

---

---

# A global sensitivity analysis of DNDC model using a Bayesian based approach

Xiaobo Qin<sup>1,2,3</sup> Hong Wang<sup>3,4</sup>, Yu'e Li<sup>1,2</sup> Kelsey Brandt<sup>3</sup>

1 Institute of Environment and Sustainable Development in Agriculture, Chinese Academy of Agricultural Sciences, Beijing 100081, China (email: [chinayrh@gmail.com](mailto:chinayrh@gmail.com));

2 The key laboratory for Agro-Environment and Climate Change, Ministry of Agriculture, Beijing 100081, China;

3 Semiarid Prairie Agricultural Research Centre, Agriculture and Agri-Food Canada, POBOX 1030, Swift Current, Saskatchewan, Canada S9H 3X2;

4 Corresponding author: [hong.wang@agr.gc.ca](mailto:hong.wang@agr.gc.ca)

---

---

**Abstract:** This study was aimed at demonstrate the application of the Bayesian based global sensitivity analysis (GSA) approach to Denitrification and decomposition (DNDC) model using the tool of Gaussian emulation machine for sensitivity analysis (GEM-SA), in order to provide information on the relative effect of parameters on major model outputs. To execute the GSA study, twenty-eight input parameters were selected and eighty-six years' DNDC simulation was run on basis of Three Hill's spring wheat system. Three interested multi-year's model outputs were chosen, whose sensitivity to inputs has been tested: yield, annual change in soil organic carbon (dSOC) and N<sub>2</sub>O flux. We found the effect of input parameters on three mentioned DNDC outputs not vary only with different simulated year but also with specific output variable. Moreover, the influence of inputs on variance of outputs varies with the form of sensitivity indices, i.e. main effects (individual contribution of each input to variance of model output) or total effects (when all inputs' interactions are considered). Consequently, multi year's SA is necessary for the nonlinear DNDC model and most sensitive parameters to specific output should be focused on further validation and calibration of that variable.

**Keywords:** DNDC, Global sensitivity analysis, Bayesian, GEM-SA

**Abbreviation:** SA, sensitivity analysis; UA, uncertainty analysis; LSA, local sensitivity analysis; GSA, global sensitivity analysis; GEM-SA, Gaussian emulation machine for sensitivity analysis

## Introduction

Ecological models have been increasingly used for up scaling and long-term prediction in research of climate change. One of the model is DNDC, it's a process based biogeochemical model, which can simulate the soil carbon and nitrogen dynamic, plant growth and biogenic greenhouse gasses (GHGs) such as CO<sub>2</sub>, CH<sub>4</sub> and N<sub>2</sub>O via sub modules (Li *et al.*, 1992a, b; Li *et al.*, 2005). Many inputs are needed for DNDC running. The initial soil properties and the current and predicted meteorological data and crop control measures are used as inputs. These variables have an associated uncertainty that will propagate through the model to produce

uncertainties in the simulated model outputs (Petropoulos *et al.*, 2009; Hastings *et al.*, 2010). Consequently, understanding the propagation of uncertainty in the inputs to predictive outputs is crucial for this process to be accurate (Hastings *et al.*, 2010). For the DNDC model, the total number of input parameters is very large. All of them may cause model uncertainty. It is worthwhile to concentrate on the most important parameters, to which model outputs are the most sensitive (Ruguet *et al.*, 2002).

Sensitivity analysis (SA) of the DNDC model has become necessary due to the multiplicity and diversity of the model's uses (Yasuhito Shirato, 2005; Abdalla *et al.*, 2009; Qiu *et al.*, 2009; Zhang *et al.*, 2009). This may involve offering a set of parameters for fitting the model to a new climatic scenario, a site specific soil and vegetation (Ruguet *et al.*, 2002). Sensitivity analysis can be used to estimate the uncertainty level in the model predictions resulting from incomplete knowledge of the inputs (Giltrap *et al.*, 2010). Saltelli (Saltelli, 2002) gave a definition to SA as the study of how the uncertainty in the output of a model can be allocated to various sources of uncertainty in the model input. In practice, SA is a methodology, which is the study of the response of selected output variables to variations in parameters and/or driving variables (Lane and Ferreira, 1980). Furthermore, SA plays an important role in model verification and validation throughout the processes of model development and improvement (Kleijnen, 1995; Fraedrich and Goldberg, 2000; Kleijnen and Sargent, 2000), and then decreases model uncertainty (Kennedy *et al.*, 2006).

There are many kinds of SA approaches (Hamby, 1994, 1995; Frey and Patil, 2002). Each methodology has its advantages and disadvantages. These methods can be classified in a variety of ways. By European Commission (EC, 2010b), the choice of SA method to perform an experiment on a model relies on a number of factors: the properties of the model under study (linearity, additivity, monotonicity, etc.), the number of inputs involved in the analysis, the computational time needed to evaluate the model, and, last but not least, the objective of the analysis (Cariboni *et al.*, 2007). SA often referred to as either "local sensitivity analysis (LSA)" or "global sensitivity analysis (GSA)", the LSA addresses sensitivity relative to point estimates of parameter values while a GSA examines sensitivity with respect to the entire parameter distribution (Hamby, 1995). By an identification study of SA methods, the One-at-a-time (OAT) method, Nominal range sensitivity analysis and Automatic Differentiation Technique belongs to LSA approach (Frey and Patil, 2002). However, methods like ANOVA based technique and Mutual Information Index (MII) approach belongs to GSA, these means appear to be the most theoretically attractive methods, because they are model free and take into account the interaction between inputs (By, Kleijnen, (Kleijnen, 1995). There are some advantages of GSA approaches over LSA methods, on one hand, GSA include the whole distribution range of input parameters, the results are independent of the researcher's individual opinion and outcomes of GSA are not limited specific site (Saltelli *et al.*, 1999); on the other hand, GSA can quantitatively educe the most sensitive input parameters, but also can estimate the interactions between them (Schwieger, 2004).

