6** Simple linear regression of estimated parameters calibrated by the hierarchical Bayesian (HB) model with soil properties (C:N ratio, silt content, clay content, and total C content). Bars indicate standard deviation.

#### 4.3.4 Model limitation and improvement

Our results confirmed previous findings showing that soil temperature and moisture are key factors affecting daily CO<sub>2</sub> flux, and that their effects on CO<sub>2</sub> flux are dependent on soil texture. Compared to the SG model constructed by [Hashimoto et al. \(2011\)](#), the HB model not only has the advantage of being simple but also reveals that soil texture should be regarded as a possible scaling factor when up-scaling the model from the site to the regional scale. Thus, the HB model simulates daily CO<sub>2</sub> fluxes at various sites using minimal input data consisting only of soil texture, daily soil temperature, and WFPS, and its results have the potential for extrapolation to the regional scale in soils with similar texture in Hokkaido.

Regarding the application and limitations when up-scaling the model from the site to regional scale, first, the limited data for low CO<sub>2</sub> flux from wet soil (*e.g.*, WFPS range from 0.55 to 0.65) from the end of April until early May resulted in an unrealistic function shape (*e.g.*, LiC), which may overemphasize the effects of soil water on CO<sub>2</sub> flux when the same parameter function is applied to the soils of similar texture. However, this effect was weak during early spring because the effect of soil water is strongly masked by soil temperature ([Smith et al., 2003](#); [Xu and Qi, 2001](#)). Therefore, even in early spring, CO<sub>2</sub> flux can be reliably predicted when both functions of soil temperature and moisture are considered in the model, and the soil water function could not constrain CO<sub>2</sub> flux prediction when the HB model was extrapolated to a larger scale. Second, although the temperature effect described by exponential function  $h(T)$  and soil water function  $g(\text{WFPS})$  is widely and reliably used in gas flux model stimulation ([Parton et al., 1996](#); [Del Grosso et al., 2000](#)), the estimated parameters were constrained by the limited amount of data measured in this study. Therefore, the estimated parameters could be applied at the regional scale in Hokkaido for the same seasonal pattern and soil texture, but it is not appropriate to scale up the HB model to a longer temporal scale and larger spatial scale across

different soil types, as the parameter functions obtained in this study may be limited in distinguishing the effects of soil temperature and moisture on a larger temporal scale, especially under low-temperature and wet conditions such as those occurring in early spring. The estimated parameters should be considered as site- or soil-specific parameters rather than global parameters.

Although the small number of studied soils and season patterns limits the application of the model to other fields, the results obtained are sufficient to establish a reliable methodology and provide conclusions that may be generalizable to other soils and climate. This study proposed a method to predict the influence of soil texture on the effects of soil temperature and moisture on CO<sub>2</sub> flux, and soil texture could thus be regarded as an up-scaling factor for future research on regional extrapolation. To enhance the reliability and applicability of the HB model on a larger scale and for other soils, future studies should evaluate data across more soils types, especially for coarse soils and seasonal patterns cover snow season and snow melting period.

## **4.4 Conclusion**

We accurately predicted the daily CO<sub>2</sub> flux and quantified the effect of environmental factors on CO<sub>2</sub> flux with consideration of uncertainty using a HB model. Our results confirm previous findings that soil temperature and WFPS are key factors affecting daily CO<sub>2</sub> flux and demonstrate that the effects on CO<sub>2</sub> flux vary with soil texture. The parameter values resulting from the multi-dataset procedure could then be applied to sites sharing the same soil texture. The posterior distributions estimated by CO<sub>2</sub>-HB model encompass all of our current measurements, and CO<sub>2</sub>-HB model could quantify the uncertainty of CO<sub>2</sub> flux by 95% confidence interval. The HB model structure requires minimal input data for soil texture and simulates daily CO<sub>2</sub> flux using daily soil temperature and WFPS, which may allow the model to be easily applied to the observed CO<sub>2</sub> fluxes.

## 5. Modeling soil nitrous oxide (N<sub>2</sub>O) and nitrogen monoxide

### (NO) flux from cropland (N-HB) model

#### 5.1 Introduction

There are two general approaches to estimating direct N<sub>2</sub>O and NO fluxes from soils in agro-ecosystems. In an empirical model, N<sub>2</sub>O and NO fluxes are proportional to some easily quantifiable factors, and is ignoring complex processes and environmental factors in N cycle ([Lokupitiya and Paustian, 2006](#)). The process-oriented ecosystem models attempt to simulate many or all of the complex components of N cycle; therefore, process-based models have a unique potential to predict N<sub>2</sub>O and NO emissions from arable soils ([Butterbach-Bahl et al., 2004](#); [Gabrielle et al., 2006a](#)). However, model testing is often limited by a lack of field data to which the simulations can be compared ([Desjardins et al., 2010](#)). The input data requirement for process-based models is also often very high, which leads to the limited use in regional or national predictions from agricultural land ([Beheydt et al., 2007](#); [Bell et al., 2012](#)). The model designed and produced to simulate soil N gaseous emissions from soils using only data which is available at national or regional scale where only a minimum amount of meteorological, land-use and soil input data is needed ([Smith et al., 2010](#)).

A remaining obstacle to the extrapolation of the N<sub>2</sub>O model is that some parameters should be measured or estimated on sites ([Lehuger et al., 2009](#)). In traditional model development, parameters of N<sub>2</sub>O and NO emissions modules in process-based models are considered universal, because variability of these parameters are not well known in different soils and land managements. However, both theory and observation suggest that the assumption of commonality in parameter values across systems may

not always be valid (Borsuk et al., 2001). For ecological modeling, parameter uncertainty estimates is essential (Beck, 1987), and a Bayesian approach provides such information (Malve and Qian, 2006). In the Bayesian framework, the problem of parameter estimation using cross-system data can be viewed as a hierarchy. HB models represent a modeling structure with capacity to exploit diverse sources of information, and yields subunit-specific parameter estimates (Clark, 2005), but shares commonality in values across systems. The HB approach is, therefore, a practical compromise between entirely site-specific and globally common parameter estimate, which could be the potential strategy to deal with model extrapolation and parameters' variability (Lehuger et al., 2009).

Therefore, this chapter designs and produces the model to simulate N<sub>2</sub>O and NO emissions from soils using only data which is available at regional scale and to quantify the uncertainty of model simulations by developing a suitable HB calibration method, and to investigate the model extrapolation and the parameters' variability using soil information.

**Table 5. 1** Description of 19 parameters of N<sub>2</sub>O and NO flux module. The prior probability distribution is defined as uniform between bounds  $\theta_{min}$  and  $\theta_{max}$  which were extracted from literature reviews. The posterior parameter distributions are characterized by the mean values of the posterior, their standard deviation (SD), and 95% CI for 15 experimental sites.

| Gas module                   | Parameter vector $\theta=[\theta_1, ..., \theta_{19}]$ |               |                | Default value                                                                                              | Prior probability distribution            |                   |                   | Posterior distribution | probability                                                                                                                                                                                   |       |       |       |       |
|------------------------------|--------------------------------------------------------|---------------|----------------|------------------------------------------------------------------------------------------------------------|-------------------------------------------|-------------------|-------------------|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------|-------|-------|-------|
|                              | Parameter                                              | Symbol        | Description    | Unit                                                                                                       |                                           | $\theta_{min}(i)$ | $\theta_{max}(i)$ | References             | Mean                                                                                                                                                                                          | SD    | 0.025 | 0.975 |       |
| N <sub>2</sub> O flux module | Site-specific                                          | $\theta_1$    | $N_{d50}$      | Soil nitrate content at which denitrification is 50% of its full potential                                 | kg N ha <sup>-1</sup> layer <sup>-1</sup> | 16.5              | 5                 | 20                     | (Stanford et al., 1975), (Maag and Vinther, 1999), (Gabrielle, 2006), (Lehuger et al., 2009), (Bell et al., 2012)                                                                             | 13.0  | 2.91  | 8.28  | 17.7  |
|                              |                                                        | $\theta_2$    | $w_1$          | soil water threshold for denitrification                                                                   | %                                         | 0.62              | 0.5               | 1                      | (Gabrielle, 2006), (Hénault and Germon, 2000), (Johnsson et al., 1991), (Lehuger et al., 2009), (Bell et al., 2012), (Parton et al., 2001), (Frolking et al., 1998)                           | 0.67  | 0.16  | 0.50  | 0.98  |
|                              |                                                        | $\theta_3$    | $w_2$          | Exponent of the power function for denitrification                                                         | uniteless                                 | 1.74              | 1.3               | 2.5                    | (Stanford et al., 1975), (Smith et al., 1998), (Johnsson et al., 1991), (Maag and Vinther, 1996), (Maag and Vinther, 1999), (Skopp et al., 1990), (Lehuger et al., 2009), (Bell et al., 2012) | 1.94  | 0.32  | 1.43  | 2.47  |
|                              | global                                                 | $\theta_4$    | $BioAct$       | Rate for soil biological activity                                                                          | uniteless                                 | 0.005             | 0                 | 0.01                   | (Bradbury et al., 1993), (Bell et al., 2012)                                                                                                                                                  | 0.005 | 0.003 | 0.000 | 0.01  |
|                              |                                                        | $\theta_5$    | $P_{NO3,f}$    | NO <sub>3</sub> content of the soil at which N is released in equal of N <sub>2</sub> and N <sub>2</sub> O | uniteless                                 | 200               | 150               | 250                    | (Frolking et al., 1998), (Bell et al., 2012)                                                                                                                                                  | 184   | 25.7  | 151   | 242   |
|                              |                                                        | $\theta_6$    | $D_P$          | Potential denitrification rate                                                                             | kg N ha <sup>-1</sup> layer <sup>-1</sup> | Site-specific     | 0                 | 1                      | (Parton et al., 1996), (Parton et al., 2001), (Bell et al., 2012)                                                                                                                             | 0.49  | 0.29  | 0.03  | 0.97  |
|                              |                                                        | $\theta_7$    | $nf$           | Proportion of N <sub>2</sub> O produced due to partial nitrification at filed capacity                     | uniteless                                 | 0.02              | 0.01              | 0.4                    | (Bell et al., 2012)                                                                                                                                                                           | 0.003 | 0.003 | 0.000 | 0.010 |
|                              |                                                        | $\theta_8$    | $P_{N2,f}$     | Denitrification proportioned into N <sub>2</sub> according to water content                                | uniteless                                 | 0.5               | 0                 | 1                      | (Frolking et al., 1998), (Bell et al., 2012)                                                                                                                                                  | 0.34  | 0.21  | 0.02  | 0.78  |
|                              |                                                        | $\theta_9$    | $n_{gas}$      | Proportion of full nitrification lost as gas                                                               | uniteless                                 | 0.02              | 0.01              | 0.09                   | (Bell et al., 2012)                                                                                                                                                                           | 0.07  | 0.02  | 0.03  | 0.10  |
|                              |                                                        | $\theta_{10}$ | $n_{no}$       | Proportion of full nitrification gaseous loss that is NO                                                   | uniteless                                 | 0.4               | 0.1               | 1                      | (Frolking et al., 1998) , (Bell et al., 2012)                                                                                                                                                 | 0.86  | 0.02  | 0.83  | 0.89  |
| NO flux module               | Site-specific                                          | $\theta_{11}$ | $Nitri_{rate}$ | Nitrification rate                                                                                         | kg N ha <sup>-1</sup> layer <sup>-1</sup> | 0.6               | 0                 | 1                      | None information                                                                                                                                                                              | 0.50  | 0.29  | 0.03  | 0.97  |
|                              |                                                        | $\theta_{12}$ | $T_1$          | Parameter for air temperature                                                                              | uniteless                                 | 47.9              | 45                | 55                     | (Bradbury et al., 1993)                                                                                                                                                                       | 49.9  | 2.89  | 45.2  | 54.7  |
|                              |                                                        | $\theta_{13}$ | $T_2$          | Parameter for air temperature                                                                              | uniteless                                 | 106               | 90                | 110                    | (Bradbury et al., 1993)                                                                                                                                                                       | 99.7  | 5.84  | 90.5  | 109   |
|                              |                                                        | $\theta_{14}$ | $T_3$          | Parameter for air temperature                                                                              | uniteless                                 | 18.3              | 15                | 25                     | (Bradbury et al., 1993)                                                                                                                                                                       | 20.0  | 2.9   | 15.3  | 24.8  |
|                              |                                                        | $\theta_{15}$ | $pH_{cons}$    | Constant for pH modifier                                                                                   | uniteless                                 | 0.56              | 0.2               | 0.7                    | (Parton et al., 1996)                                                                                                                                                                         | 0.45  | 0.14  | 0.21  | 0.69  |
|                              |                                                        | $\theta_{16}$ | $pH_{modif}$   | Shape of pH modifier                                                                                       | uniteless                                 | 0.45              | 0.2               | 0.7                    | (Parton et al., 1996)                                                                                                                                                                         | 0.45  | 0.14  | 0.21  | 0.69  |
|                              |                                                        | $\theta_{17}$ | $pH_{Tr}$      | pH threshold for pH rate change                                                                            | uniteless                                 | 5                 | 4                 | 6                      | (Parton et al., 1996), (Mortland, 1970), (Gilmour, 1984)                                                                                                                                      | 5.00  | 0.58  | 4.06  | 5.94  |
|                              |                                                        | $\theta_{18}$ | $m_{w0}$       | Soil water rate modifier for decomposition                                                                 | %                                         | 0.2               | 0.1               | 0.3                    | (Bell et al., 2012)                                                                                                                                                                           | 0.28  | 0.04  | 0.14  | 0.30  |
|                              |                                                        | $\theta_{19}$ | $Cmax$         | Maximum rate of nitrification possible                                                                     | uniteless                                 | 50                | 40                | 60                     | (Parton et al., 1996)                                                                                                                                                                         | 40.2  | 0.21  | 40.0  | 40.8  |

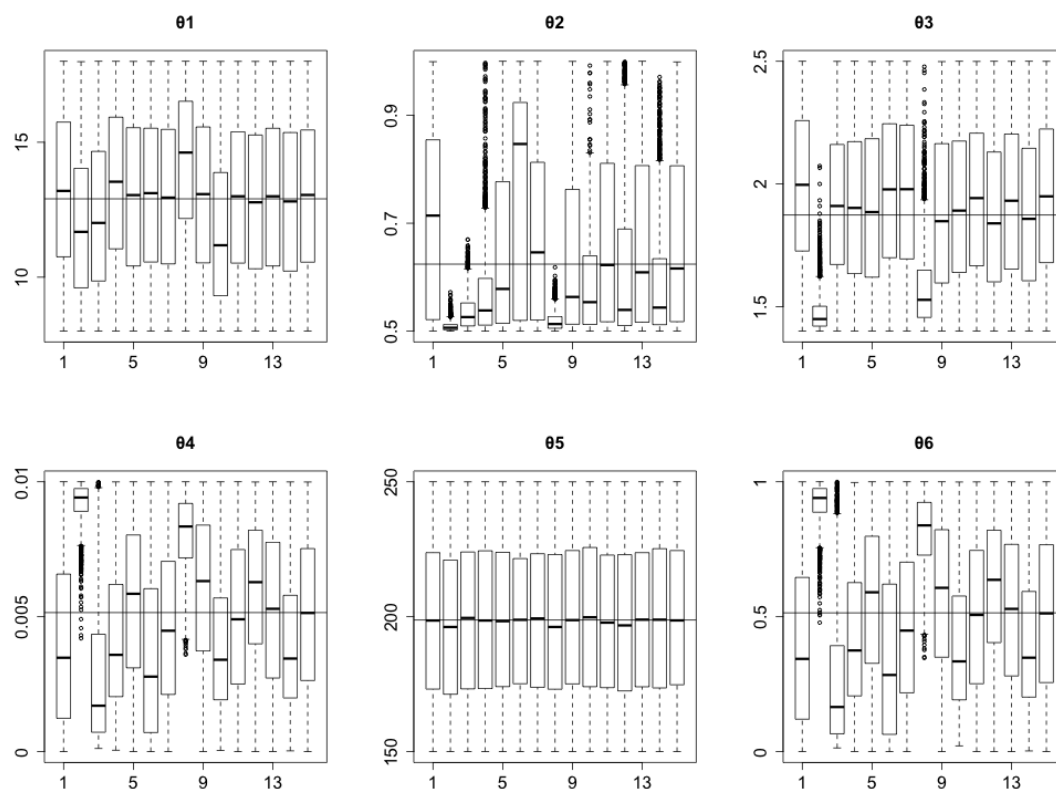
## 5.2 Results

### 5.2.1 Posterior parameter distributions

Figure 5.1 shows boxplots of the posterior parameter distributions in N<sub>2</sub>O ( $\theta_1$  to  $\theta_6$ ) flux module after HB calibration. The y-axis corresponding to the prior range of parameter variation, and the x-axis represented 15 sites. The priors allow for uncertainty. Such representation made it possible to visualize differences between parameter pdfs across sites, while the shape of the boxplot revealed the dispersion and symmetry of the marginal distributions.