To estimate the uncertainty in model outputs, OAT method was used to conduct SA study of DNDC. Li et al. (Li *et al.*, 1992a) carried out four SA tests using OAT method to see the response of sub-module and the complete model to variation of relevant parameters from baseline conditions by varying one parameters and fixing others during one cycle. This

method was also employed by recent studies (Nakagawa *et al.*, 2008; Abdalla *et al.*, 2009). Nevertheless, OAT is one of LSA methods, it is the most primitive SA tool, in the context of model validation or modification, the use of OAT methods is illicit and unjustified, unless the model under analysis is proved to be linearity (Saltelli *et al.*, 2006). The other LSA approach, i.e. most sensitive factor (MSF) method was developed to estimate uncertainty of DNDC outputs (Li *et al.*, 1996; Li *et al.*, 2001; Li *et al.*, 2002). MSF was employed by some studies (Liu *et al.*, 2006; Fumoto *et al.*, 2008). In MSF mode, DNDC was run twice for each grid cell with the min and max values of the most sensitive soil factors commonly observed in the grid cell, the simulated two fluxes formed a range, which was wide enough to include the real flux from the grid cell with a high probability (Li *et al.*, 2004). This simplified method is applied to majority regional simulations (Giltrap *et al.*, 2010). However, the MSF method belongs to LSA too, the method is model dependent and takes no account of interactions between input parameters, which is the necessary for SA studies on the nonlinear model. Whereas DNDC is not an absolutely linearity model, only 50% of driving variables have linear relations with major model outputs (Hastings *et al.*, 2010). Besides OAT and MSF, Monte Carlo (MC) simulation was investigated in many studies on SA of DNDC (Li *et al.*, 2004; Li *et al.*, 2005; Hutchinson *et al.*, 2007; Werner *et al.*, 2007; Tonitto *et al.*, 2009). In the MC mode, DNDC was run for one year, range of each input cell will be divided into 8 intervals, DNDC will randomly select an interval from each of the soil properties to form a scenario to conduct a simulation (Li *et al.*, 2004). Nevertheless, this MC method is computational expensive, i.e. it needs thousands of times original model runs (Li *et al.*, 2004), by the DNDC help document, the lowest number for MC simulation is 4000 (DNDC, 2009). Generally speaking, the OAT, MSF and MC both has its obvious disadvantage, thus, the GSA method should be used for the complicated DNDC model.

In 2001, Kennedy and O'Hagan (Kennedy and O'Hagan, 2001) developed an approach of Bayesian analysis of computer code output (BACCO). The method based on Bayes' theorem and Gaussian process. The hypothesis of the BACCO is that the output is an unknown function of input parameters, and then emulate it as a stochastic process (Kennedy and O'Hagan, 2001), a tutorial form of BACCO was explicitly provided by O'Hagan (O'Hagan, 2006). Gaussian emulation machine for sensitivity analysis (GEM-SA) is a GSA software based on BACCO approach and was developed by Centre for Terrestrial Carbon Dynamics (CTCD) (Kennedy and O'Hagan, 2006). GEM-SA is a variance based (also known as importance measures or sensitivity indices) SA tool with the desirable properties of GSA methods: model free, quantitative, ability of testing the strength and relationship of analysis in the occurrence of uncertainties (Saltelli, 2002). Some studies have employed the tool for SA in different fields (Kennedy *et al.*, 2006; Voyer *et al.*, 2008; White *et al.*, 2008; Finley *et al.*, 2009).

For this study, we chose the GEM-SA because of its advantages over the other GSA tools (MC based methods). It's a Bayesian based solution with the capability of investigate multiple sources of uncertainty influencing model performance. Results directly from the emulator include: the decompositions of output uncertainty due to uncertainty in single input or pairs of inputs as well the measure of the uncertainty of emulation (Kennedy, 2004; Petropoulos *et al.*, 2009). By O'Hagan (O'Hagan, 2006), GEM-SA has specific advantages compared to other conventional GSA methods (those reviewed in (Saltelli *et al.*, 2000)), these strong points

include: 1) the emulator is derived from a relatively small number of model runs (the highest number is 400); 2) the emulator covering a multidimensional input space; 3) once the emulator is built, is not necessary to perform any additional runs with the model, regardless of how many analyses are required to assess the simulator's behavior; 4) most particularly, the emulator embeds a self-measure of its performance in matching the original model code, thereby offering an accurate and reliable indication of the trustworthiness of its analysis.

Accordingly, the aim of this article includes: for the first time, demonstrate the multi year's SA study of DNDC using the GEM-SA; secondly, identifying the most sensitive parameters with respect to major model outputs, ranking them by their influence to model outputs; last but not least, providing an objective judgment on the sensitivity and stability of the whole model performance, offering a reference for further model validation and modification.

## **Materials and methods**

### **DNDC model and site information**

DNDC has evolved into a comprehensive ecological model that can be used in most agricultural systems (Li *et al.*, 1992a, b; Li *et al.*, 1994; Zhang *et al.*, 2002; Levy *et al.*, 2007; Pattey *et al.*, 2007; Saggar *et al.*, 2007). DNDC is a deterministic sequential model, consisting of five sub modules (Li *et al.*, 1992a; Li *et al.*, 1994; Li, 2000): thermo-hydraulic module, aerobic composition module, denitrification module, fermentation module and crop growth module. These submodels are driven by input parameters, i.e. climate drivers (daily precipitation and temperature or solar radiation), soil features (initial value of SOC, clay content, soil density, wilt point and field capacity, pH etc.), vegetation coefficients (crop, grass or trees and their physiology) together with farming practices (vegetation managements, fertilizer usage, tillage, irrigation etc.). The time step of DNDC is one day. DNDC model output is a daily update on the soil GHGs and carbon exchange (from denitrification, decomposition and fermentation module), crop production (crop growth module) and N leaching (denitrification module) (Hastings *et al.*, 2010).

However, uncertainties in the input parameters that drive DNDC propagates through them, resulting in uncertainties in the model output (Hastings *et al.*, 2010). With the increasing applications of DNDC, sensitivity analysis is necessary for simulation of specific climatic condition, soil property and crop system. The default parameters of DNDC model are based on US's soil average value (Giltrap *et al.*, 2010), so re-parameterization of the soil and climate attributes is needed to fit the local condition before using the model. For the large number of parameters of DNDC, we should focus on those whose effect on major model outputs is relatively large than the others. Consequently, we employed the GSA tool described below to rank the most sensitive parameters with respect to specific model outputs.

Input parameters of this study are based on experiment data from Three Hills, Alberta (51°42'N, 113°13'W, 907m), the site located in semiarid prairie of west Canada with a Thin Black Chernozemic clay loam soil. The site is moderately well drained with undulating slopes of about 2%, the soil has an average field capacity of 40% and a wilting point of 26% by volume (Wang *et al.*, 2007). Spring wheat is the main food crop of this region. The relationship between crop yield and environmental factors are getting more and more

concerns. Consequently, we chose the wheat yield, dSOC and N<sub>2</sub>O flux from DNDC (current version DNDC93) model outputs to see how of their variance were affected by input parameters. For the sophisticated DNDC model, many input factors may lead to model uncertainty. Among them, 28 input parameters were chosen, it include climatic, soil properties and field managements parameters (Table 1). According to the GEM-SA software introduced later, maximum number of inputs can be analyzed is 30. Most of former studies have found the annual precipitation and air temperature were the most sensitive factors affect DNDC model outputs (Li *et al.*, 1992a; Li *et al.*, 1996; Li *et al.*, 2004; Giltrap *et al.*, 2010), so we did not consider these two parameters in this study. Because of sensitive parameters to model outputs may vary with the simulated year. 11 different simulated year's results were selected to see the dynamic trend of sensitive scenarios. The years has been chosen are: 1a, 10a, 20a, 30a, 40a, 50a, 60a, 70a, 80a, 86a, and 86avg, the 86 year's average value also has been computed for comparison. 86 years' Three Hill's climate files needed for DNDC simulations were obtained from website of Environment Canada ([http://climate.weatheroffice.gc.ca/Welcome\\_e.html](http://climate.weatheroffice.gc.ca/Welcome_e.html)).

## **GEM-SA**

By European Commission (EC, 2000), a good sensitivity analysis should conduct analyses over the full range of plausible values of key parameters and their interactions, to assess how impacts change in response to changes in key parameters. GEM-SA is a BACCO based GSA approach, just has the characters of ideal SA mentioned above. For the theoretical foundation and the software behavior, O'Hagan (O'Hagan, 2006) made a comprehensive introduction to the BACCO method in a form of tutorial. Petropoulos *et al.* (Petropoulos *et al.*, 2009) also offered an exceptional detailed description of theoretical basis of the approach. The variance based GSA has the essential feature of an ideal SA (Saltelli, 2002; EC, 2010a): 1) Deal with the influence of scale and form, the BACCO incorporates the effect of the range of input variation with the figure of its probability density function (PDF, uniform or normal); 2) Embrace multidimensional averaging, BACCO evaluate the effect of an input while with all others are varying; 3) Model free, BACCO is a model independent SA approach, it works in spite of the additivity or linearity of the original model, it has the ability to introduce the interaction effect; 4) Cope grouped factors supposing they are single factors, the synthetic property of BACCO is crucial for the nimbleness of the explanation of the SA results.

Actually, three crucial stages are involved in the GEM-SA performance: 1) building an emulator of original model from a set of training points (inputs design and outputs of original model); 2) using the training data to measure the emulator's performance in fitting the original model; 3) calculate the SA of interest using the emulator. Using of GEM-SA is just the process of emulator building (Kennedy, 2004). The software provides some powerful tools to ensure the emulator work with high quality (Kennedy, 2004): 1) For training data sampling, two methods, i.e. the Maximin Latin Hypercube and LP-TAU design are embedded in the software, we chose the latter, the built-in method is an excellent random sampling method with high efficiency and powerful when dealing with stochastic process (Holvoet *et al.*, 2005), we can edit the input design flexibly in the GEM interface after sampling; 2) input uncertainty distributions option (normal or uniform), We chose the default option that all the input is represented by a uniform distribution. Besides, 3) the cross-validation was built-in the

software to check the fitting accuracy of emulator, we use the “leave final 20% out” option, then the emulator mean and variance of the final 20% of data output points is computed as if they had been left out of the training data, the result is a more conservative estimate of the emulator accuracy (Kennedy, 2004).

## **Framework of this study**

Based on what has been discussed above, a framework of this study was designed as described in Figure one (Figure 1), the whole work consists of 4 tiers tasks:

- Tier 1: Input design. 28 input parameters were selected; each one of them was given a theoretical range (minimum and maximum) based on Three Hill’s experiments and some literatures. 400 training points within the given range for each parameter (400 model simulations is the maximum possible sampling size that can be currently built using the GEM SA tool) were sampled by LP-TAU design, the training data is a  $28 \times 400$  matrix, it defined the distribution of input parameters, each column in the data has 400 training points for each parameter, and each row has 28 values for one DNDC model run.
- Tier 2: DNDC model simulation. Each row from the input design (training data) must be used to generate outputs by running DNDC model. We employed Perl program statements to make 400 DND files using the above training data for DNDC 400 batch runs (each run last for 86 years with the Three Hill’s climatic files). And then the interested model outputs were extracted: wheat yield, dSOC and  $N_2O$  flux. 11 different year’s results were summarized to see the dynamic trend of sensitive scenarios.
- Tier 3: Run GEM-SA. GEM-SA software needs an inputs file and an outputs file. The inputs file is the mentioned training points, and the outputs file is the extracted file above. The outputs file contains 3 column outputs from 400 runs (each column stand for yield, dSOC and  $N_2O$  flux from given year respectively). One cycle of GEM-SA run can only analyze one column of the outputs.
- Tier 4: Analyzing and summary the results. It’s worth noting that, the GEM-SA output the emulator performance data, we should make a judgment to see how the emulator has been fitted, if it performed not too good, re-sampling maybe required; if it well performed, the left is analyzing and summary work.

## **Results and discussion**

### **Analyze of emulator performance**

GEM-SA Gaussian emulator has a built-in self check mechanism, after running the software, three items were computed to test the linearity between model output and input and check the accuracy of emulator fit.

Each input parameter has its own roughness value, it’s a unitless value, specifying what kind of relationship exist between model output and input (linearity or nonlinear) (Kennedy, 2004). For each DNDC output, such as wheat yield, roughness value of 28 input parameters was calculated, also with the multi-year’s results (Figure 2). We can see the roughness value vary

with different model output and also with different simulated period of time. But most of the values are lower than 1, only few of the value in specific years is exception. It indicated that the model output can be approximately a linearity function of the inputs.

Besides the roughness value, sigma-squared value is one of the measurements for checking the emulator accuracy. It expresses the variance of the emulator after standardizing the output (Petroopoulos *et al.*, 2009), its an efficient tool to measure the linearity of the emulator (Kennedy, 2004). From Table 2, we found the sigma-squared values are low for all of the SA experiments, its ranging from 0.60 to 1.73, meaning that these parameters exhibit only moderate deviations from linearity.

Cross validation was calculated to check the accuracy of the emulator fit. Each given year's "cross validation root mean square error" (CVRMSE) and "cross validation root mean square standardized error" (CVRMSSE) was computed (Table 3 and Table 4). The CVRMSE is the simple value of square root of the mean square error of the emulator predictions at the training points, whereas the CVRMSSE expresses the residual divided by an estimate of its standard deviation. All the CVRMSSE values are close to 1, with values between 0.95~1.06, this indicates reasonable emulator accuracy. These results are accordance with former study (Kennedy *et al.*, 2006).