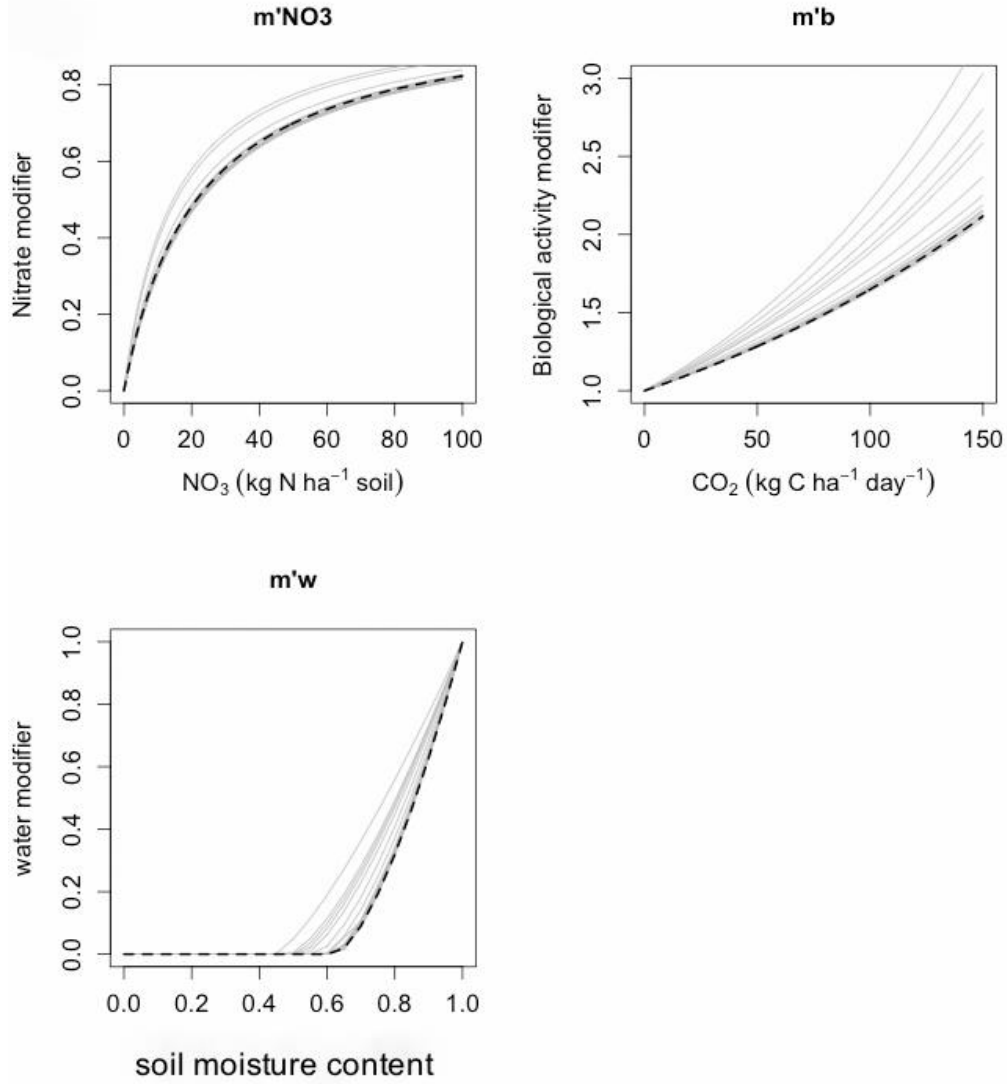
Figure 5.1 demonstrates that the posterior distributions of some parameters in N<sub>2</sub>O flux module became narrower compared to the uniform prior distributions (corresponding to y-axis), which was due to the efficiency of the HB calibration procedure. Van Oijen et al. (2005) and Lehuger et al. (2009) revealed that the choice of an uniform distribution for the prior had little influence for posterior pdfs, as the measured data gradually became much more dominant than the prior distribution in the calibration process. For example, the posterior distributions of the soil water threshold triggering denitrification ( $\theta_2$ ) had a narrow range for all sites compared to the prior range (corresponding to y-axis) suggesting that the HB calibration drastically reduced its uncertainty. Conversely, NO<sub>3</sub><sup>-</sup> content of the soil at which N is released in equal of N<sub>2</sub> and N<sub>2</sub>O ( $\theta_5$ ) remained spread across their prior range of variation (corresponding to y-axis), and centered around their prior mean values. This means that the calibration did not significantly reduce their uncertainty. In addition, some posterior distributions were flattened on one of the prior bounds (corresponding to y-axis), implying that their optimal values were outside the prescribed range. This was particular true for soil biological activity ( $\theta_4$ ), for the site number of 2, 3 and 8 (Site BL, C, GL, respectively). We should therefore reconsider the prior ranges for

these parameters. The posterior distributions of parameters ( $\theta_{11}$ – $\theta_{19}$ ) in NO flux module are not variable across sites revealed that these parameters in nitrification may be considered universally constant (Figure of posterior distributions of some parameters in NO flux module was not showed here).

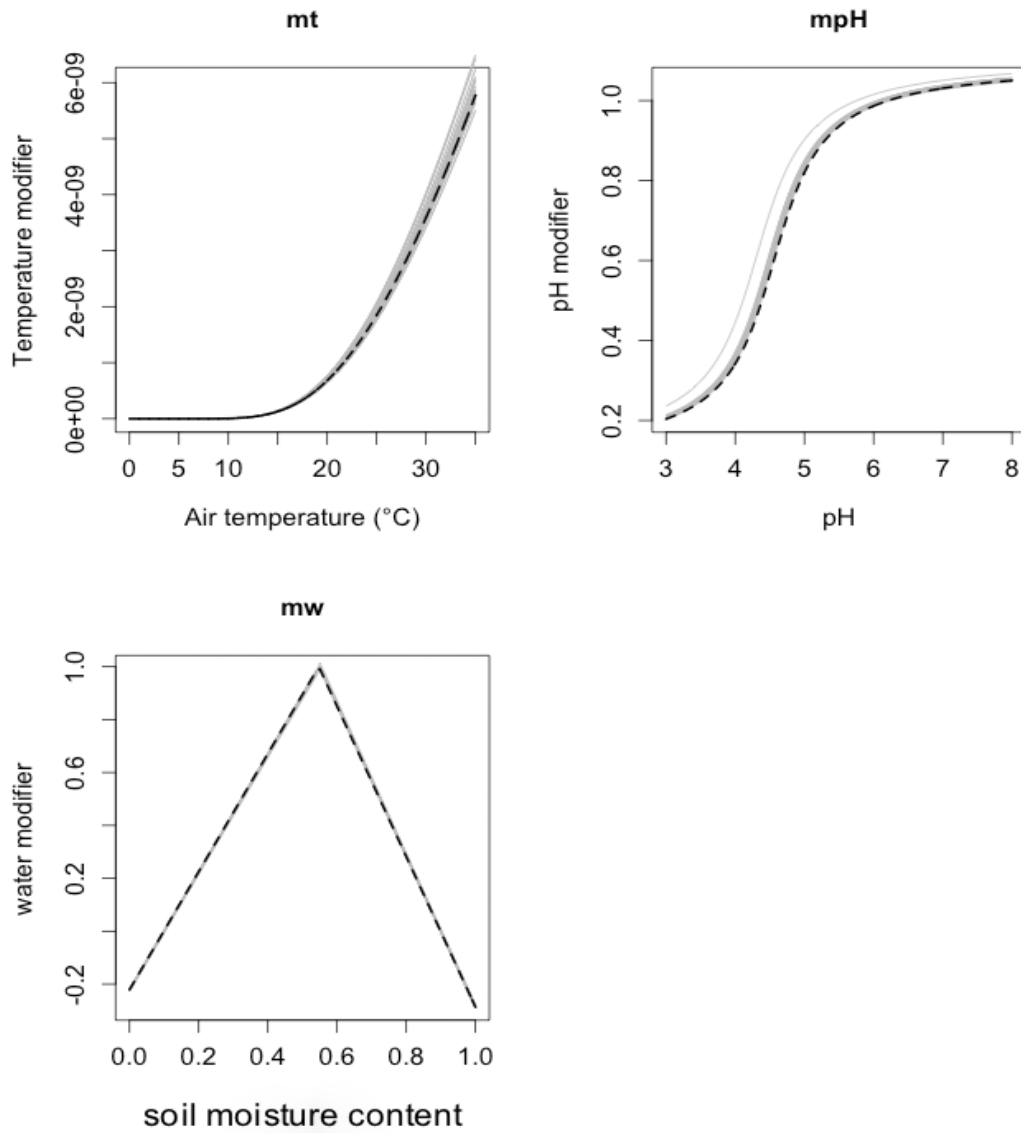


**Figure 5. 1** Posterior distribution of the 6 calibrated parameters ( $\theta_1$  to  $\theta_6$ ) in  $N_2O$  flux module represented as boxplots over the prior range of variation (corresponding to the range of the y-axis). The boxplots are computed from hierarchical Bayesian calibration with 15 experimental sites. The horizon line represents the global cross-sites parameter. The boxplots depict the median (solid line), the 2nd and 3rd quartiles (bars), the 1st and 4th quartiles (dotted line), and the extreme values (excluding outliers). The x-axis present 15 sites.

Figure 5.2 and Figure 5.3 depicts the ranges of response functions of the  $\text{N}_2\text{O}$  and NO flux resulting from the N-HB model calibrations. These response functions of  $\text{N}_2\text{O}$  (Fig. 5.2) were more variable than function of NO (Fig. 5.3), which matches with the higher variability of parameters in  $\text{N}_2\text{O}$  flux module (Fig. 5.1) than that of NO (Figure of posterior distributions of some parameters in NO flux module was not showed here). The calibrated response of denitrification to biological activity ( $m'_b$ ) was highly variable, along with the response of denitrification to soil  $\text{NO}_3^-$  content ( $m'_{\text{NO}_3}$ ) and the response of denitrification to soil water content ( $m'_w$ ). Response of denitrification to soil water content ( $m'_w$ ) varied widely, as a consequence of the large variations of soil water threshold for denitrification ( $\theta_2$ ). Hénault et al. (2005) showed that the denitrification was highly sensitive to the soil water threshold,  $\theta_2$ , and that this parameter dependent on soil type. The response functions of NO had a similar shape across the sites (Fig. 5.3) corresponding to the low variation of posterior distribution of calibrated parameters in NO module, which lead to the conclusion that the parameters for NO module could be considered to be universal.



**Figure 5. 2** Response functions of the N<sub>2</sub>O flux module traced with different sites: mean of the posterior for each study site calibration (line), and the global cross-sites posterior for the 15 experimental sites calibration (dashed line).



**Figure 5. 3** Response functions of the NO flux module traced with different sites: mean of the posterior for each study site calibration (line), and the global cross-sites posterior for the 15 experimental sites calibration (dashed line).

### 5.2.2 N<sub>2</sub>O and NO simulation

Under the hierarchical approach, each different fifteen experimental sites had its own parameter set (data not shown here), the mean posterior probability for the globally common model was summarized in Table 5.1. Table 5.2 summarized the  $R$  squared ( $R^2$ ), and the root-mean-square error ( $RMSE$ ) of N<sub>2</sub>O and NO fluxes simulated by N-HB model. The HB calibrated model's  $RMSE$  over the 15 sites ranged from 0.8 to 22.0 kg N ha<sup>-1</sup> day<sup>-1</sup> for N<sub>2</sub>O, from 0.9 to 37.5 kg N ha<sup>-1</sup> day<sup>-1</sup> for NO. Although the  $R^2$  at none of the 15 sites was high on a daily time step, the model simulation could predict the N<sub>2</sub>O and NO across the 15 sites (Table 5.2). Comparison of simulated and measured soil state variables of site\_GL was displayed in the Figure 5.5, which indicated that the model adequately simulated the direction, timing and magnitude of the measured data. The peaks of N<sub>2</sub>O and NO fluxes were correctly predicted following fertilizer addition, and there was no mistiming of the model response for fertilizer application.

**Table 5. 2** Sample size ( $N$ ),  $R$  squared ( $R^2$ ) and root mean square errors ( $RMSE$ ) computed with the predicted and measured  $N_2O$  and  $NO$  fluxes at 15 sites.

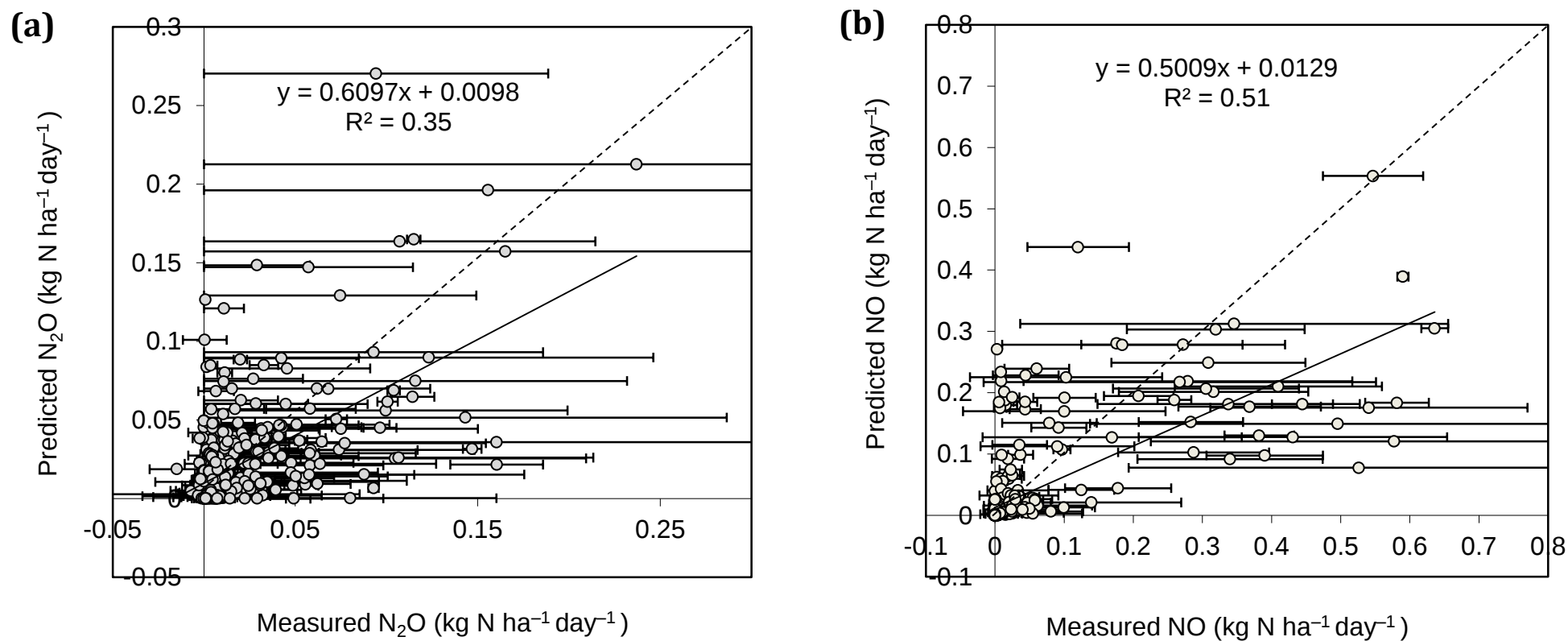
| Site | Site_No. | $N$ | $N_2O$                                  |            | $NO$                                    |            |
|------|----------|-----|-----------------------------------------|------------|-----------------------------------------|------------|
|      |          |     | kg N ha <sup>-1</sup> day <sup>-1</sup> |            | kg N ha <sup>-1</sup> day <sup>-1</sup> |            |
|      |          |     | $R^2$                                   | $RMSE(\%)$ | $R^2$                                   | $RMSE(\%)$ |
| B    | 1        | 34  | 0.35                                    | 2.38       | 0.35                                    | 7.82       |
| BL   | 2        | 112 | 0.36                                    | 21.98      | 0.20                                    | 16.64      |
| C    | 3        | 29  | 0.33                                    | 1.02       | 0.31                                    | 0.90       |
| D    | 4        | 62  | 0.50                                    | 0.93       | 0.62                                    | 3.08       |
| E    | 5        | 96  | 0.28                                    | 0.80       | No data                                 |            |
| F    | 6        | 31  | 0.36                                    | 4.51       | 0.22                                    | 2.66       |
| G    | 7        | 24  | 0.21                                    | 7.32       | 0.32                                    | 37.53      |
| GL   | 8        | 339 | 0.42                                    | 1.22       | 0.46                                    | 1.23       |
| P    | 9        | 83  | 0.08                                    | 1.45       | 0.28                                    | 12.58      |
| R    | 10       | 267 | 0.12                                    | 1.78       | 0.30                                    | 1.66       |
| S    | 11       | 17  | 0.37                                    | 0.88       | 0.41                                    | 1.47       |
| T    | 12       | 84  | 0.17                                    | 1.78       | 0.08                                    | 1.30       |
| U    | 13       | 46  | 0.29                                    | 1.34       | 0.24                                    | 7.85       |
| V    | 14       | 220 | 0.34                                    | 2.11       | 0.32                                    | 1.86       |
| W    | 15       | 84  | 0.48                                    | 1.77       | 0.16                                    | 3.78       |

The model performance of  $N_2O$  and  $NO$  simulation applied across 15 sites for calibration and verification were shown in Table 5.2 and Figure 5.4. Simulation of  $N_2O$  flux showed appropriate correlation corresponding to observations on a daily time-step, with  $R^2$  value of 0.38 in calibration and 0.27 in validation. Although this correlation ( $R^2$ ) was weak, it was statistically significant, with  $RMSE$  value smaller than  $RMSE_{95}$ . Simulation of the  $NO$  flux showed better correlation corresponding to observations on a daily time-step, with  $R^2$  value of 0.49 in calibration and 0.55 in verification, and it was statistically significant.

**Table 5. 3** Model performance for calibration (2003–2009) and verification (2010–2011); and model performance efficiency through the years 2003–2011.

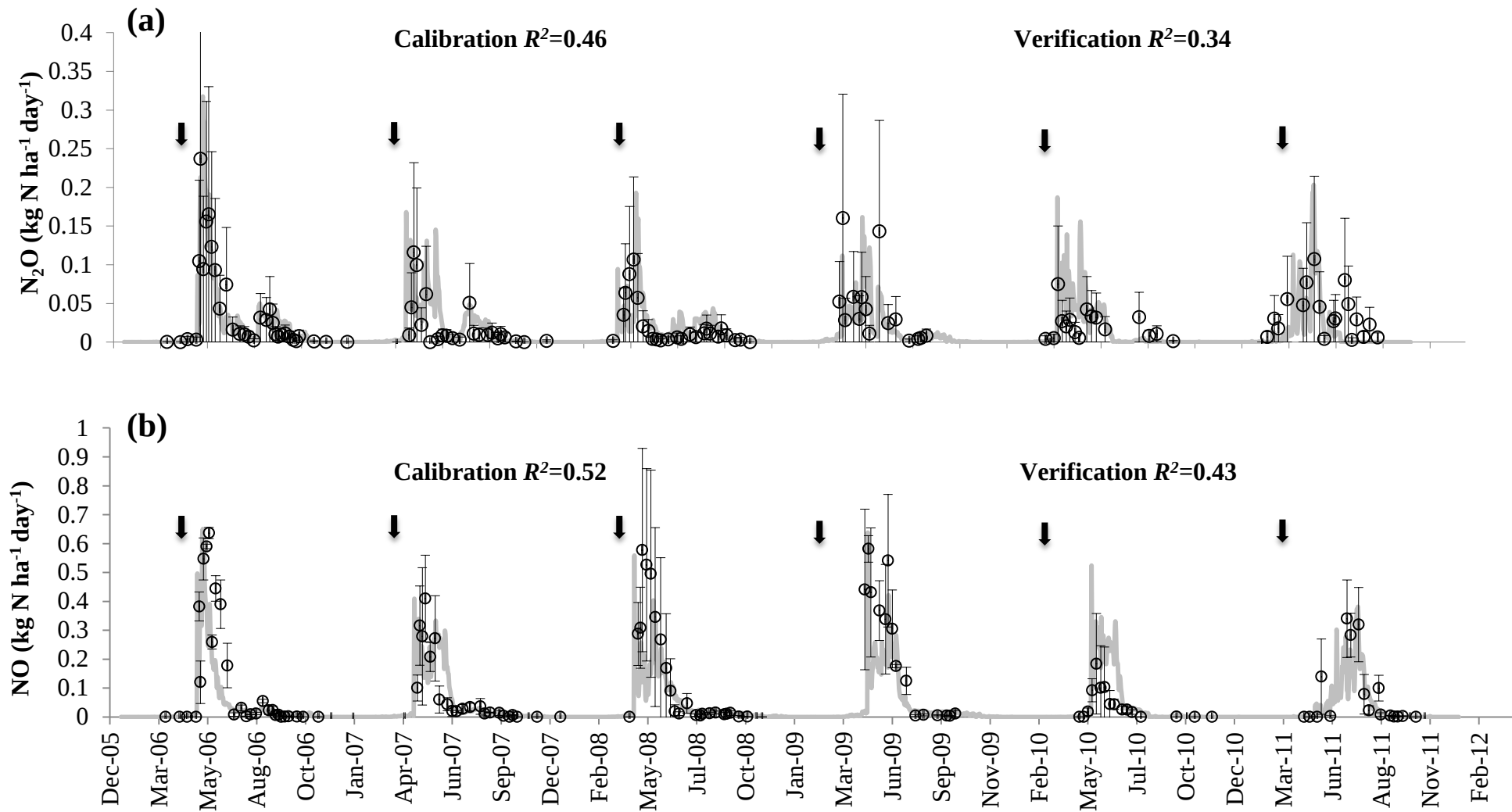
|                                          | N <sub>2</sub> O |              |                   | NO          |              |                   |
|------------------------------------------|------------------|--------------|-------------------|-------------|--------------|-------------------|
|                                          | Calibration      | Verification | Model performance | Calibration | Verification | Model performance |
| Year Data                                | 2003–2009        | 2010–2011    | 2003–2011         | 2003–2009   | 2010–2011    | 2003–2011         |
| $R^2$                                    | 0.38             | 0.27         | 0.35              | 0.49        | 0.55         | 0.51              |
| $r$ = Correlation Coeff.                 |                  |              | 0.57              |             |              | 0.70              |
| $T$ value                                |                  |              | 17.26             |             |              | 23.92             |
| Critical $T$ value at $P=0.05$           |                  |              | 2.13              |             |              | 2.13              |
| Significant association?                 |                  |              | Yes-Good          |             |              | Yes-Good          |
| $RMSE$ = Root mean square error of model | 0.57             | 0.28         | 1.77              | 0.43        | 0.23         | 2.14              |
| $RMSE$ (95% Confidence Limit)            | 27.74            | 22.5         | 28.19             | 24.19       | 20.18        | 19.39             |
| Significant total error?                 | No-Good          | No-Good      | No-Good           | No-Good     | No-Good      | No-Good           |
| $M$ = Mean Difference                    |                  |              | 0.00              |             |              | 0.00              |
| $T$ value                                |                  |              | –0.01             |             |              | –0.20             |
| Critical $T$ value at $P=0.05$           |                  |              | 1.96              |             |              | 1.96              |
| Significant bias?                        |                  |              | No-Good           |             |              | No-Good           |
| $E$ = Relative Error                     |                  |              | –0.55             |             |              | –0.03             |
| $E$ (95% Confidence Limit).              |                  |              | 19.63             |             |              | 9.79              |
| Significant bias?                        |                  |              | No-Good           |             |              | No-Good           |
| Number of Values                         |                  |              | 607               |             |              | 607               |

$R^2$  is the coefficient determination.  $r$  is the correlation coefficient and the significance was quantified using an  $F$  test at 95% confidence limit.  $RMSE$  is the root mean squared error and the significance was quantified by  $RMSE$  at the 95% confidence limit.  $M$  is the mean difference and then undertaking a  $t$  test to check for significance.  $E$  is the relative error and compare to the  $E$  at 95% confidence limit.



**Figure 5. 4** Predicted vs. Observed  $\text{N}_2\text{O}$  (a) and NO (b) flux in study sites for calibration and verification (2003–2011) from N-HB model performance. Bar indicate S.D. ( $n=3$ ) for observed data.

Figure 5.5 shows the simulated daily N<sub>2</sub>O and NO fluxes for GL (Site\_No. 8). The model could predict daily N<sub>2</sub>O and NO fluxes well, except for the fluxes with high experimental error, which it failed to predict in some cases. Here, some discrepancies between measurements and simulations remained, due to uncertainty on both sides. The two N<sub>2</sub>O spikes measured in 2009 May and July had a large experimental error, but did not appear to constrain the calibration as much as the more frequent lower N<sub>2</sub>O fluxes with much lower standard deviations. The same failed estimation were found in NO fluxes simulation in 2008 May, which with much higher standard deviations.



**Figure 5. 5** Simulated vs. Observed N<sub>2</sub>O (a); NO (b) at Site GL (Site\_No.8). Arrows indicates fertilizer application.

## 5.3 Discussion

### 5.3.1 Spatial variability of model parameters

We sought to calibrate model parameters by hierarchical structure in order to minimize model error and simultaneously on all datasets to find parameter values that would be universally applicable, expressed by the mean value of posterior distribution. Such values would be extremely useful to apply the model to new soil conditions and to spatially extrapolate it. Measurements of denitrification show extreme higher spatial and temporal variability with typical coefficients of variation exceeding 100% compared with nitrification, which lead to large uncertainty in denitrification simulation (Hénault et al., 2005). The parameters in denitrification revealed by HB calibration in this study are highly variable, which suggested that the simulation of  $\text{N}_2\text{O}$  flux using the universal parameters for denitrification is not appropriate and the site-specific parameterization of denitrification process in process-based model is required (Heinen, 2006; Lehuger et al., 2009). In contrast, HB calibration revealed that parameters in nitrification and response function of NO are less variable, therefore, nitrification process could be parameterized on universal basis.

Heinen (2006) concluded that defining a set of denitrification response functions to soil  $\text{NO}_3^-$  and soil water (Fig. 5.2), and parameter values for denitrification that would equally apply to sandy, loamy and peat soil types was not easily possible. Our HB calibration gave further evidence to that response functions for denitrification (Eqs. 5.9, 5.10, 5.11, 5.12) were highly variable, and the soil  $\text{NO}_3^-$  at which denitrification is 50% of its full potential ( $\theta_1$ ), soil water threshold for denitrification ( $\theta_2$ ), exponent of soil water power function in denitrification ( $\theta_3$ ), soil biological activity ( $\theta_4$ ) in these functions were in large variations in pdfs across sites. Parameters of denitrification are required to be site-specific due to the fact that soil structure and aggregate

characteristics exert a major influence on denitrification (Gabrielle et al., 2006a).

In our study, non-linear relationships between the soil water threshold for denitrification and soil texture was found, however, our result indicated that the exponent of the power function for soil water ( $\theta_3$ ) decrease linearly with soil silt content ( $P < 0.05$ ) (Table 5.4). Some authors have suggested that the threshold of soil water for an existing denitrification activity ( $\theta_2$ ) was especially sensitive, and it could vary with soil texture or corresponds to the soil's field capacity (Hénault et al., 2005; De Klein and Van Logtestijn, 1996). Generally, the soil water content has a complex effect on denitrification by controlling aeration, diffusion of substrates and microbial activity, which also indicated by the variable denitrification response functions for soil water in this study (Fig. 5.3). Results from previous studies investigated the relationships among soil water, texture and denitrification rate are not consistent or even contradictory. Several studies (Sexstone et al., 1988; Weier et al., 1993) found that a stronger effect of soil water content on denitrification rate in clay loam, compared to a sandy loam. Groffman and Tiedje (1991) indicated that when soil water content increased, denitrification rates increased more sharply in coarse soil than in a finer-texture soil.

Denitrification response function to  $\text{CO}_2$  was highly variable, however, the linear relationship between the soil biological activity with soil sand contents (Table 5.4), which conflicted with the concept that fine-texture soils can absorb organic matter and prevented it from being decomposed by microorganisms (Sorensen, 1975). The denitrification- $\text{CO}_2$  production relationship was more complicated. Fine-texture soils have smaller pores thus are more easily become anaerobic than the coarse soils, which was likely to favor denitrification (Groffman and Tiedje, 1991). Therefore, denitrification response factor to  $\text{CO}_2$  production cannot be considered as simple isolated SOMD in denitrification simulation.

Denitrification response function for  $\text{NO}_3^-$  varied less from site to site, compared

with denitrification response function for CO<sub>2</sub> production and soil water (Fig. 5.3).

We also observed the soil NO<sub>3</sub><sup>-</sup> content at which denitrification is 50% of its full potential ( $\theta_1$ ) was not very sensitive at different sites (Hénault et al., 2005).

Our study indicated that the potential denitrification rate ( $\theta_6$ ) decrease linearly with soil sand content ( $P < 0.05$ ) (Table 5.4). Hénault et al. (2005) suggested that parameter potential denitrification rate ( $\theta_6$ ) could be used for comparing soil capacities for denitrification.  $\theta_6$  was widely used in process-based model: NEMIS (Hénault et al., 2005), CERES-EGC (Gabrielle et al., 2006a) and ECOSSE model (Bell et al., 2012), which varied as a function of soil texture and soil biota, and was calculated on site by experimentally creating optimal conditions for denitrification in the soil (Bell et al., 2012). Hénault et al. (2005) reported that potential denitrification rate was also a seasonal variable, which is different in summer season from autumn, winter or spring season with the assumption that there is little anaerobic denitrification during summer because the soil is too dry. Although potential denitrification rate measured on a few French soils seemed to be positively influenced by the organic C in the soil, no model could include this because of the weak observed relation (Wheatley and Williams, 1989). Our study didn't test the seasonal variability and there was no relation between potential denitrification rate and organic C content was found, however, the result indicated that potential denitrification rate,  $\theta_6$ , in soil includes implicitly different soil characteristics, which decrease linearly with soil sand content ( $P < 0.05$ ) (Table 5.4). It is possible that potential denitrification rate assessments based on soil texture or establish a dataset of potential denitrification rate,  $\theta_6$ , based on soil classification.

As Bayesian calibration assumes that there is a 'true' parameter value that is incrementally approached with increasing sample size, the hierarchical approach differs from this assumption in the sense that a parameter can varies, that equals hierarchical approach admits that parameter has its own variability. Thus, hierarchical approach identifies two "hyper parameters" to described the posterior distribution of

each subunit-specific parameter variability. [Figure 5.1](#), demonstrated posterior distribution of calibrated parameters represented as boxplots over the prior range (range of y-axis). In this case, the posterior density describes parameters' variability. For example, variability in soil water threshold for denitrification ( $\theta_2$ ) in this study is accomplished by conditioning on two hyper parameters  $\alpha$  and  $\beta$  ( $\mu_{\theta_2}$  and  $\sigma_{\theta_2}$  for  $\theta_2$ ) in Eq. (5.22) (posterior distribution of hyper parameters was not shown here). Hyper parameter  $\mu_{\theta_2}$  and  $\sigma_{\theta_2}$  have the estimation error, while the individual parameter  $\theta_{2,j}$  have distributions that depend on data for the  $j$ th individual site and for the entire sites. Two hyper parameters  $\mu_{\theta_2}$  and  $\sigma_{\theta_2}$  define a conditional distribution of the  $\theta_{2,j}(\pi(\theta_{2,j}|\mu_{\theta_2},\sigma_{\theta_2}))$ , and this distribution does not collapse with increasing sample size. Unlike the hierarchical model, the nonhierarchical model does not admit variability in  $\theta_2$ . It simply expresses our posterior belief in values of  $\theta_2$  (Eq. 3.1), which collapses to a point estimate with large sample size ([Clark, 2003](#)). The spread in parameter distributions ([Fig. 5.1](#)) describes the parameters' variability by hierarchical model that could have been missed by the nonhierarchical model.

**Table 5. 4** The linear regression relation between calibrated parameter and soil texture.

| Linear regression relation                           | $R^2$ | $P$ value |
|------------------------------------------------------|-------|-----------|
| $\theta_3 = -0.0071 \times \text{silt} + 2.1816$     | 0.21  | 0.08      |
| $\theta_4 = -0.0008 \times \text{sand} + 0.0728$     | 0.53  | 0.002     |
| $\theta_6 = -0.007756 \times \text{sand} + 0.727487$ | 0.52  | 0.002     |

### 5.3.2 Model application

We have established a database on  $\text{N}_2\text{O}$  fluxes for central Hokkaido, Japan and sought to calibrate the model parameters on different sites in order to minimize the uncertainty and to find the parameter values that would be universally applicable. Generally, the parameters with less variability would be regarded as the global parameters and be extremely useful for spatial extrapolation, however, the parameters

with the large variability need to be parameterized on site-specific basis. The simple linear relationship of calibrated parameters and soils provide a pre-requisite for simulation over space. Ensuring the accurate parameterization is a pre-requisite to develop the model with the purpose of providing predictions over a large domain in space and time. Although the studied soil types in this study are limited, our HB approach developed in this study is universal rather than the calibrated parameter itself. The HB approach is the recommended strategy to improve the model simulations at separately field scale, and to find the universal values of parameters to spatially extrapolate the model. When attempting at simulating N<sub>2</sub>O fluxes in a new site where no measured data available, following strategy is suggested. Firstly, the user should make the calibrated parameter sets based on the variability range of parameters refers to the previous studies of used model. Hence the most important/sensitive parameters must be identified before. Take the ECOSSE used in this study as an example. The less variable parameters, such as parameters of nitrification may serve as the default values for the spatial extrapolation of the model at regional scale regardless of soil types or soil physic-chemical characteristics. Secondly, the user should check if calibrated parameters sets, especially for high variability parameters, already exist for similar soil types, based on soil taxonomy or physic-chemical characteristics, such as the soil nitrate content at which denitrification is 50% of its full potential ( $\theta_1$ ), soil water threshold for denitrification ( $\theta_2$ ), exponent of soil water power function in denitrification ( $\theta_3$ ), soil biological activity ( $\theta_4$ ) and potential denitrification rate ( $\theta_6$ ) in this study. If these parameters are not exist for similar soil types, these parameters derived from the multi-dataset calibration may be used to encompass a wide range of space and time condition at regional scale, though at the cost of a larger error between simulations and observations with site-specific sets.