### **DNDC model sensitivity analysis**

Multi year's summary of the main effects (SME) of 28 inputs and their interactions (INTER, include first order interactions and higher order interactions) with respect to selected DNDC model outputs were computed (Table 5). It can easily be seen, maximum of SME occurs in the first simulated year (1a, highlighted in bold) for 3 outputs, the other year's SME relatively low. But opposite situation appears in INTER, the INTER is lower in first simulated year than the other selected year. This indicates the high joint effects exist between some of the model inputs (pair of parameters and/or ternary of parameters, etc). It can be derived that sensitivity of DNDC outputs to inputs not depend only on different analyzed year but also outputs variable; more over, the average of all simulated year's data (86avg) can not present the real sensitivity situation; in addition, only one year's simulation is not nearly enough to conduct SA as previous studies did (Li *et al.*, 1992a; Li *et al.*, 2004).

By average of 28 input parameters' main effects (AME, individual contribution of each input to variance of model output) and total effects (ATE, main effects and joint effects), we selected five most sensitive parameters (MSP) with respect to each DNDC outputs.

According to AME, wheat yield and dSOC is most sensitive to WILP (soil wilting point), AME of WILP to the two outputs is great than 10%, but for N<sub>2</sub>O flux, MSP is PORO (soil porosity) (Table 6). Its easy to understand, annual precipitation determine soil water regime because there is no manual irrigation, model outputs uncertainty (CV) is larger in low yield year (1a, 10a, 30a and 80a) than high yield year (20a, 40a, 50a, 70a and 86a) (Figure 4). We calculated the correlation coefficient of DNDC outputs and annual precipitation (Table 8), there is a strong relationship between yield and annual precipitation as well as dSOC and annual precipitation ( $p < 0.01$ ,  $p < 0.05$  respectively), this suggests that yield and dSOC is strongly controlled by water regime. But for N<sub>2</sub>O flux, a weak negative correlation with annual precipitation was founded ( $p > 0.05$ ), it is because the conclusion: if anaerobic

conditions last too longer, the denitrification process tend to generate more N<sub>2</sub> rather than N<sub>2</sub>O (Li *et al.*, 1992a), moreover, the high precipitation may block the emission of N<sub>2</sub>O from soil by affecting the soil porosity. There are 4 parameters correlated with soil water regime (PORO, HYDC, WILP and FC) in the given 5 MSP, the other study also found that the water filled porosity at field capacity had the largest effects on the amount of N<sub>2</sub>O emissions (Nakagawa *et al.*, 2008).

However, based on ATE, wheat yield, dSOC and N<sub>2</sub>O flux is most sensitive to SOC at surface (5cm), SOC and soil pH respectively, where as WILP and SOC became the second most sensitive parameters for 3 outputs (Table 7). SOC content may impacts all of the biochemical processes around the plant-soil sphere. In fact, the reflection of effect of soil water regime on crop growth is the variation of SOC pool. Consequently, if we consider all of the factors which affect the yield and dSOC, the SOC at soil surface become the most important one. It's well known that N<sub>2</sub>O can come from nitrification and dinitrification process; the two procedures always occur simultaneously in the pedosphere. So the generation and emission of N<sub>2</sub>O at soil-atmosphere interface is really complex and can be influenced by many factors. For N<sub>2</sub>O flux, the soil pH become to the MSP instead of PORO, it's unexpected that the latter did not occur in the 5 MSP selected. Soil pH is the representation of biochemical and biophysical processes in rhizosphere, if we take interactions into account, soil pH value can reflect comprehensively the total effects of other factors. In fact, DNDC was designed to stop denitrification process if soil pH less than 5 (Giltrap *et al.*, 2010). Besides, SOC is the second MSP for N<sub>2</sub>O flux due to its ability of providing substrates for N<sub>2</sub>O production processes.

Actually, it's always sophisticated in the processes relevant to yield, dSOC and N<sub>2</sub>O flux, so the total effects of SA results has more persuasive. Among all the selected parameters, the soil attributes exhibit tremendous effects on production of vegetation, soil carbon dynamic and biogenic gasses. SOC content at soil surface is the most sensitive parameter for 3 DNDC outputs. This result is accordance with some studies (Li *et al.*, 1992a; Plant, 1998; Butterbach-Bahl *et al.*, 2004; Li *et al.*, 2004). Similarly, Abdalla *et al.* (Abdalla *et al.*, 2009) considered that DNDC overestimates the effect of SOC on nitrification and denitrification process in Irish agricultural soil, and then concluded that DNDC is unsuitable for predicting N<sub>2</sub>O emission from Irish grassland. There are no agricultural practices factors (crop management parameters, see table 1) included in the 5 most sensitive parameters (Table 6 and Table 7). Li *et al.* (Li *et al.*, 1996) considered that most of the agricultural practices simulated showed little effect on N<sub>2</sub>O emission after a series SA studies on DNDC, in another study, fertilizer type was found have very significant effect on N<sub>2</sub>O emission but depends on baseline soil conditions (Brown *et al.*, 2002). In practice, many management practices have a significant impact on greenhouse gas emissions, although the degree of impact can often depend on the soil and climate properties (Giltrap *et al.*, 2010). As a matter of fact, effect of whether climate or management factors must be reflected by soil properties. From table 6 and table 7, we also can see the effects values of 5 MSP for N<sub>2</sub>O flux is less than the values for yield and dSOC, it indicates that the effects of parameters on N<sub>2</sub>O flux is more uniform than yield and dSOC, it can be explained that the mechanic of production and emission of N<sub>2</sub>O flux is more complicated than the other two outputs.

## Conclusions

Most of the previous SA studies of DNDC are belong to local sensitivity analysis. LSA has some limits due to its unable to calculate interactions between parameters. It's the first time to employ a GSA tool to DNDC model by means of GEM-SA. The BACCO based method can conduct the Bayesian based GSA on computational model with high efficiency and accuracy. BACCO also has been used to other models (Voyer *et al.*, 2008; White *et al.*, 2008).

Effect of input parameters on variance of DNDC model outputs depends on several factors. Above all, it due to different analyzed time period. In general, the effect is larger in first simulated year than other period, and the effect of one parameter on one model output vary in different period. Most of previous SA study on DNDC is based on one year's simulation, now by our results, it's not nearly enough, multi year's analysis is necessary. Furthermore, the sensitivity of DNDC outputs to input parameters varied with output variables. For wheat yield, dSOC and N<sub>2</sub>O flux, all the 5 most sensitive parameters located in soil property category, but with significant different among them. Consequently, the most influential parameter for output variable should be focused for the latter's calibration. Last but not least, the influence of input parameters on DNDC outputs was affected by form of sensitivity indices, i.e. main effects and total effects. The former is the individual contribution of one parameter to output, whereby the latter consider the interactions between parameters. Actually, some parameter's total effects is far greater than main effects, it means that the effect of the parameter on output must influence by the other factors. Therefore, GSA method should be used to complex nonlinear model, instead of the simplified LSA approach.