Our results do not provide robust evidence that the parameters of N<sub>2</sub>O fluxes could be estimated from soil texture. It is difficult to apply the linear relation to other soils due to the limited breadth of input soil textures, however, it agrees with other models' result that the soil or landscape characteristics could control these parameters. Such as potential denitrification rate ( $\theta_6$ ), though several studies revealed that it varies as a function of soil texture, how  $\theta_6$  changes in soil taxonomy is still unknown (Hénaul and Germon, 2000; Bell et al., 2012). Therefore, it will be interesting to apply HB calibration across different soils and establish a database of parameters based on soil taxonomy.

## 5.4 Conclusion

N-HB model was successfully applied to simulate N<sub>2</sub>O and NO emission from agriculture field. The parameters were calibrated against sites to improve model simulations at field scale and to find universal values of parameters described by the mean value of posterior parameter distributions to spatially extrapolate the model. The posterior parameter encompassing all our observations at the study sites gave us the possibility of quantifying the real parameter variability. Parameters for nitrification could be considered universal while parameters for denitrification were much less constant across sites.

Based on our result, we recommended a strategy to develop a HB approach across more soil types globally. The spatial variability of parameters for soil classification could deal with model extrapolation; and could serve as prior information to infer the parameters of the N<sub>2</sub>O module to decrease uncertainty in N<sub>2</sub>O simulation.

## **6. Carbon balance at regional scale during the last four decades**

### **6.1 Introduction**

The C balance in terrestrial ecosystems has large implications on the variation in atmospheric CO<sub>2</sub> emission. Soil have the potential to sequester organic matter and thus to significantly contribute to the terrestrial C sink. Agriculture profoundly affects global C, water and nutrient cycles, as well as the planetary surface energy balance ([Bondeau et al., 2007](#)) . Assessment of soil C stock changes over time is typically based on application of two methods, namely (i) repeated soil inventory and (ii) determination of the NBP by continuous measurement of CO<sub>2</sub> exchange in combination with quantification of other C imports and exports ([Leifeld et al., 2011](#)).

Long-term trends in agricultural productivity and residue inputs to soil, driven by technological and management changes, impact the magnitude and direction of change in soil C storage ([Johnsson et al., 1991](#)). Because of the high net primary productivity (NPP) of many agricultural crops, relative to non-cropland vegetation, agricultural systems can substantially increase short-term C exchanges between the land surface and the atmosphere in regions converted to agricultural land use. Interannual variability and changes in crop species distribution, as well as interannual variability in net ecosystem C storage, may have significant implications for estimating short-term changes in terrestrial C balances, for both atmospheric-based estimates of regional C cycling and ground-based soil C inventories. Spatial and temporal variability of C inputs present significant challenges for estimating the C balance in agricultural ecosystems. A large proportion of NPP (about 40–50% of above ground biomass in grain crops) is removed as yield and thus the long-term C

balance in croplands is instead governed by the amount of crop residues, which is remained on the field.

In principal, an indication for the uncertainty in NBP should be provided and thus a direct quantitative evaluation of methods is available. Meanwhile, the NBP value for an agricultural system should be directly comparable with the C stock change measured by repeated sampling of soil, but up to now, there has been few field study that directly compared the two approaches at an agricultural system at the regional scale.

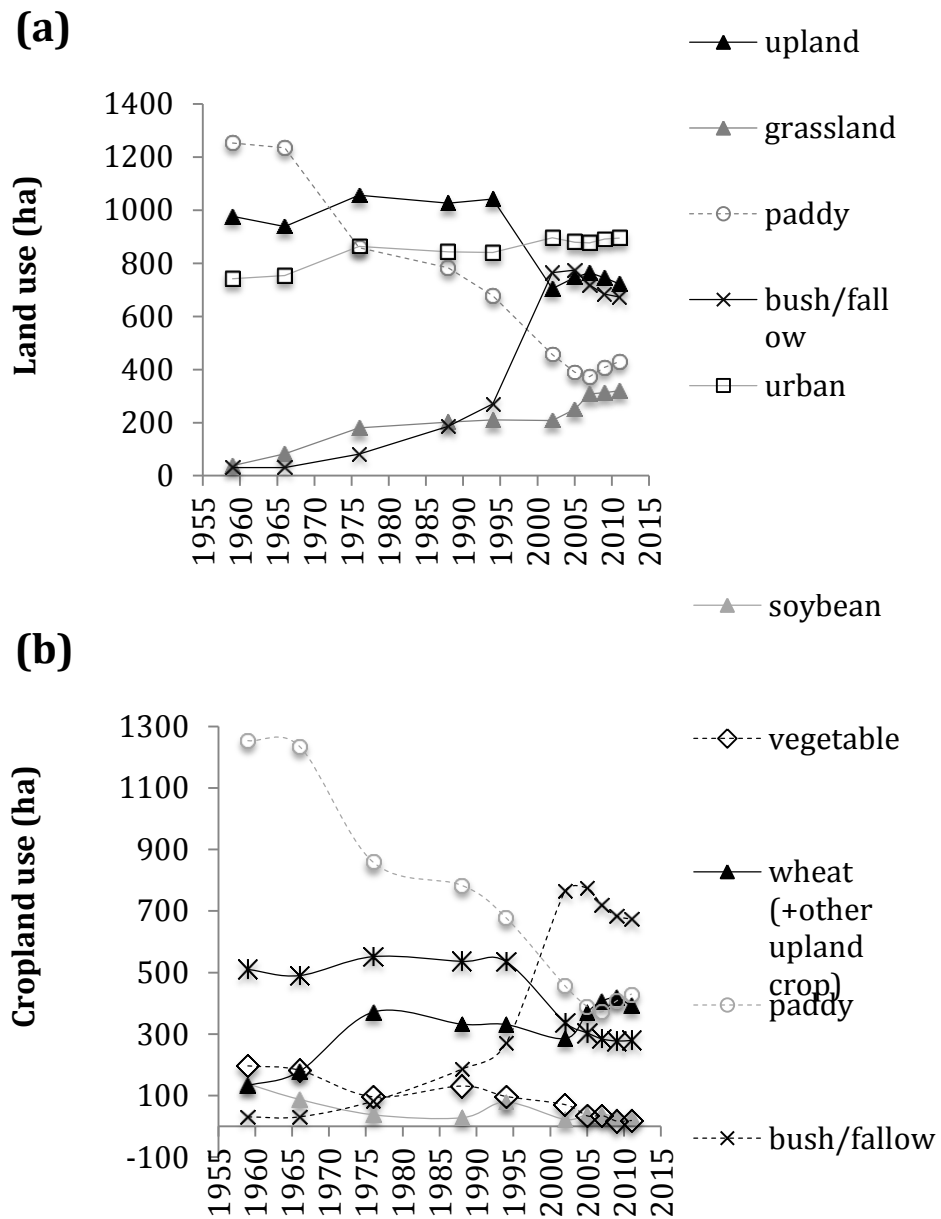
The first goal of our study was to explore trends and interannual variability of NBP at regional scale, focusing on the spatial and temporal patterns of NPP, crop residue inputs and NBP at the main land use: upland, paddy, grass from 1959 to 2011. Secondly, verifying the ecosystem C budget change estimated by NBP at individual land use (upland, paddy, grass) from 2005 to 2011, by comparing the soil C change estimated by repeated soil inventory.

## **6.2 Results**

### **6.2.1 Land use Change from 1959 to 2011**

Urban area was the largest artificial land use, occupying about 28% of the landscape throughout the study year ([Fig. 6.1a](#)). Urban area slightly increased from 24% in 1959 to 28% in 2011. The grassland increased from 38 ha in 1959 to 320 ha in 2011. In cropland, paddy area declined from 1254 ha in 1959 to 430 ha in 2011, upland area keeps stable from 1959 to 1994, and then decline from 977 ha in 1994 to 723 ha in 2011, bush/fallow area keeps slightly increase from 1959 to 1994 and then increased from 270 ha in 1994 to 673 ha in 2011. The main land use type in cropland was shown in [Fig. 6.1b](#). In upland crop, the area of soybean and vegetable declined slighted from 1959 to 2011, onion showed decrease from 1994, while wheat (+other upland crop) increased from 132 ha in

1959 to 392 ha in 2011.



**Figure 6. 1** Land use change from 1959 to 2011. (a) The main land use change. (b) The cropland use change.

## 6.2.2 Regional annual net primary production, carbon harvest and carbon inputs from plants

Average yield of soybean, vegetable, wheat, paddy and grass showed an overall increasing trend, and yield of onion showed an overall decreasing trend over the period of 1959–2011, although there were considerable variations from year to year. Average yield of buckwheat, maize, greenhouse and melon showed slightly increasing trend, and yield of fruits, potato remained relatively stable, while yield of pumpkin showed a decreasing trend from 1959 to 2011 (see Table 3.8). Crop-dependent NPP, C harvest and plant C inputs in the study region are presented in Fig. 6.3 (see Tables 6.1, 6.2 and 6.3 for crop NPP, C harvest and plant C inputs in each study year, respectively). Of all the crops, the crop-dependent NPP was highest for greenhouse ( $11.84 \pm 0.74 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$ ) and following to vegetable ( $10.12 \pm 2.92 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$ ), paddy ( $5.03 \pm 0.82 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$ ), wheat ( $4.67 \pm 1.69 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$ ), fruits ( $0.93 \pm 0.06 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$ ), and lowest in buckwheat ( $0.74 \pm 0.08 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$ ). Greenhouse had the highest plant C inputs per cropland hectare, followed by vegetable, wheat, maize, soybean and paddy. Onion and potato had relatively low plant C input. Ratios of plant C inputs to NPP varied significantly, depending on crop species (Fig. 6.2), with larger ratios being recorded for buckwheat (58%) and maize (54%) and smaller ratios for onion (10%) and potato (12%). Consequently, 38% of crop NPP was returned to the field at the regional scale.

**Table 6. 1** Crop net primary productivity (Mg C ha<sup>-1</sup> yr<sup>-1</sup>) data in the Ikushunbetsu watershed from 1959 to 2011.

|                            | 1959 | 1966 | 1976  | 1988  | 1994  | 2002  | 2005  | 2007  | 2009  | 2012  |
|----------------------------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|
| Soybean                    | 1.44 | 0.69 | 1.81  | 1.93  | 2.39  | 2.11  | 2.26  | 2.70  | 2.22  | 2.70  |
| Potato                     |      |      |       |       | 2.64  | 3.11  | 3.11  | 3.42  | 2.93  | 2.81  |
| Buckwheat                  |      |      |       |       | 0.64  | 0.79  | 0.79  | 0.67  | 0.67  | 0.85  |
| Vegetable                  | 4.42 | 5.27 | 10.00 | 10.46 | 10.79 | 12.03 | 12.17 | 12.61 | 11.06 | 12.39 |
| Onion                      | 5.23 | 3.74 | 4.49  | 4.01  | 3.37  | 4.24  | 4.07  | 2.98  | 2.98  | 3.99  |
| Maize                      |      |      |       |       | 2.80  | 3.11  | 2.97  | 2.85  | 2.85  | 3.08  |
| Greenhouse                 |      |      |       |       | 10.79 | 12.03 | 12.17 | 12.61 | 11.06 | 12.39 |
| Fruits <sup>a</sup>        |      |      |       |       | 0.99  | 0.81  | 0.95  | 0.95  | 0.95  | 0.95  |
| Melon <sup>a</sup>         |      |      |       |       | 1.63  | 1.63  | 1.79  | 1.87  | 1.87  | 1.97  |
| Pumpkin <sup>a</sup>       |      |      |       |       | 1.61  | 1.24  | 1.19  | 0.88  | 0.91  | 1.04  |
| Wheat                      | 2.70 | 1.56 | 4.09  | 5.33  | 5.04  | 5.78  | 6.02  | 6.40  | 3.27  | 6.48  |
| Grass                      | 6.41 | 5.07 | 7.29  | 8.01  | 8.21  | 7.99  | 8.11  | 7.91  | 7.74  | 7.76  |
| Paddy                      | 3.26 | 4.04 | 4.68  | 5.09  | 5.47  | 5.58  | 5.48  | 5.59  | 5.11  | 5.95  |
| Bush / Fallow <sup>a</sup> | 6.85 | 6.85 | 6.85  | 6.85  | 6.85  | 6.85  | 6.85  | 6.85  | 6.85  | 6.85  |

<sup>a</sup> NPP was estimated from dry weight of total plant, main plant product and by plant product using the linear regression from Osaki (1992).

**Table 6. 2** Crop C harvest (Mg C ha<sup>-1</sup> yr<sup>-1</sup>) data in the Ikushunbetsu watershed from 1959 to 2011.

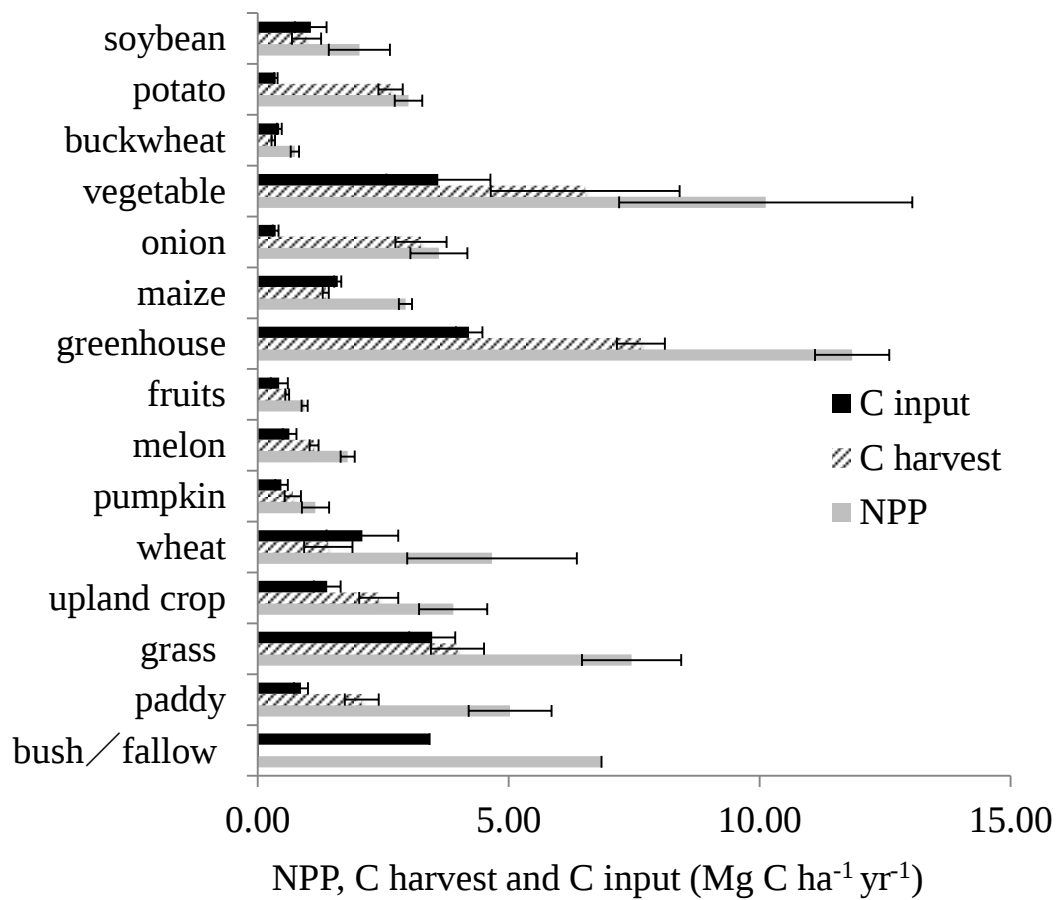
|                            | 1959 | 1966 | 1976 | 1988 | 1994 | 2002 | 2005 | 2007 | 2009 | 2011 |
|----------------------------|------|------|------|------|------|------|------|------|------|------|
| Soybean                    | 0.69 | 0.33 | 0.87 | 0.92 | 1.15 | 1.01 | 1.08 | 1.29 | 1.06 | 1.29 |
| Potato                     |      |      |      |      | 2.32 | 2.74 | 2.74 | 3.01 | 2.58 | 2.48 |
| Buckwheat                  |      |      |      |      | 0.27 | 0.33 | 0.33 | 0.28 | 0.28 | 0.35 |
| Vegetable                  | 2.85 | 3.40 | 6.45 | 6.75 | 6.96 | 7.75 | 7.84 | 8.13 | 7.13 | 7.98 |
| Onion                      | 4.71 | 3.37 | 4.05 | 3.62 | 3.04 | 3.82 | 3.67 | 2.69 | 2.69 | 3.60 |
| Maize                      |      |      |      |      | 1.29 | 1.43 | 1.36 | 1.31 | 1.31 | 1.42 |
| Greenhouse                 |      |      |      |      | 6.96 | 7.75 | 7.84 | 8.13 | 7.13 | 7.98 |
| Fruits <sup>a</sup>        |      |      |      |      | 0.62 | 0.51 | 0.59 | 0.59 | 0.59 | 0.59 |
| Melon <sup>a</sup>         |      |      |      |      | 1.02 | 1.02 | 1.12 | 1.17 | 1.17 | 1.23 |
| Pumpkin <sup>a</sup>       |      |      |      |      | 0.98 | 0.76 | 0.72 | 0.53 | 0.55 | 0.63 |
| Wheat                      | 0.78 | 0.45 | 1.18 | 1.57 | 1.49 | 1.71 | 1.78 | 1.89 | 1.31 | 1.87 |
| Grass                      | 3.42 | 2.71 | 3.89 | 4.28 | 4.38 | 4.27 | 4.33 | 4.22 | 4.13 | 4.15 |
| Paddy                      | 1.34 | 1.66 | 1.93 | 2.09 | 2.25 | 2.30 | 2.26 | 2.30 | 2.10 | 2.45 |
| Bush / Fallow <sup>a</sup> | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |

<sup>a</sup> C harvest was estimated from dry weight of total plant, main plant product and by plant product using the linear regression from Osaki (1992).