The Gaussian emulation machine worked well with exact emulator fit. But the GEM-SA tool is just a type of static SA method, we need manually run the software a year by a year for that year's model outputs, so, the static SA method is computational expensive. Actually, we always need run DNDC in many years, especially for the long-term prediction. Therefore, a dynamic sensitivity analysis approach is required for further study, not only for the time saving analysis, but also for the dynamic sensitivity scenarios.

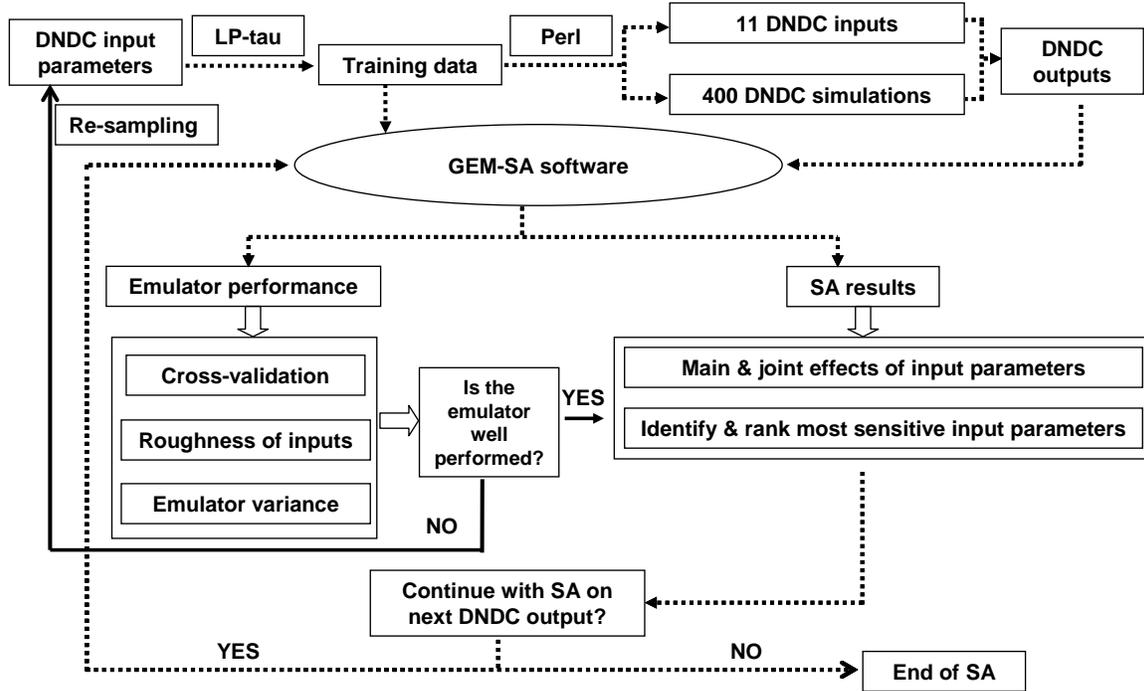
### **Acknowledgement**

The authors want to thank Xuelin Yu from University of Regina for his hard work on data processing.

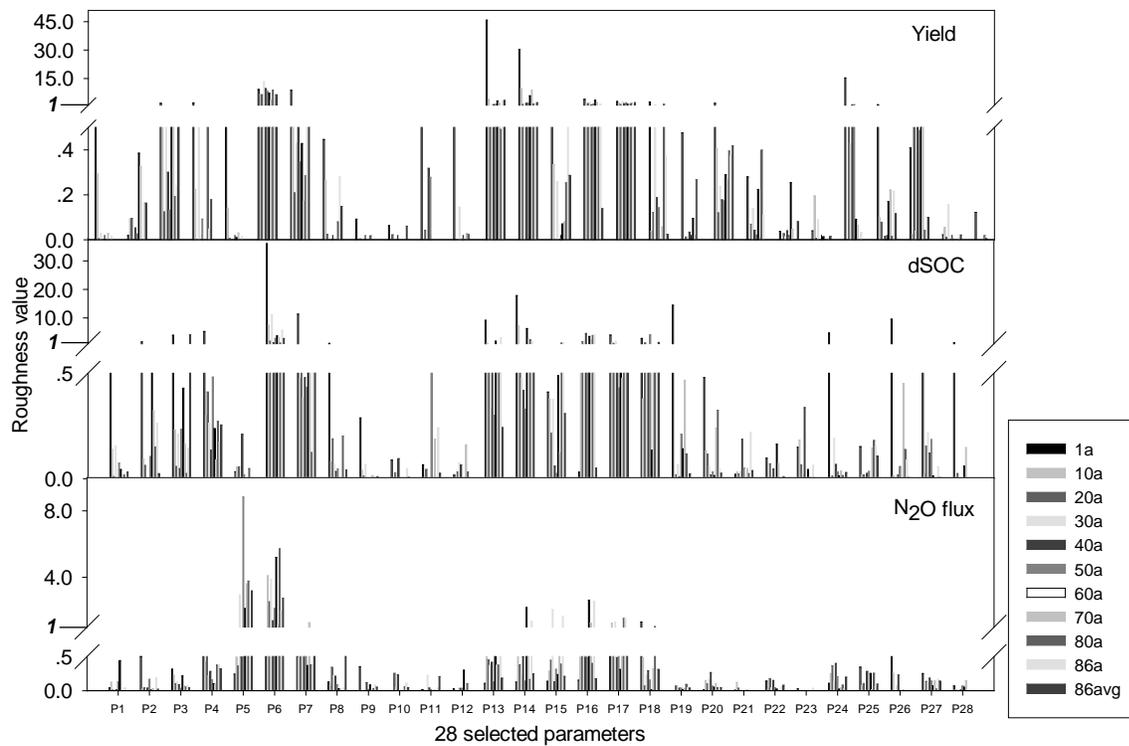
**Table 1** Selected 28 input parameters of DNDC model

Selected parameters			Actual name of the model input	Default value DNDC	Three hills value	Min value	Max value
Climate	NRAIN	P1	Atmosphere N deposition (concentration in rainfall) (ppm)	N/A	1.75	1.3	1.9
	NATM	P2	Atmosphere background NH <sub>3</sub> concentration (µgN/m <sup>3</sup> )	0.06	0.06	0.01	0.1
	CO2	P3	Atmosphere CO <sub>2</sub> concentration (ppm)	350	350	320	450
Soil properties (for clay loam soil)	DEN	P4	Soil bulk density(g/cm <sup>3</sup> )	N/A	1.2	1.1	1.9
	PH	P5	Soil pH	N/A	5.7	4.5	6.5
	SOC	P6	SOC (Soil organic carbon) at surface (0-5cm) (kgC/kg)	N/A	0.035	0.015	0.075
	CLAY	P7	Soil clay content	0.41	0.41	0.25	0.65
	LITSOC	P8	Litter SOC	1	0.01	0.005	0.02
	NO3	P9	Soil NO <sub>3</sub> <sup>-</sup> -N density (mgN/kg)	N/A	10.5	8.5	15.5
	NH4	P10	Soil NH <sub>4</sub> <sup>+</sup> -N density (mgN/kg)	N/A	1.05	0.85	1.5
	MOI	P11	Soil moisture	N/A	0.42	0.27	0.65
	TEM	P12	Soil temperature(°C)	N/A	-2.34	-10.5	10.5
	FC	P13	Field capacity (WFPS)	0.57	0.57	0.25	0.75
	WILP	P14	Wilting point	0.27	0.27	0.15	0.65
	HYDC	P15	Hydro-conductivity (m/hr)	0.00882	0.008	0.01	0.025

	PORO	P16	Soil porosity	0.476	0.476	0-1	0.476
	SOCPA	P17	Depth of soil profile with uniform SOC content (m)	0.05	0.05	0.1	0.5
	SOCPB	P18	SOC decrease rate below top soil (0.5-5)	4	4	0.5	5
	GRESA	P19	Ground residue (ratio)	N/A	1	0	1
	MYD	P20	Yield(kgC/ha)	1200	3000	1000	2000
	CNG	P21	Grain C/N ratio	25	25	20	35
	CNS	P22	Shoot C/N ratio	50	50	45	55
Crop managements	CNR	P23	Root C/N ratio	60	60	55	65
(for spring wheat)	WTREQ	P24	Water requirement demand(g water/g DM)	150	150	100	250
	NFIX	P25	Nitrogen fixation index	1.2	1.2	1	2
	DTILL	P26	Tillage depth(cm)	N/A	3	1	4
	DFERTI	P27	Fertilization depth(cm)	N/A	15	0.2	20
	UREA	P28	Urea (kgN/ha)	N/A	74	60	80



**Figure 1:** Schematic of sensitivity analysis study



**Figure 2:** Roughness value of each input parameters to selected model outputs  
 Note: P1~P28 stand for 28 input parameters (see Table 1)

**Table 2** Sigma-squared value of each input parameters to selected model outputs (the value great than 1.5 is highlighted in bold)

	1a	10a	20a	30a	40a	50a	60a	70a	80a	86a	86avg
Yield	0.7310	1.1682	<b>1.7288</b>	1.1199	1.2886	<b>1.6450</b>	1.1880	1.2482	1.1851	1.2619	<b>1.6936</b>
dSOC	0.5978	1.1611	0.8871	1.1873	1.2038	1.4883	0.9740	0.9629	0.8769	1.0525	0.7359
N <sub>2</sub> O	0.7664	1.0420	<b>1.6009</b>	1.4299	1.2384	1.2987	1.4115	0.9871	<b>1.5099</b>	1.4292	1.0500

**Table 3** Cross-validation of root mean square error

	1a	10a	20a	30a	40a	50a	60a	70a	80a	86a	86avg
Yield	99.75	176.47	111.64	205.41	130.22	117.19	117.31	150.15	176.38	161.65	115.41
dSOC	179.85	257.30	154.71	279.17	126.31	123.25	162.64	175.19	294.87	213.71	72.34
N <sub>2</sub> O	11.81	9.31	7.42	8.98	6.74	6.17	7.26	9.21	8.80	5.38	4.68

**Table4** Cross-validation of root mean squared standardized error

	1a	10a	20a	30a	40a	50a	60a	70a	80a	86a	86avg
Yield	1.0399	0.9523	0.9835	0.9840	0.9803	0.9537	0.9520	0.9693	0.9834	0.9659	0.9698
dSOC	0.9754	0.9947	1.0610	1.0021	0.9994	0.9996	0.9712	0.9892	1.0035	0.9494	1.0290
N <sub>2</sub> O	1.0175	1.0409	1.0076	1.0124	1.0379	1.0315	0.9836	0.9979	0.9785	1.0199	1.0381

**Table 5** SME and INTER of 28 input parameters to selected DNDC outputs

		1a	10a	20a	30a	40a	50a	60a	70a	80a	86a	86avg
Yield	SME	<b>79.52</b>	30.076	39.388	44.161	40.776	27.026	20.55	33.205	58.757	35.909	30.39
	INTER	20.48	69.924	60.612	55.839	59.224	72.974	79.45	66.795	41.243	64.091	69.61
dSOC	SME	<b>81.602</b>	58.056	70.56	64.278	69.651	58.477	48.472	62.264	67.68	34.151	84.214
	INTER	18.398	41.944	29.44	35.722	30.349	41.523	51.528	37.736	32.32	65.849	15.786
N <sub>2</sub> O flux	SME	<b>77.064</b>	67.954	56.491	57.766	68.044	67.446	48.972	69.808	59.26	46.54	75.11
	INTER	22.936	32.046	43.509	42.234	31.956	32.554	51.028	30.192	40.74	53.46	24.89

**Table 6** 5 MSP for selected 3 DNDC model outputs by main effects (%)

Yield		dSOC		N <sub>2</sub> O flux	
Parameter	AME	Parameter	AME	Parameter	AME
WILP	11.32	WILP	10.65	PORO	6.00
FC	8.71	PORO	9.03	HYDC	2.99
PORO	7.98	FC	4.04	SOCPA	2.83
WTREQ	1.09	SOCPA	1.87	WILP	2.55
HYDC	1.64	SOCPB	1.79	FC	1.50

Note: parameters name are described in Table 1

**Table 7** Five MSP for selected three DNDC model outputs by total effects (%)

Yield		Dsoc		N <sub>2</sub> O flux	
Parameter	ATE	Parameter	ATE	Parameter	ATE
SOC	43.86	SOC	40.01	PH	29.72
WILP	38.52	WILP	29.99	SOC	25.00
FC	31.33	PORO	29.03	CLAY	25.14
PORO	27.09	FC	17.95	HYDC	21.60
SOCPA	23.38	HYDC	15.59	WILP	19.76

Note: parameters name are described in Table 1

**Table 8** Relationship between multi-year's DNDC outputs and annual precipitation

	Coefficient of correlation	Significant level
Yield & precipitation	0.8175	$p < 0.01$
dSOC & precipitation	0.6909	$p < 0.05$
N <sub>2</sub> O flux & precipitation	-0.4563	$P > 0.05$