**Table 6. 3** Plant C input (Mg C ha<sup>-1</sup> yr<sup>-1</sup>) data in the Ikushunbetsu watershed from 1959 to 2012.

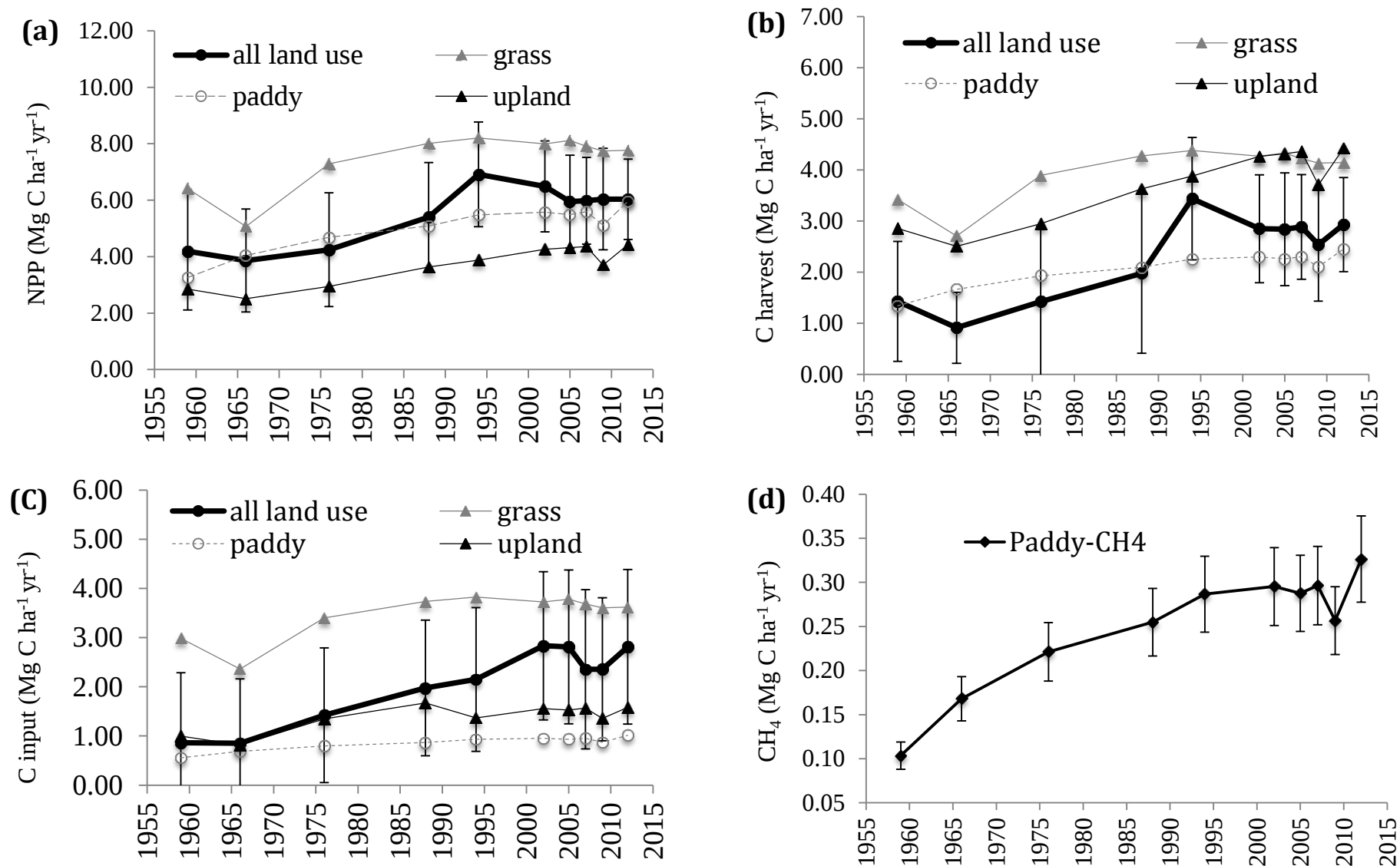
|                            | 1959 | 1966 | 1976 | 1988 | 1994 | 2002 | 2005 | 2007 | 2009 | 2011 |
|----------------------------|------|------|------|------|------|------|------|------|------|------|
| Soybean                    | 0.75 | 0.36 | 0.94 | 1.00 | 1.25 | 1.10 | 1.17 | 1.41 | 1.15 | 1.41 |
| Potato                     |      |      |      |      | 0.31 | 0.37 | 0.37 | 0.41 | 0.35 | 0.34 |
| Buckwheat                  |      |      |      |      | 0.37 | 0.46 | 0.46 | 0.39 | 0.39 | 0.49 |
| Vegetable                  | 1.57 | 1.87 | 3.55 | 3.72 | 3.84 | 4.28 | 4.32 | 4.48 | 3.93 | 4.40 |
| Onion                      | 0.52 | 0.37 | 0.44 | 0.40 | 0.33 | 0.42 | 0.40 | 0.29 | 0.29 | 0.39 |
| Maize                      |      |      |      |      | 1.51 | 1.68 | 1.61 | 1.54 | 1.54 | 1.67 |
| Greenhouse                 |      |      |      |      | 3.84 | 4.28 | 4.32 | 4.48 | 3.93 | 4.40 |
| Fruits <sup>a</sup>        |      |      |      |      | 0.37 | 0.78 | 0.36 | 0.36 | 0.36 | 0.36 |
| Melon <sup>a</sup>         |      |      |      |      | 0.37 | 0.61 | 0.67 | 0.70 | 0.70 | 0.74 |
| Pumpkin <sup>a</sup>       |      |      |      |      | 0.63 | 0.61 | 0.47 | 0.35 | 0.36 | 0.41 |
| Wheat                      | 1.16 | 0.67 | 1.76 | 2.34 | 2.21 | 2.54 | 2.65 | 2.81 | 1.95 | 2.78 |
| Grass                      | 2.99 | 2.36 | 3.40 | 3.73 | 3.82 | 3.72 | 3.78 | 3.68 | 3.61 | 3.62 |
| Paddy                      | 0.56 | 0.69 | 0.80 | 0.87 | 0.93 | 0.95 | 0.93 | 0.95 | 0.87 | 1.01 |
| Bush / Fallow <sup>a</sup> | 3.43 | 3.43 | 3.43 | 3.43 | 3.43 | 3.43 | 3.43 | 3.43 | 3.43 | 3.43 |

<sup>a</sup> C input was estimated from dry weight of total plant, main plant product and by plant product using the linear regression from Osaki (1992).



**Figure 6. 2** Crop NPP, C harvest and plant C input through the study period. The error bar indicates standard deviation.

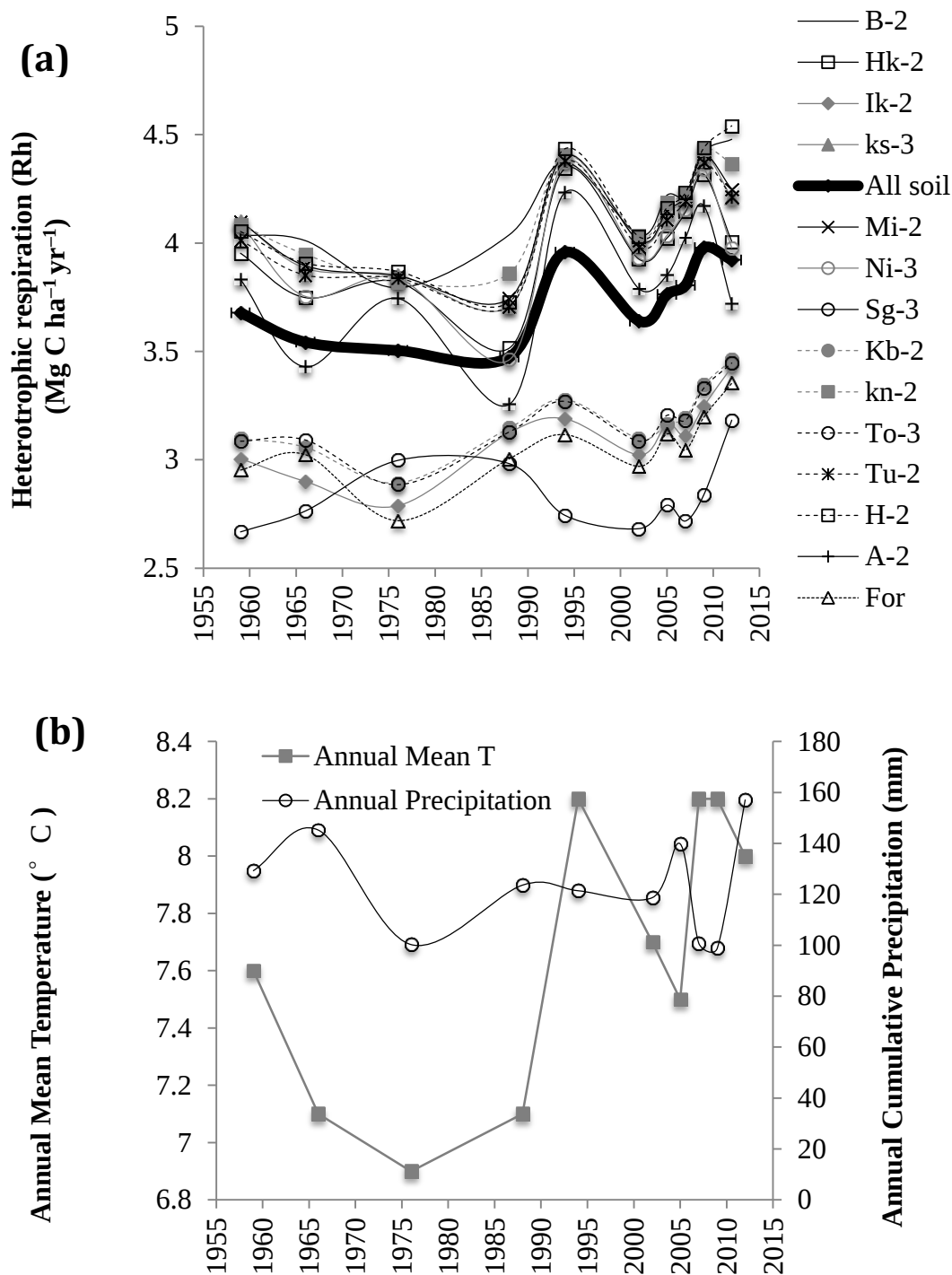
Total annual NPP of all land use (upland + paddy + grass) over the analysis period averaged  $5.51 \pm 1.05 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$ . At regional scale, NPP of all land use over the study period ranged from  $4.19 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$  (in 1959) (Fig. 6.6b) to  $6.03 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$  (in 2011) (Fig. 6.6g) (Fig. 6.3a), while the plant C inputs over the period ranged from  $1.11 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$  in 1959 (Fig. 6.6d) to  $2.81 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$  in 2011 (Fig. 6.6i) (Fig. 6.3c). NPP of upland (not included bush/fallow) ranged from  $2.85 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$  in 1959 to  $4.42 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$  in 2011. NPP of paddy ranged from  $3.26 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$  in 1959 to  $5.95 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$  in 2011. NPP of grass ranged from  $6.41 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$  (in 1959) to  $7.76 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$  (in 2011) (Fig. 6.3a). As a result, the annual C harvest from all the field combined increased from 1959 to 2011, by  $1.94 \text{ Mg C ha}^{-1}$  in all land use, by  $0.58 \text{ Mg C ha}^{-1}$  in upland (not included bush/fallow), by  $0.56 \text{ Mg C ha}^{-1}$  in paddy, and by  $0.63 \text{ Mg C ha}^{-1}$  in grass (Fig. 6.3b). Total annual C input from all the field combined increased from 1959 to 2011, by  $1.85 \text{ Mg C ha}^{-1}$  in all land use, by  $0.01 \text{ Mg C ha}^{-1}$  in upland crop (not included bush/fallow), by  $1.58 \text{ Mg C ha}^{-1}$  in paddy, by  $0.63 \text{ Mg C ha}^{-1}$  in grass (Fig. 6.3c). In bush/fallow field, the overall trend was considered as neither increasing nor decreasing over the study period.



**Figure 6.3** Temporal trends of NPP (a) , C harvest (b), C input (c) during the study period for main land use at the regional scale, and temporal trends of CH<sub>4</sub> emission in paddy (d). The error bar for all filed indicates the range of standard deviation.

### 6.2.3 Soil heterotrophic respiration and CH<sub>4</sub> emission at regional scale

Heterotrophic respiration (Rh) over the study period of 1959–2011 showed clear seasonality, with high levels in warm year and low levels in cold year (Figs. 6.4a, 6.4b). Rh was estimated at  $3.14 \pm 0.27 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$  at regional scale, which takes a fraction of 59% ( $\pm 12\%$ ) of the total NPP. The CH<sub>4</sub> emission from the paddy over the analysis period 1959–2011 averaged  $0.25 \pm 0.07 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$ . CH<sub>4</sub> emission from paddy increased from  $0.1 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$  in 1959 to  $0.33 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$  in 2011 (Fig. 3d).



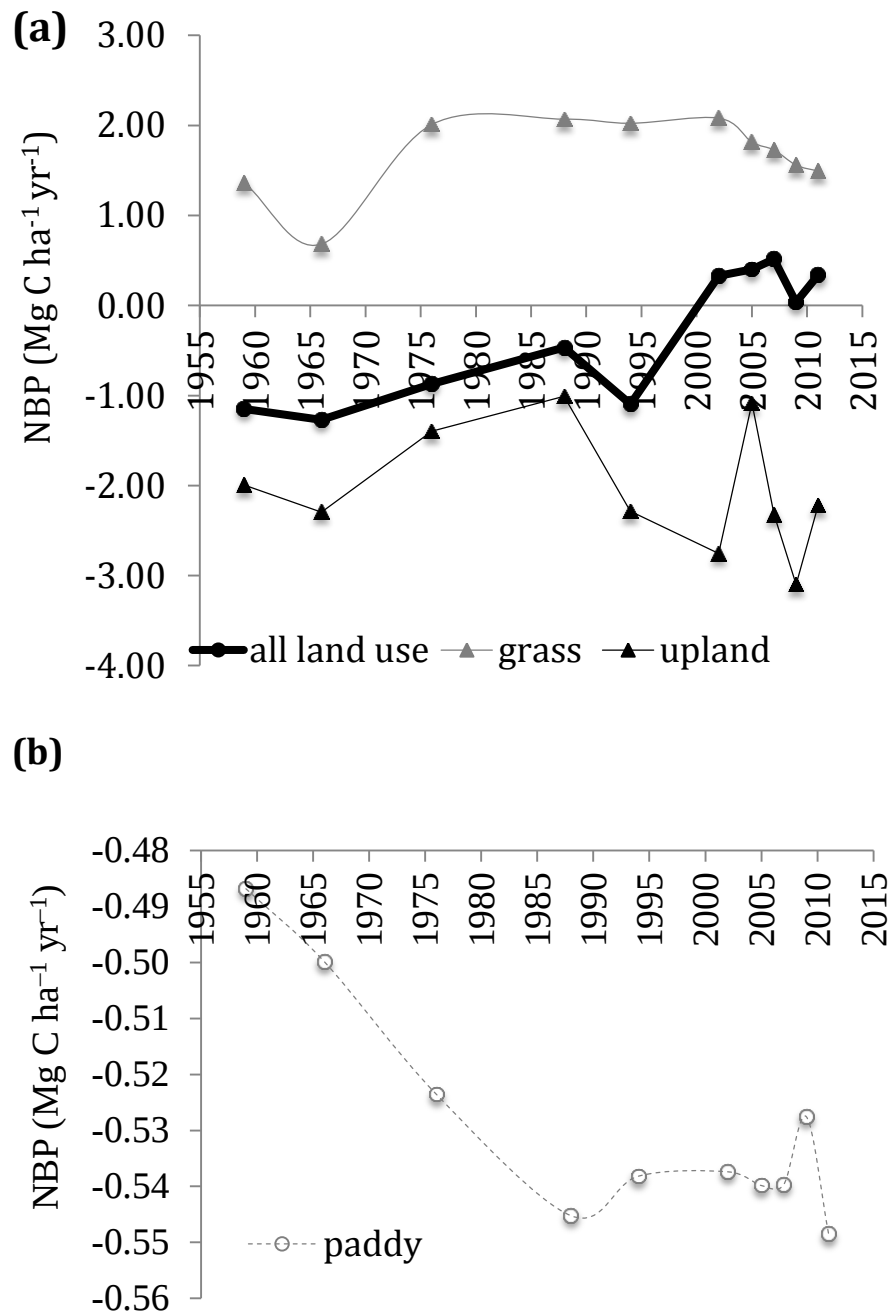
**Figure 6. 4** (a) Soil heterotrophic respiration estimated at 15 soil types. Soils of B-2, Hk-2, A-2, H-2 and forest (for) are the sub soil of Grey lowland; Soils of Ik-2, M-3, Sg-3, To-3 and Tu-3 are the sub soil of Brown lowland; Soils of Ks-3, Mi-2 and Kb-2 are the sub soil of Gely lowland; Soils of Ni-3 and Kn-2 are the sub soil of Pseudogleys ([Hokkaido Central Agriculture Experiment Station, 1971](#)). (b) Mean annual temperature and mean annual precipitation from 1959 to 2011.

## 6.2.4 Regional annual net biome productivity

Though the mean NBP in all land use (upland + paddy + grassland) was estimated to  $-0.32 \pm 0.72 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$  through to the period from 1959 to 2011, the time series of NBP in all land use increased over the study period and the change in NBP showed a slowly upward trend, which estimated an average increase of NBP ( $1.48 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$ ) from 1959 to 2011 (Fig. 6.5). Interannual variability of NBP in all land use ranged between  $-1.42$  to  $0.48 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$  (Table 6.4). The NBP in 1959 and 2011 in all land use ranged from  $-1.27 \pm 2.53 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$  to  $0.52 \pm 2.77 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$  (Table 6.6; Fig. 6.5; Figs. 6.6e, 6.6j). NBP of upland (not included bush/fallow) ranged from  $-1.99 \pm 0.53 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$  in 1959 to  $-2.22 \pm 0.57 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$  in 2011 (Table 6.4). NBP of paddy ranged from  $-0.49 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$  in 1959 to  $-0.55 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$  in 2011 (Table 6.4). NBP of grass ranged from  $1.36 \pm 0.84 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$  in 1959 to  $1.49 \pm 0.86 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$  in 2011 (Table 6.4; Fig. 6.5). The C sequestration efficiency (CE), defined as the ratio of NBP/NPP, ranged from  $-0.13$  to  $-0.03$  for croplands (upland + paddy + fallow), and equal to  $0.22 \pm 0.04$  for grassland.

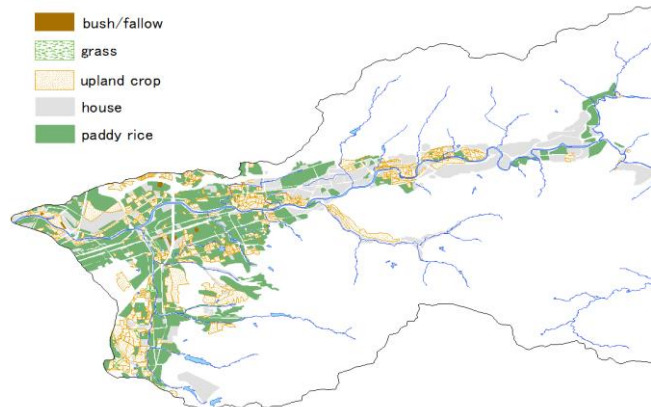
**Table 6. 4** The carbon budget of different land use based on a full carbon flux budget (NBP) from 1959–2011.

| Year                                                                   | Upland         | Paddy          | Grass         | All land use   |
|------------------------------------------------------------------------|----------------|----------------|---------------|----------------|
| 1959                                                                   | $-1.99 (0.53)$ | $-0.49 (0.68)$ | $1.36 (0.84)$ | $-1.15 (2.84)$ |
| 1966                                                                   | $-2.29 (0.55)$ | $-0.50 (0.68)$ | $0.68 (0.85)$ | $-1.27 (2.53)$ |
| 1976                                                                   | $-1.40 (0.54)$ | $-0.52 (0.69)$ | $2.01 (0.85)$ | $-0.87 (2.96)$ |
| 1988                                                                   | $-1.01 (0.59)$ | $-0.55 (0.70)$ | $2.07 (0.88)$ | $-0.47 (2.93)$ |
| 1994                                                                   | $-2.29 (0.57)$ | $-0.54 (0.70)$ | $2.02 (0.87)$ | $-1.09 (2.95)$ |
| 2002                                                                   | $-2.76 (0.56)$ | $-0.54 (0.71)$ | $2.08 (0.86)$ | $0.33 (2.76)$  |
| 2005                                                                   | $-1.08 (0.55)$ | $-0.54 (0.71)$ | $1.82 (0.85)$ | $0.40 (2.83)$  |
| 2007                                                                   | $-2.32 (0.58)$ | $-0.54 (0.70)$ | $1.73 (0.88)$ | $0.52 (2.77)$  |
| 2009                                                                   | $-3.10 (0.60)$ | $-0.53 (0.70)$ | $1.56 (0.89)$ | $0.04 (2.87)$  |
| 2011                                                                   | $-2.22 (0.57)$ | $-0.55 (0.71)$ | $1.49 (0.86)$ | $0.34 (2.66)$  |
| Positive numbers are sinks. Numbers in brackets are total uncertainty. |                |                |               |                |

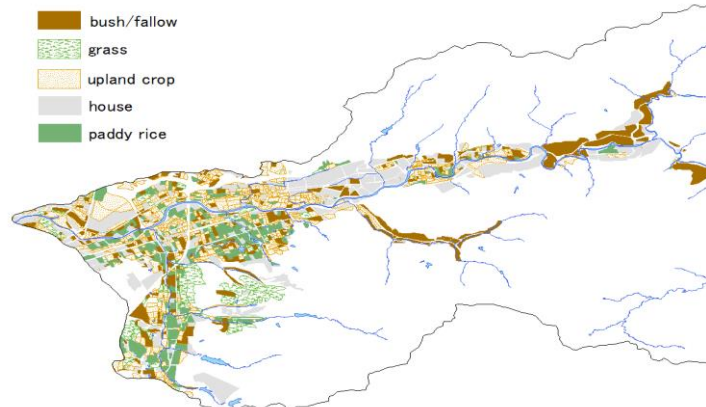


**Figure 6. 5** Temporal trends of net biome productivity (NBP) during the study period for (a) all land use, grass and upland, (b) paddy.

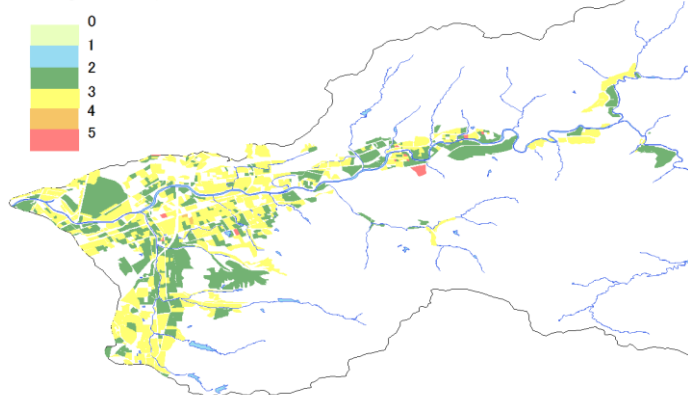
(a) land use 1959



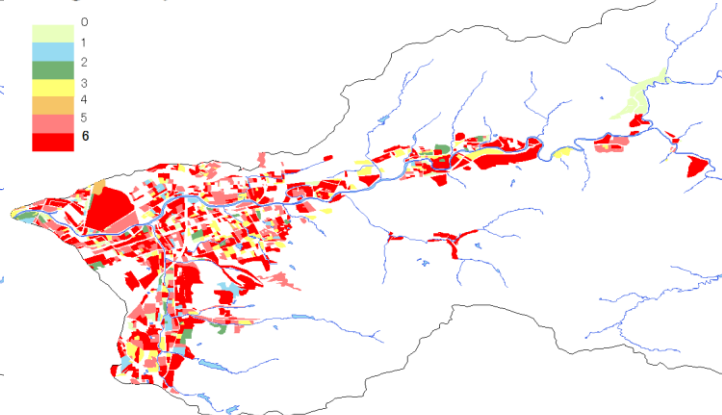
(f) land use 2012



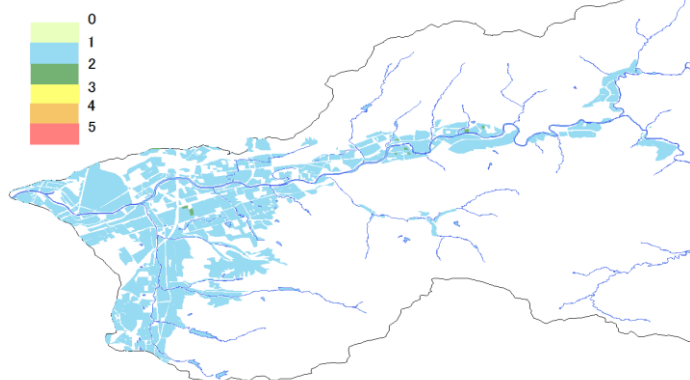
(b) NPP 1959  
Mg C ha<sup>-1</sup> yr<sup>-1</sup>



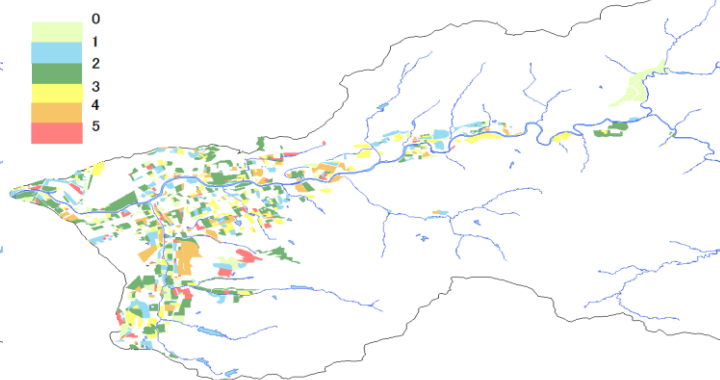
(g) NPP 2012  
Mg C ha<sup>-1</sup> yr<sup>-1</sup>

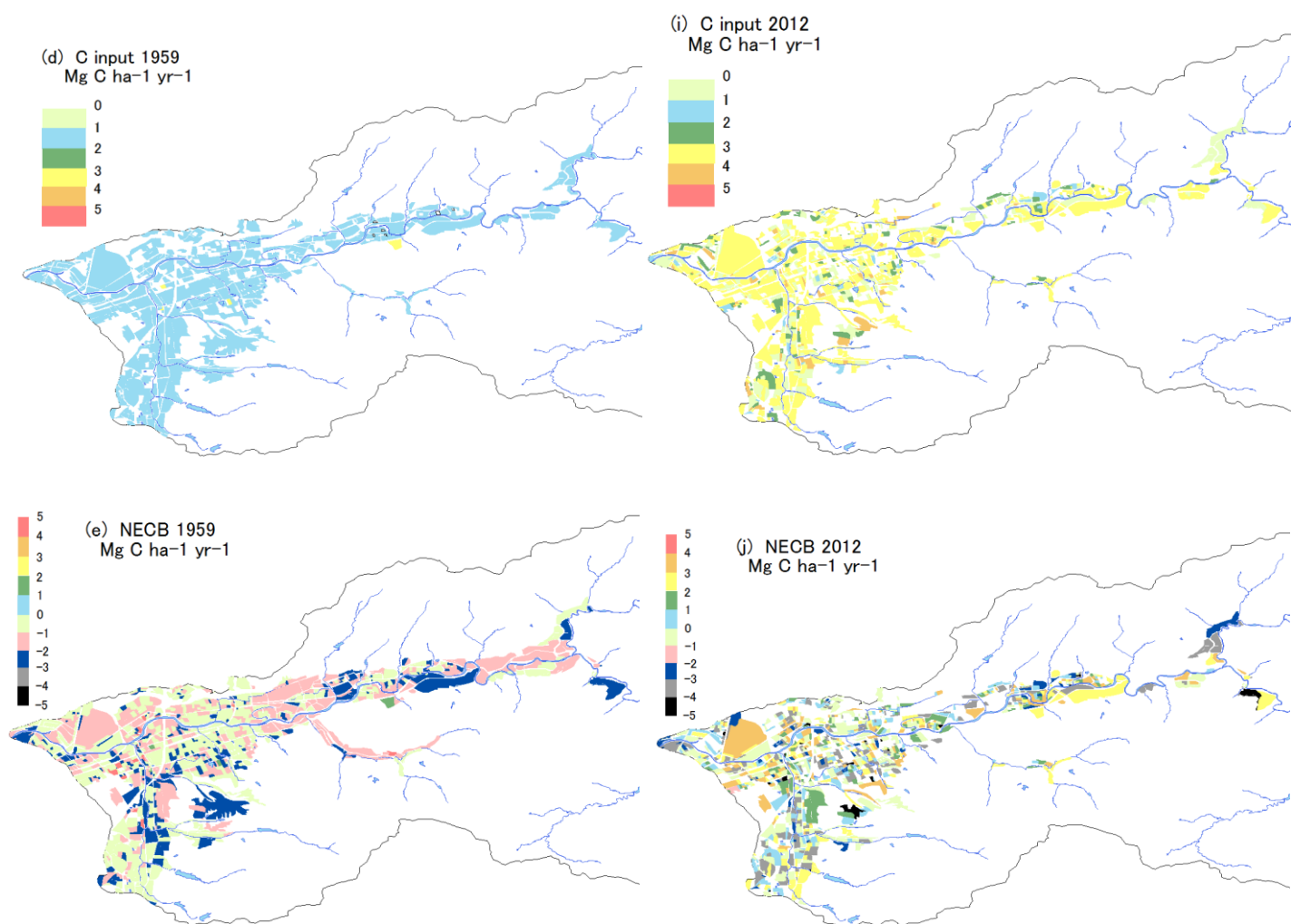


(c) C harvest 1959  
Mg C ha<sup>-1</sup> yr<sup>-1</sup>



(h) C harvest 2012  
Mg C ha<sup>-1</sup> yr<sup>-1</sup>





**Figure 6. 6** Land use (a,f), NPP (b,g) , C harvest (c,h), C input (d,i), NECB (e,j) at study site in 1959 and 2011.

## 6.2.5 Temporal variation in net primary production and residue carbon inputs

The Pearson correlation of weather condition with NPP, C harvest, plant C input and NBP was shown in Table 6.5. The NPP for the all land use was positively correlated with annual mean temperature ( $r=0.74$ ,  $P<0.05$ ) and was positively correlated with the mean growing season temperature ( $r=0.48$ ,  $P<0.05$ ) over the study period (1959–2011). At individual land use level, such a positive correlation with annual mean temperature could be found for upland ( $r=0.62$ ,  $P<0.05$ ), paddy ( $r=0.40$ ,  $P<0.05$ ), and grass ( $r=0.46$ ,  $P<0.05$ ). The observed temporal variation of NPP can be well described by climate relationships in upland, grass and all land use (Table 6.5).