## References

- Abdalla, M., Wattenbach, M., Smith, P., Ambus, P., Jones, M., Williams, M., 2009. Application of the DNDC model to predict emissions of N<sub>2</sub>O from Irish agriculture. *Geoderma* 151, 327-337.
- Brown, L., Syed, B., Jarvis, S.C., Sneath, R.W., Phillips, V.R., Goulding, K.W.T., Li, C., 2002. Development and application of a mechanistic model to estimate emission of nitrous oxide from UK agriculture. *Atmospheric Environment* 36, 917-928.
- Butterbach-Bahl, K., Kesik, M., Miehle, P., Papen, H., Li, C., 2004. Quantifying the regional source strength of N-trace gases across agricultural and forest ecosystems with process based models. *Plant and Soil* 260, 311-329.
- Cariboni, J., Gatelli, D., Liska, R., Saltelli, A., 2007. The role of sensitivity analysis in ecological modelling. *Ecological Modelling* 203, 167-182.
- DNDC, 2009. User's Guide for the DNDC Model (Version 9.3).  
<http://www.dndc.sr.unh.edu/Models.html>.
- EC, 2000. European Commission's Communication on Extended Impact Assessment Brussels, 05/06/2002 COM (2002) 276 final. . Guidelines for implementing the directive are available at the Governance page of the EC, [http://europa.eu.int/comm/governance/docs/index\\_en.htm](http://europa.eu.int/comm/governance/docs/index_en.htm)
- EC, 2010a. Sensitivity analysis methods. European commission, Joint Research Centre, <http://sensitivity-analysis.jrc.ec.europa.eu/methods/>.
- EC, 2010b. What's Sensitivity analysis. European commission, Joint Research Centre, [http://sensitivity-analysis.jrc.it/docs/what\\_is\\_SA.htm](http://sensitivity-analysis.jrc.it/docs/what_is_SA.htm).
- Finley, S., Sidwell, V., Marzocca, P., Willmert, K., 2009. Application of Variance Based Sensitivity Analysis to Blade Outer Air Seals. *Advanced Modeling and Optimization II*, 115-138.
- Fraedrich, D., Goldberg, A., 2000. A methodological framework for the validation of predictive simulations. *European Journal of Operational Research* 124, 55-62.
- Frey, H.C., Patil, S.R., 2002. Identification and Review of Sensitivity Analysis Methods. *Risk Analysis* 22, 553-578.
- Fumoto, T., Kobayashi, K., Li, C., Yagi, K., Hasegawa, T., 2008. Revising a process-based biogeochemistry model (DNDC) to simulate methane emission from rice paddy fields under various residue management and fertilizer regimes. *Global Change Biology* 14, 382-402.
- Giltrap, D.L., Li, C., Saggar, S., 2010. DNDC: A process-based model of greenhouse gas fluxes from agricultural soils. *Agriculture, Ecosystems & Environment* 136, 292-300.

Hamby, D.M., 1994. A review of techniques for parameter sensitivity analysis of environmental models. *Environmental Monitoring and Assessment* 32, 135-154.

Hamby, D.M., 1995. A Comparison of Sensitivity Analysis Techniques. *Health Physics* 68, 195-204.

Hastings, A.F., Wattenbach, M., Eugster, W., Li, C., Buchmann, N., Smith, P., 2010. Uncertainty propagation in soil greenhouse gas emission models: An experiment using the DNDC model and at the Oensingen cropland site. *Agriculture, Ecosystems & Environment* 136, 97-110.

Holvoet, K., van Griensven, A., Seuntjens, P., Vanrolleghem, P.A., 2005. Sensitivity analysis for hydrology and pesticide supply towards the river in SWAT. *Physics and Chemistry of the Earth, Parts A/B/C* 30, 518-526.

Hutchinson, J.J., Grant, B.B., Smith, W.N., Desjardins, R.L., Campbell, C.A., Worth, D.E., Vergé, X.P., 2007. Estimates of direct nitrous oxide emissions from Canadian agroecosystems and their uncertainties. *Canadian Journal of Soil Science* 87, 141-152.

Kennedy, M.C., 2004. Description of the Gaussian process model used in GEM-SA. GEM-SA help documentation.

Kennedy, M.C., Anderson, C.W., Conti, S., O'Hagan, A., 2006. Case Studies in Gaussian Process Modelling of Computer Codes. *Reliability Engineering & System Safety* 91, 1301-1309.

Kennedy, M.C., O'Hagan, A., 2001. Bayesian calibration of computer models. *J. R. Stat. Soc. Ser. B. Stat. Methodol* 63, 425-464.

Kennedy, M.C., O'Hagan, T., 2006. <http://www.tonyohagan.co.uk/academic/GEM/>.

Kleijnen, J.P.C., 1995. Sensitivity analysis and optimization of system dynamics models: Regression analysis and statistical design of experiments. *System Dynamics Review* 11, 275-288.

Kleijnen, J.P.C., Sargent, R.G., 2000. A methodology for fitting and validating metamodels in simulation. *European Journal of Operational Research* 120, 14-29.

Lane, L., Ferreira, V., 1980. Sensitivity analysis. In *CREAMS: Chemicals, Runoff and Erosion from Agricultural Management Systems*, Knisel WG (ed.). USDA-ARS Conservation Research Report No. 26: US.

Levy, P.E., Mobbs, D.C., Jones, S.K., Milne, R., Campbell, C., Sutton, M.A., 2007. Simulation of fluxes of greenhouse gases from European grasslands using the DNDC model. *Agriculture Ecosystems & Environment* 121, 186-192.

Li, C., Qiu, J., Frohking, S., Xiao, X., Salas, W., Moore, B., III, Boles, S., Huang, Y., Sass, R., 2002. Reduced methane emissions from large-scale changes in water management of China's rice paddies during 1980-2000. *Geophys. Res. Lett.* 29, 1972.