Plant C input varied with changing weather condition over the study period (Table 6.5). Annual plant C input for the all land use was positively correlated with annual mean temperature ( $r=0.48$ ,  $P<0.05$ ) and was positively correlated with the mean growing season temperature ( $r=0.44$ ,  $P<0.05$ ) over the study period (1959–2011). At individual land use level, such a positive correlation with annual mean temperature could be found for upland ( $r=0.25$ ,  $P<0.05$ ), paddy ( $r=0.40$ ,  $P<0.05$ ) and grass ( $r=0.46$ ,  $P<0.05$ ). The observed temporal variations in plant C input in upland was well described by a quadratic relationship, which incorporated annual total precipitation (Annppt), annual mean temperature (Annt), growing season precipitation (Gppt), squared growing season precipitation ( $Gppt^2$ ), ratio of precipitation and potential evapotranspiration in growing season (Gratio) in upland. C input =  $-1.78 + 0.004 \times Annt + 0.13 \times Gppt - 0.001 \times Gppt^2 - 0.24 \times Gratio$  ( $R^2=0.83$ ,  $P=0.04$ ) for upland (Table 6.6).

**Table 6. 5** Pearson correlations of weather condition with net primary productivity (NPP), C harvest, plant C input, net biome productivity (NBP) ( $P < 0.05$ ) from 1959–2011.

|              |                         | Annppt | Annt  | Gppt  | Gtmean | Annratio | Gratio |
|--------------|-------------------------|--------|-------|-------|--------|----------|--------|
| Upland       | NPP                     | -0.23  | 0.62  | -0.19 | 0.31   | -0.18    | -0.29  |
|              | Charvest                | -0.20  | 0.80  | -0.02 | 0.36   | -0.16    | 0.01   |
|              | Cinput                  | -0.19  | 0.25  | -0.34 | 0.14   | -0.28    | -0.64  |
|              | NBP                     | 0.25   | -0.69 | -0.04 | -0.29  | 0.30     | -0.08  |
| Paddy        | NPP/Charvest/Cinput/NBP | -0.13  | 0.40  | -0.09 | 0.31   | -0.03    | -0.19  |
| Grass        | NPP/Charvest/Cinput     | -0.31  | 0.46  | -0.53 | 0.31   | -0.25    | -0.40  |
|              | NBP                     | -0.49  | 0.10  | -0.73 | 0.09   | -0.12    | -0.46  |
| All land use | NPP                     | -0.11  | 0.74  | -0.32 | 0.48   | -0.07    | 0.04   |
|              | Charvest                | -0.07  | 0.52  | -0.28 | 0.42   | 0.06     | 0.03   |
|              | Cinput                  | 0.11   | 0.48  | -0.12 | 0.44   | 0.02     | -0.21  |
|              | NBP                     | 0.21   | 0.35  | 0.24  | -0.12  | -0.23    | -0.25  |

ppt: precipitation; t: temperature, ratio: ratio of precipitation and potential evapotranspiration. “Ann” stands for annual mean value; “G” stands for growing season.

**Table 6. 6** The relationship of NPP, C harvest, C input and NBP with climate data in different land use from 1959–2011.

| Land use     | Equation                                                                                                               | $R^2$ | $P$  |
|--------------|------------------------------------------------------------------------------------------------------------------------|-------|------|
| Upland       | $NPP = -3.02 + 0.88 \times Annt$                                                                                       | 0.39  | 0.05 |
|              | $Charvest = -7.39 - 0.001 \times Annppt + 1.29 \times Annt + 0.0004 \times Gppt^2 - 0.383 \times Gratio$               | 0.82  | 0.04 |
|              | $Cinput = -1.78 + 0.04 \times Annt + 0.13 \times Gppt - 0.001 \times Gppt^2 - 0.24 \times Gratio$                      | 0.83  | 0.04 |
| Grass        | $NPP = 2.70 - 0.18 \times Annt - 0.06 \times Gppt + 0.0005 \times Gppt^2 + 0.002 \times Gtmean^2 - 0.07 \times Gratio$ | 0.92  | 0.02 |
|              | $NBP = 3.01 - 0.28 \times Annt - 0.0004 \times Gppt^2 + 0.006 \times Gtmean^2$                                         | 0.72  | 0.04 |
| All land use | $NPP = -6.43 + 1.56 \times Annt$                                                                                       | 0.54  | 0.02 |
|              | $NBP = 0.87 + 0.22 \times Annt - 0.07 \times Gppt + 0.001 \times Gppt^2 - 0.21 \times Gratio$                          | 0.75  | 0.09 |

ppt: precipitation; t: temperature, ratio: ratio of precipitation and potential evapotranspiration. “Ann” stands for annual mean value; “G” stands for growing season.

## 6.2.6 Method comparison

C budget for upland, paddy, grass from 2005–2011 based on NBP method was listed in [Table 6.7](#) together with the results from the repeated soil inventory. For individual fields, both methods NBP and soil inventory indicate a decrease of soil C from 2005–2011, however, a higher C loss measured by soil inventory and a much smaller C decline for NBP. Soil inventory showed that the higher C loss ( $-3.21 \pm 2.51 \text{ Mg C ha}^{-1} \text{ yr}^{-1} \text{ layer}^{-1}$ ) in 3<sup>rd</sup> layer than in 1<sup>st</sup> and 2<sup>nd</sup> layer in upland. Though in paddy, soil acts as C sink in 1<sup>st</sup> layer, the higher C

loss in 2<sup>nd</sup> layer cause the soil to be C source ( $-0.38 \pm 2.56 \text{ Mg C ha}^{-1} \text{ yr}^{-1} \text{ layer}^{-1}$ ) in 30cm soil depth. In grass, the higher C loss was found ( $-0.95 \pm 6.43 \text{ Mg C ha}^{-1} \text{ yr}^{-1} \text{ layer}^{-1}$ ) by means of soil inventory than  $-0.32 \pm 1.21 \text{ Mg C ha}^{-1} \text{ yr}^{-1} \text{ layer}^{-1}$ ) by means of NBP method.

**Table 6. 7** Six year (2005–2011) carbon budget of different land use based on a full carbon flux budget (NBP) and repeated soil carbon inventories.

| Land use     | NBP<br>$\text{Mg C ha}^{-1} \text{ yr}^{-1}$ | Soil inventory<br>$\text{Mg C ha}^{-1} \text{ yr}^{-1} \text{ layer}^{-1}$ |              |              |             |
|--------------|----------------------------------------------|----------------------------------------------------------------------------|--------------|--------------|-------------|
|              |                                              | 30cm (1st ~ 3rd layer)                                                     | 1st layer    | 2nd layer    | 3rd layer   |
| Upland       | -1.13 (0.79)                                 | -1.55 (3.76)                                                               | -0.34 (2.24) | -0.62 (2.17) | -3.21(2.51) |
| Paddy        | -0.01(0.95)                                  | -0.38 (2.56)                                                               | 0.14 (1.56)  | -0.73 (2.79) |             |
| Grass        | -0.32 (1.21)                                 | -0.95 (6.43)                                                               | -1.21 (3.14) | -0.93 (5.98) |             |
| Paddy-upland |                                              | -1.05 (8.24)                                                               | 0.17 (4.69)  | -2.34 (4.69) |             |

Positive numbers are sinks. Numbers in brackets are total uncertainty. "paddy-upland" represented land use change from paddy to upland.

## 6.3 Discussion

### 6.3.1 Influence of residue management on net biome productivity

Over the whole study region during 1988–2011, mean cropland NPP ( $\pm$ SD) was  $5.51 \pm 1.05 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$ . Compared to NPP for other regions, the NPP was  $6.66 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$  for Tokachi region of Hokkaido over the period of 1971–2010 (Koga et al., 2011),  $5.5 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$ , for the European cropland (Ciais et al., 2010) and  $3.5\text{--}4.2 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$  for Canadian cereal-based cropland (Bolinder et al., 2007). The average amount of C input ( $\pm$ SD) at regional scale in this study area over the period of 1959–2011 was  $2.04 \pm 0.80 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$ , and this plant C input represented 37% of the NPP. This result was close to the result in arable farmlands of northern Japan estimated by Koga et al. (2011), which the regional annual plant C input was  $2.52 \pm 0.32 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$  and the C input represented 38% of the NPP.

Crop production increased markedly between 1959 and 2011, which augmented the amount of residue and root input to the soil (Figs. 6.3a; 6.3c). Under field conditions, merely

15–50% of the C input will remain in soil un-decomposed after one year (Sleutel et al., 2006). The average amount of C input ( $\pm$ SD) in upland and paddy in this study over the period of 1959–2011 was  $1.38 \pm 0.27$  Mg C ha<sup>-1</sup> yr<sup>-1</sup> and  $0.86 \pm 0.14$  Mg C ha<sup>-1</sup> yr<sup>-1</sup>. Even though the increasing C input to the soil over the years, NBP in upland and paddy showed decreasing trend from 1959–2011, especially for upland, because the C input in Ikushunbetsu watershed was far more smaller than the value of Japanese C input to mention soil C level mentioned by Yokozawa et al. (2010). Our study demonstrated that C budget by NBP decreased in upland and paddy in central Hokkaido under the recent C input scenario. Yokozawa et al. (2010) used Roth C to simulate soil C stocks in Japanese upland and paddy at a national scale, showed that the required C input to upland and paddy are 5.06–5.66 Mg C ha<sup>-1</sup> yr<sup>-1</sup> and 2.76 Mg C ha<sup>-1</sup> yr<sup>-1</sup>, respectively, to maintain the soil C level in 1990. This illustrates that crop residues play a crucial role in maintaining soil C stocks in croplands and that the removal of residues or smaller return of C to the soil has adverse effects on soil C storage and the mitigation of GHG emissions from agricultural lands (Zhang et al., 2006; Koga et al., 2011).

The C sequestration efficiency (CE) of croplands (upland + paddy + fallow), defined as the ratio of NBP/NPP, ranged from –0.13 to –0.03. This CE value is low compared to the values of European cropland, ranged from –0.03 to 0.01 (Ciais et al., 2010). The grasslands CE equal to 0.22 ( $\pm$ 0.04), which is higher than the grasslands CE in European (0.13) (Ciais et al., 2010). The smaller CE values in croplands reflect a smaller return of C to the soil, coupled with an accelerated composition of soil organic matter due to plowing and tillage (e.g. destruction of soil micro aggregates and oxygenation). Another reason is that our estimates do not include manure additions that are accounted for in the cropland inventory estimates. At face value, improved cropland management can greatly increase cropland soil C sequestration (Smith et al., 2007a). Smith et al. (2005) suggested that croplands could become a net C sink under improved technology, but the uncertainty (due to climate projections and interactions between decomposition, NPP and technology) was also large, with a 9% uncertainty due to forecast changes in technology alone. The major contribution of

croplands to longer term sequestration of C, and hence mitigation of the greenhouse effect, is likely to be in soil C accumulation, especially in “no-till” agriculture where the land is not ploughed ([Prince et al., 2001](#)).

### **6.3.2 Influence of climate condition on net biome productivity**

Regional patterns in crop production in agricultural ecosystems are driven by differences in the productivity potential of different crop species, which are largely governed by climate, but modified by management (i.e. irrigation). Temporal trends in production are influenced by developing technology (i.e. crop genetics, fertilization) and changes in management and agricultural policies, and by long-term trends in climate and CO<sub>2</sub> concentrations. In longer trends, the interannual variability of production, largely driven by weather variability and climate cycles, and also vary spatially across the regional scale related to differences in soil quality, moisture and nutrient availability that may be directly or indirectly related to climatic differences ([Lokupitiya et al., 2012](#)).

To simulate both spatial and temporal changes in ecosystem C balance at a regional scale, detailed information regarding C inputs from crop residues, green manure and composted manure is necessary. However, accurate measurements or simulations of annual plant C inputs (part of crop NPP) to croplands are difficult due to the unpredictability of a number of regional-specific factors such as crop species, cultivars and field management practices, as well as variable micrometeorological and soil conditions. The temporal variability of cropland NPP and plant C input is determined by fluctuating climate conditions ([Ciais et al., 2005](#); [Lokupitiya et al., 2012](#)). According to our study, yields and plant C inputs showed an increase trend for most crops over the 1959–2005. Our study revealed that plant C inputs could be well predicted by a quadratic relationship. Plant C inputs in this study tended to be positively proportional to the annual mean temperature (Annt) and growing season temperature (Gtmean) ([Table 6.5](#)). Increasing temperature may increase NPP where it can increase the length of the seasonal and daily growing cycles, but it may decrease NPP in

water-stressed ecosystems as it increases water loss (Gómez et al., 2006). Lokupitiya et al. (2012) found a negative relation over the 16-year period in US croplands, for instance, a 1°C increase in the growing season temperature (and a decrease in precipitation of 80 mm compared to the previous year), a decrease of 0.76 Mg ha<sup>-1</sup> in plant C input rate was observed. Reduction in productivity in region with increases in growing season temperature, due to the higher temperature and drought occurred in North Central region, US in 1993. Fungal epidemics in corn, soybean and alfalfa caused by high moisture, and outbreak of soybean sudden death syndrome in the US in 1993, may have led to the low productivity and low plant C inputs observed.

In this study, we estimated trends in C budget by NBP at regional scale based on residue inputs and climate impacts on Rh modeling (Chapter 4). Our study revealed that NBP could be well predicted by a quadratic relationship based on climate condition in grass and all land use (Table 6.4), however, this relationship cannot be found in upland and paddy. Much more complicated C budget was in managed upland and paddy than permanent grass, because plowing and tillage intensity impacts on Rh, crop species change within upland, smaller return of C to the soil might have the major impact on C budget.

### 6.3.3 Influence of land use change on net biome productivity

The land area of upland and paddy was found to decrease from 1956 to 2011, however, the yield and plant C input in all land use showed an overall increase (Fig. 6.3c). The upland and paddy are the main land use contributing the increase of plant C input at the regional scale. The long-term trend of increasing yields for most major crops such as soybean, vegetable, wheat and paddy are largely attributed to an array of technology and management developments (i.e., crop genetics, fertilization, plant breeding and pesticide use, etc.). The declined in paddy area has been encouraged by the set aside policy of the Japanese government (Ministry of Agriculture, Forestry and Fisher, 2006). The decline in onion area might be due to the low market price of onion from 2002. The fallow land area increased

from 1989 due to the closure of mine activity in 1989 (Mikasa City, 1994) and agricultural activity in this area (Kimura et al., 2004).

The upland in this study showed decreased NBP over the period of 1959–2011. In Japanese upland cropland, Koizumi (2001) reported that the amount of C loss from the soil was within 1.58–3.14 Mg C ha<sup>-1</sup> yr<sup>-1</sup> in fields under upland crop cultivation. Another field experiments in upland under wheat, onion and soybean cultivation in the northern part of Japan showed significant loss of 1.47–4.10 Mg C ha<sup>-1</sup> yr<sup>-1</sup> from the soil (Hu et al., 2004; Mu et al., 2006). The NBP in upland declined from 1988 was caused by the increased wheat cultivation from 79 ha in 1959 to 188 ha in 2012. However, there is large uncertainty in this estimate because the historical land use changes are poorly quantified in terms of both spatial and temporal before 1994 in our study. Generally, the range of estimated NBP shown in this study is similar to those literatures in cropland (Koizumi, 2001). Other previous studies showed quite different results, with NBP near zero or with significant C accumulation into the soil, however, these results were only found in no-tillage cultivation (Hollinger et al., 2005; Nouchi and Yonemura, 2005).

The paddy in this study showed decreased NBP over the period of 1959–2011. We ignored the low CH<sub>4</sub> emission from the upland aerobic soils. Methanogenesis is restricted to completely anaerobic soil conditions as occur in paddy when the soils are flooded. C input in paddy increased over the study period along with increasing paddy rice yield, however, the increased C input leads to higher CH<sub>4</sub> emission loss from paddy field. These CH<sub>4</sub> emissions were estimated at 1.28±0.27 Mg C ha<sup>-1</sup> yr<sup>-1</sup> over the study period. Paddy was not a C source in fallow season, due to non harvest, retention of crop residues, and the fact that biomass incorporated into the soil was not completely decomposed during the season. Our estimation was based the over one year including fallow season, therefore, the paddy showed a C source during study period. The land area of paddy declined from 1254 ha in 1959 to 430 ha in 2012, which land use of paddy changed to upland, grassland and bush/fallow (Figs. 6.6a; 6.6f). Though land use change from paddy cultivation to upland cultivation might cause significant

loss of C from cropland soil; 1.05 Mg C ha<sup>-1</sup> yr<sup>-1</sup> C loss from 2005–2011 in this study ([Table 6.7](#)). In the case of increased agricultural abandonment (fallow/bush) from 1988, C pools slowly start to build up.

In our study, we find a tendency for a C sink in grassland. Our study indicated that cropland to grassland conversion sequester C from 2002. The NBP in all land use across the whole region showed a slowly increase. Though upland and paddy showed decreased NBP over the period of 1959–2011, the increased land use of grassland and bush/fallow contributed to less C loss from field, which lead to the increased NBP at regional scale.