- Li, C.S., 2000. Modeling trace gas emissions from agricultural ecosystems. *Nutrient Cycling in Agroecosystems* 58, 259-276.
- Li, C.S., Frolking, S., Frolking, T.A., 1992a. A MODEL OF NITROUS-OXIDE EVOLUTION FROM SOIL DRIVEN BY RAINFALL EVENTS .1. MODEL STRUCTURE AND SENSITIVITY. *Journal of Geophysical Research-Atmospheres* 97, 9759-9776.
- Li, C.S., Frolking, S., Frolking, T.A., 1992b. A MODEL OF NITROUS-OXIDE EVOLUTION FROM SOIL DRIVEN BY RAINFALL EVENTS .2. MODEL APPLICATIONS. *Journal of Geophysical Research-Atmospheres* 97, 9777-9783.
- Li, C.S., Frolking, S., Harriss, R., 1994. MODELING CARBON BIOGEOCHEMISTRY IN AGRICULTURAL SOILS. *Global Biogeochemical Cycles* 8, 237-254.
- Li, C.S., Frolking, S., Xiao, X.M., Moore, B., Boles, S., Qiu, J.J., Huang, Y., Salas, W., Sass, R., 2005. Modeling impacts of farming management alternatives on CO<sub>2</sub>, CH<sub>4</sub>, and N<sub>2</sub>O emissions: A case study for water management of rice agriculture of China. *Global Biogeochemical Cycles* 19.
- Li, C.S., Mosier, A., Wassmann, R., Cai, Z.C., Zheng, X.H., Huang, Y., Tsuruta, H., Boonjawat, J., Lantin, R., 2004. Modeling greenhouse gas emissions from rice-based production systems: Sensitivity and upscaling - art. no. GB1043. *Global Biogeochemical Cycles* 18, B1043-B1043.
- Li, C.S., Narayanan, V., Harriss, R.C., 1996. Model estimates of nitrous oxide emissions from agricultural lands in the United States. *Global Biogeochemical Cycles* 10, 297-306.
- Li, C.S., Zhuang, Y.H., Cao, M.Q., Crill, P., Dai, Z.H., Frolking, S., Moore B, III, Salas, W., Song, W.Z., Wang, X.K., 2001. Comparing a process-based agro-ecosystem model to the IPCC methodology for developing a national inventory of N<sub>2</sub>O emissions from arable lands in China. *Nutrient Cycling in Agroecosystems* 60, 159-175.
- Liu, Y., Yu, Z., Chen, J., Zhang, F., Doluschitz, R., Axmacher, J.C., 2006. Changes of soil organic carbon in an intensively cultivated agricultural region: A denitrification-decomposition (DNDC) modelling approach. *Science of The Total Environment* 372, 203-214.
- Nakagawa, Y., Chin, Y., Shiono, T., Miyamoto, T., Kameyama, K., Shinogi, Y., 2008. Evaluating the Validity and Sensitivity of the DNDC Model for Shimajiri Dark Red Soil. *Jarq-Japan Agricultural Research Quarterly* 42, 163-172.
- O'Hagan, A., 2006. Bayesian analysis of computer code outputs: A tutorial. *Reliability Engineering & System Safety*. The Fourth International Conference on Sensitivity Analysis of Model Output (SAMO 2004) - SAMO 2004 91, 1290-1300.

Pattey, E., Edwards, G.C., Desjardins, R.L., Pennock, D.J., Smith, W., Grant, B., MacPherson, J.I., 2007. Tools for quantifying N<sub>2</sub>O emissions from agroecosystems. *Agricultural and Forest Meteorology* 142, 103-119.

Petropoulos, G., Wooster, M.J., Carlson, T.N., Kennedy, M.C., Scholze, M., 2009. A global Bayesian sensitivity analysis of the 1d SimSphere soil-vegetation-atmospheric transfer (SVAT) model using Gaussian model emulation. *Ecological Modelling* 220, 2427-2440.

Plant, R., 1998. GIS-Based Extrapolation of land Use-Related Nitrous Oxide Flux in the Atlantic Zone of Costa Rica. *Water, Air, & Soil Pollution* 105, 131-141.

Qiu, J.J., Li, C.S., Wang, L.G., Tang, H.J., Li, H., Van Ranst, E., 2009. Modeling impacts of carbon sequestration on net greenhouse gas emissions from agricultural soils in China. *Global Biogeochemical Cycles* 23.

Ruget, F., Brisson, N., Del Moral, R., Faivre, R., 2002. Sensitivity analysis of a crop simulation model, STICS, in order to choose the main parameters to be estimated. *Agronomie* 22, 133-158.

Saggar, S., Giltrap, D.L., Li, C., Tate, K.R., 2007. Modelling nitrous oxide emissions from grazed grasslands in New Zealand. *Agriculture Ecosystems & Environment* 119, 205-216.

Saltelli, A., 2002. Sensitivity analysis for importance assessment. *Risk Analysis* 22, 579-590.

Saltelli, A., Ratto, M., Tarantola, S., Campolongo, F., 2006. Sensitivity analysis practices: Strategies for model-based inference. *Reliability Engineering & System Safety* 91, 1109-1125.

Saltelli, A., Tarantola, S., Campolongo, F., 2000. Sensitivity Analysis as an Ingredient of Modeling. *Statistical Science* 15, 377-395.

Saltelli, A., Tarantola, S., Chan, K.P.-S., 1999. A quantitative model-independent method for global sensitivity analysis of model output. *Technometrics* 41, 39-56.

Schwieger, V., 2004. Variance-based sensitivity analysis for model evaluation in Engineering Surveys. INGENIO 2004 and FIG Regional central and Eastern European Conference on Engineering Surveying, Bratislava, Slovakia, 1-10.

Tonitto, C., David, M., Drinkwater, L., 2009. Modeling N<sub>2</sub>O flux from an Illinois agroecosystem using Monte Carlo sampling of field observations. *Biogeochemistry* 93, 31-48.

Voyer, D., Musy, F.o., Nicolas, L., Perrussel, R., 2008. Impact of uncertainties in 2D hyperthermia using stochastic spectral and collocation methods.

Wang, H., Lemke, R., Goddard, T., Sprout, C., 2007. Tillage and root heat stress in wheat in central Alberta Canadian *Journal of Soil Science* 87, 3-10.

Werner, C., Butterbach-Bahl, K., Haas, E., Hickler, T., Kiese, R., 2007. A global inventory of N<sub>2</sub>O emissions from tropical rainforest soils using a detailed biogeochemical model. *Global Biogeochem. Cycles* 21, GB3010.

White, T., Luckai, N., Larocque, G.R., Kurz, W.A., Smyth, C., 2008. A practical approach for assessing the sensitivity of the Carbon Budget Model of the Canadian Forest Sector (CBM-CFS3). *Ecological Modelling* 219, 373-382.

Yasuhito Shirato, 2005. Testing the Suitability of the DNDC Model for Simulating Long-Term Soil Organic Carbon Dynamics in Japanese Paddy Soils. *Soil Science and Plant Nutrition* 51, 183-192.

Zhang, L.M., Yu, D.S., Shi, X.Z., Weindorf, D.C., Zhao, L.M., Ding, W.X., Wang, H.J., Pan, J.J., Li, C.S., 2009. Simulation of global warming potential (GWP) from rice fields in the Tai-Lake region, China by coupling 1:50,000 soil database with DNDC model. *Atmospheric Environment* 43, 2737-2746.

Zhang, Y., Li, C.S., Zhou, X.J., Moore, B., 2002. A simulation model linking crop growth and soil biogeochemistry for sustainable agriculture. *Ecological Modelling* 151, 75-108.