### **6.3.4 Comparison of repeated soil inventory and net biome productivity method**

In this study, for the same period and in same land use, the soil inventory method showed a tendency towards higher C loss than NBP method ([Table 6.7](#)). Hardly any direct comparisons of the NBP approach and repeated soil inventories are reported in cropland in the literature. One study comparing NBP and soil C inventories over a 3 year period for maize-soybean rotations found similar C budgets between methods with non significant changes in soil inventories and no or small changes in NBP, however, no indication for the uncertainty in NBP was provide and thus a direct quantitative evaluation of methods proved difficult. [Leifeld et al. \(2011\)](#) made a comparison of soil inventory and NBP to detect soil C stock after conversion from cropland to grasslands, and showed that the soil inventory method showed a tendency towards higher C loss / smaller C gain than NBP method. Though grassland was calculated as a C sink from 1959–2011 by NBP method in our study site, both methods showed that C loss occurs in grassland from 2005–2011. [Ciais et al. \(2010\)](#) reported that European grasslands to be a C sink by means of NBP. However, the long-term grass use does not go along with a change in soil C by means of soil inventory ([Hopkins et al., 2009](#)). Together, these data tentatively indicate that an underestimation measured by means of NBP or an overestimation by means of repeated C inventories in this study cannot be excluded.

### 6.3.5 Uncertainty

The capability of the two methods to detect changes in soil C stocks is limited by their total uncertainty resulting from various error sources. The temporal uncertainty of NBP in all land use at regional scale was estimated to be  $0.72 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$  described by standard deviation value as the inter-annual variation between 1959 and 2011. Another uncertainty result from systematic errors in individual land use was described in [Table 6.4](#). The NBP approach uncertainty resulting from temporally random-like errors is generally not very problematic, because of the large number of measurements during a multiyear experiment. Instead, the NBP method encounters a number of sources for systematic errors, including limited field size, field heterogeneity, and measurement limitations, such as imperfect quantification/correction of high-frequency damping and of (correlated) density fluctuations. Thus, it is important that they are accounted for in the NBP uncertainty estimation ([Leifeld et al., 2011](#)). Random-like uncertainty that strongly depend on the number of distributed samples and the heterogeneity of the investigated field dominate the uncertainty of the soil inventory approach.

Estimates of NBP in cropland remain uncertain and vary strongly in the literature ([Bondeau et al., 2007](#)). [Bondeau et al. \(2007\)](#) indicated that the larger uncertainties for NBP than for net ecosystem productivity ( $\text{NEP} = \text{NPP} - \text{Rh}$ ), which were mostly related to uncertainties in C removal by harvest and in C inputs or organic fertilization. The highest uncertainties are associated with the estimates of NBP. This is presumably due to the fact that many of the components that contribute to the cropland C balance are site-specific, reflecting the impact of geographic factors, such as soil type, climate, or the types of crops/cropping practice on the total C budget. This is important as differences among sites in the contribution of the different components to the overall budget result in a high level of variation in NBP at regional scale ([Osborne et al., 2010](#)). Our uncertainty ranges calculated for annual NBP are larger than those published in other grassland studies ([Rogiers et al., 2008](#)) and cropland studies ([Ciais et al., 2010](#)). Yet, many authors even presented and interpreted their C budget

results without indicating any uncertainty ([Lloyd, 2006](#)).

## 6.4 Conclusion

Cropland NPP and residue C input rate over the study period showed significant interannual variability, depending on the changes in crop production and weather variability. Variation in plant C input can be predicted by climate conditions. For the whole region, overall NBP for all land use was slightly increased 1959 to 2011. Though upland and paddy showed decreased NBP over the period of 1959–2011, in the case of increased agricultural abandonment (fallow/bush) and grassland from 1988, the regional C pools slowly start to build up. The combination of allometric relationship-based estimation of plant C inputs and Rh simulation modeling used in the present study allows us to simulate C balance in an agro-ecosystem where various crops are grown under different environmental (climate and soil) conditions across large scale.

None of the agro-ecosystem studies published used NBP and soil inventories combination. Our study provides this comparison in upland, paddy and grassland, and indicates that C loss occurs in each individual land use from 2005–2011. However, differences and large uncertainties in both methods stress the need for more direct comparisons to evaluate whether the observed difference in the outcome of the two approaches reflects a general methodological bias, and the uncertainty analysis would have important implications for regional C budgets.

## **7. General Discussion**

### **7.1 Achievements of this study**

Whilst there are a growing number of models for estimating soil GHG emission, the final choice of model is ultimately dependent on both the specific question being asked by the user and the availability of sufficiently detailed input data. For example, to develop sub-regional mitigation strategies based on C and N management would normally require high resolution of soil, climate and management data and a fully functional mechanistic or advanced empirical soil-plant simulation approach. In contrast, a regional or national emissions inventory may only require simple regression approaches with coarse resolution soil and climate data. However, the national-scale study indicates that integrating process-based models with spatial databases can form a powerful tool to assess the effectiveness of GHG mitigation strategies at large scales. Quantifying soil GHG emissions is a scientific challenge that requires capacity to extend the understanding at a microbial or soil chemical scale to a regional or global scale. Process-based theory modeling, spatial data acquisition and computing techniques in this study have provided potentials to quantify soil GHG emission across the scales in space and time.

One of the major purposes for developing process-based models is to extend our understanding gained at specific sites to regional, national or global scales. In fact, policy decisions can only be made based on their effectiveness at regional or national scales. When a process-based model is applied to a regional scale, an issue of uncertainty will arise even when the model may have been well calibrated and validated at a site scale. The uncertainty mainly results from spatial heterogeneity of the input parameters used for the upscaling. For applying this type of model to a region, the region is routinely divided into many grid cells or polygons, with an assumption that each grid cell is uniform in all its properties. This

assumption is against the fact that some of the input parameters, especially soil properties, usually vary even within small scales, such as a county or a farm. Averaging the variations of the input data may not resolve the problem because the correlation between the modeled output (e.g. GHG flux or other concerned items) and the drivers is non-linear. There are a number of measures to cope with this challenge. A relatively approach such as, the Most Sensitive Factor (MSF) method ([Li et al., 2004](#)), Monte Carlo method ([Li et al., 2004](#)) are widely used, and the method used in this study Bayesian Calibration are becoming popular. Bayesian method is clearly not the only way to address uncertainty; it stands out as an approach that can accommodate complex systems in a fully consistent framework. Compared to Bayesian calibration, the hierarchical approach would be beneficial to identify “hyper parameters”, which may explain spatial variability. The advantage of hierarchical methods come as complexity increase ([Clark, 2005](#)), therefore it would be beneficial to apply HB calibration across different soils globally to deal with parameters’ variability based on soil classification.

The magnitude of CO<sub>2</sub>, N<sub>2</sub>O and NO fluxes from arable land has been successfully simulated on a daily time-step using the CO<sub>2</sub>-HB and N-HB models. Although the small number of studied soils and seasonal patterns limits the application of the model to other fields, the results obtained are sufficient to establish a reliable methodology and provide conclusions that may be generalizable to other soils and climate. This study proposed a method to predict the influence of soil texture on the effects of parameters on CO<sub>2</sub>, N<sub>2</sub>O and NO flux, and soil texture could thus be regarded as an upscaling factor for future research on regional extrapolation. We sought to calibrate the model parameters on different sites in order to minimize the uncertainty and to find the parameter values that would be universally applicable. Although the studied soil types in this study are limited, the results of our calibration could be suitable for simulating N<sub>2</sub>O and NO fluxes in a new site where no measured data are available.

Our uncertainty ranges calculated for annual NBP (Table 6.4) are larger than those published in other grassland studies (e.g., Rogiers et al., 2008) and cropland studies (e.g., Ciais et al., 2010). Yet, many authors even presented and interpreted their C budget results without indicating any uncertainty (e.g., Lloyd, 2006; Allard et al., 2007). The NBP in all land use across the whole region showed a slowly increase. Though upland field and paddy field showed decreased NBP over the period of 1959–2012, in the case of increased agricultural abandonment (fallow/bush) and grassland from 1988, the regional C pools slowly start to build up. The combination of allometric relationship-based estimation of plant C inputs and CO<sub>2</sub>-HB modeling used in the present study allows us to simulate C balance in an agro-ecosystem where various crops are grown under different environmental (climate and soil) conditions. None of the agro-ecosystem studies published used NBP and soil inventories combination. Our study provides this comparison in upland, paddy and grassland, and indicates that C loss occurs in each individual land use from 2005–2011. However, the soil inventory showed a tendency towards higher C loss than NBP. Thus either method may be suitable for tracking absolute changes in soil C unless with indication of uncertainty analysis, but both give similar answers respect to relative changes.

## 7.2 Suitability and benefits of Hierarchical Bayesian calibration

In recent years, hierarchical method has been successfully applied in different fields (Li et al., 2015; Ganesan et al., 2014; Riccio et al., 2006; Cressie et al., 2009). Under the hierarchical model, each site is unique but shares some commonality of behavior with other sites. Hierarchical modeling is the compromise between entirely site-specific and globally common parameter estimates (Malve and Qian, 2006). If the data do not demonstrate substantial inter-site variation, then the parameters of hierarchical structure will be closely identical to the global cross-site parameter.

Hierarchical method is clearly not the only way to address uncertainty; it stands out as an approach that can accommodate complex systems in a fully consistent framework. The

hierarchical method solves for a larger number of parameters, including a small additional computational cost. [Ganesan et al. \(2014\)](#) indicated that based on traditional computational methods, as the size of the observation and/or parameter grows, the cost of computing will be approximately  $n^3$ . Our application in N-HB model involves 19 parameters, which 15 parameters were site-specific. Our data including total 15 different experimental sites and 26 different site/treatment combinations cross 9 years. In this study, the computational burden was released by HB calibration. The advantage of hierarchical methods come as complexity increase ([Clark, 2005](#)), therefore it would be beneficial to apply HB calibration across different soils globally to deal with parameters' variability based on soil classification.

### 7.3 Model application

The CO<sub>2</sub>-HB model established in Chapter 4 requires only a few inputs (soil temperature, soil water texture, soil texture), they can be easily applied on a range of scales and incorporated into other models, such as shown in the establishment of N-HB model in Chapter 5. The CO<sub>2</sub>-HB model was not designed for tracing detailed processes. Compared to the SG model constructed by [Hashimoto et al. \(2011\)](#), the CO<sub>2</sub>-HB model not only has the advantage of being simple but also reveals that soil texture should be regarded as a possible scaling factor when upscaling the model from the site to the regional scale.

The N-HB model shown in Chapter 5 is designed based on process-based theory to simulate soil N gaseous emissions from agriculture soils. The main advantages of using the N-HB model in estimating cropland N<sub>2</sub>O and NO fluxes arise as follows: (i) flexibility over the scale range. N-HB model was validated to performance well in predicting N<sub>2</sub>O and NO flux at plot scale. The N-HB model shares the same N-cycle theory with other process-based models ([Gabrielle et al., 2006a](#)), NEMIS ([Hénault et al., 2005](#)), CERES-EGC ([Gabrielle et al., 2006a](#)) and ECOSSE model ([Bell et al., 2012](#)) and therefore is easily incorporation into other models as a sub-model. The N-HB model follows the alternative approach, using only the

measurements that are available at large scale to drive the model at the range of scales. When attempting to stimulate emissions for a large scale, detailed information on plant/ soil input/ characteristics is not available. As such simulation at site level using the N-HB do not require this information, enabling the same model structure/process to be used at the large scale. This means that evaluations of the N-HB model using field scale measurements can be used directly to determine the uncertainty in simulation at larger scale. (ii) parameter variability. The N-HB model offers a critical guidance for parameterization. Generally, the parameters with less variability would be regarded as the global parameters and are extremely useful for spatial extrapolation, however, the parameters with the large variability need to be parameterized on site-specific basis. The simple linear relationship of calibrated parameters and soils provide a pre-requisite for simulation over space. Parameters of the NO module could be considered constant for model extrapolation to regional scale. The calibrated parameters derived from soil-specific calibration could be served as default values for the N<sub>2</sub>O module extrapolation for similar soil types. Otherwise, the mean value of posterior distribution of calibration parameters could be served as global-parameter for new sites or soils.

## **7.4 Shortages & perspective**

Although, both CO<sub>2</sub>-HB and N-HB models showed several parameters significantly related to soil texture, to enhance the reliability and applicability of the CO<sub>2</sub>-HB and N-HB models up-scaled to a larger scale and for similar soils, future studies should evaluate data across more soils types and seasonal patterns. It is difficult to apply the liner relation to other soils due to the limited breadth of input soil textures, however, it agrees with other models' result that the soil or landscape characteristics could control these parameters. Therefore, it will be interesting to apply HB calibration across different soils and establish a database of parameters based on soil classification.

Agriculture soils are so diverse in terms of crops grown, rotation, management, soil types, and climatic conditions that it is not possible to directly upscale results from individual cropland sites to the large scale, even with an extensive network of sites. Instead, the data are most valuable to calibrate and parameterize or validate ecosystem models, which are then combined with detailed spatial datasets, to allow a more process-based understanding at the plot scale to be up-scaled to the continent's total agriculture area. Through this combination of detailed measurement, improved understanding, and model development, we will be able to better estimate and project agricultural GHG fluxes, as well as advance our understanding of the factors controlling GHG fluxes in agriculture.

## 8. Summary

The carbon (C) balance in terrestrial ecosystems has large implications on the variation in atmospheric carbon dioxide (CO<sub>2</sub>) emission. Soils are the main source of nitrous oxide (N<sub>2</sub>O) emission and nitrogen monoxide (NO) emissions via the microbial processes of nitrification and denitrification. Modeling is an effective supplementary tool to estimate soil gas fluxes that allows the extrapolation of the results from the site scale to the large scale. Hierarchical Bayesian (HB) theory is useful tools for modeling multifaceted, nonlinear phenomena such as those encountered in ecology, and potentially used to reduce the uncertainty of estimated parameters.

The first goal of this study was to modeling CO<sub>2</sub>, N<sub>2</sub>O and NO flux at Ikushunbetsu River watershed, central Hokkaido, Japan by using HB theory. Secondly, the spatial and temporal patterns of net biome productivity (NBP) impacted by land management, climate condition and land use were estimated during the last four decades, and the C stocks change from 2005 to 2011 was compared with soil inventory method.

### 1. Modeling soil CO<sub>2</sub> flux from cropland (CO<sub>2</sub>-HB model)

The CO<sub>2</sub>-HB model was developed to simulate soil CO<sub>2</sub> flux derived from heterotrophic respiration (Rh) based on soil temperature (T), water-filled pore space (WFPS) and soil texture using HB theory. The simulation-observation fit of the CO<sub>2</sub> flux model was  $R^2 = 0.64$  ( $P < 0.001$ ). More than 90% of the observed daily data were within the 95% confidence interval. The CO<sub>2</sub>-HB model calibration revealed differing sensitivity of CO<sub>2</sub> flux to T and WFPS in different soil texture classes. The CO<sub>2</sub>-HB model provided a method for predicting how the effects of soil temperature and moisture on CO<sub>2</sub> flux change with texture, and soil texture could be regarded as an up-scaling factor for model extrapolation.

### 2. Modeling soil N<sub>2</sub>O and NO flux from cropland (N-HB model)

The N-HB model was developed based on the nitrogen transformation process theory using HB method. Simulation of N<sub>2</sub>O and NO fluxes showed appropriate correlation corresponding to observations on a daily time-step, with  $R^2$  value of 0.35 in N<sub>2</sub>O simulation and 0.51 in NO simulation. The main advantages of using N-HB model in estimating cropland N<sub>2</sub>O and NO fluxes arise as follows: (i) flexibility over the scale range. The N-HB was validated to performance well in predicting N<sub>2</sub>O and NO flux at plot scale, and it is easily incorporation into other models as a sub-model, which demonstrate its ability to adequately simulate soil N<sub>2</sub>O flux at large scale. (ii) parameter variability. The N-HB model offers a critical guidance for parameterization. Parameters of the NO module could be considered constant for model extrapolation. The calibrated parameters derived from soil-specific calibration could be served as default values for the N<sub>2</sub>O module extrapolation for similar soil types. Otherwise, the mean value of the calibration parameters could be served as global-parameter for similar soils.

### **3. NBP at regional scale during the last four decades**

The complete crop-level yields, the CO<sub>2</sub>-HB model and Geographic Information System (GIS) land use data were used to estimate the spatio-temporal changes of net primary productivity (NPP), plant C inputs, and NBP from 1959–2011. For the whole region (2193 ha), overall annual plant C inputs to the soil representing 37% of the whole region NPP. Plant C inputs in upland field (without bush/fallow) could be predicted by climate conditions. Overall NBP for all land use increased from  $-1.15 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$  in 1959 to  $0.34 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$  in 2011. Though upland and paddy showed decreased NBP over the period of 1959–2011, in the case of increased agricultural abandonment (fallow/bush) and grassland from 1988, the regional C pools slowly start to build up. The comparison of soil inventory and NBP method in upland, paddy and grassland indicates that C loss occurs in each individual land use from 2005–2011, however, the soil inventory showed a tendency towards higher C loss than NBP.

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