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A long-term sensitivity analysis of the denitrification and decomposition model

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ABSTRACT

Although sensitivity analysis (SA) was conducted on the DeNitrification–DeComposition (DNDC) model, a global SA over a long period of time is lacking. We used a method of Bayesian analysis of computer code outputs (BACCO) with the Gaussian emulation machine for sensitivity analysis software (GEM-SA) to conduct a long-term SA of DNDC for predicting the annual change of soil organic carbon (dSOC), nitrous oxide emission (N_2O) and grain yield of spring wheat. Twenty seven non-weather input parameters with wide ranges were selected for SA using weather data recorded from Three Hills, Alberta over 86 years (1921–2006). The SA had two steps: 1) a preliminary BACCO GEM-SA was conducted to identify a more accurate emulator sampling method and to screen out parameters with insignificant influence on model outcomes; and 2) final BACCO GEM-SA was conducted with optimal input design set for emulator training runs varying only the significant input parameters. Results indicated that the Maximin Latin Hypercube sampling method outperformed the LP-τ method with higher emulator accuracy. Most of the 27 input parameters contributed little to the three outputs by the first step BACCO GEM-SA. In the second step of BACCO GEM-SA there were only three (in the case of dSOC) and six (in the cases of N_2O and yield) input parameters whose influence contributed to more than 10% of the total output variances by their total effects. Among the selected parameters, initial soil organic carbon and clay content are very important and were important in determining results for all three outputs. Sensitivities of some parameters, such as clay content and urea fertilizer amount changed dramatically over the years. This indicates that a single year SA may overestimate or underestimate a long-term parameter effect on the model prediction. The two-step procedure with the BACCO GEM-SA method improved the accuracy of SA and provided important information for model validation and parameterization.

1. Introduction

Developing ecosystem models is essential for the assessment of agricultural best management practices to address climate change and climate variability. DeNitrification and DeComposition (DNDC) is a process-oriented simulation model that was initially developed for predicting carbon sequestration and trace gas emissions from agricultural soils in the United States (Li et al., 1992a, 1994; Palosuo et al., 2012). In recent years, it has been tested by many researchers worldwide with promising results for simulating the impacts of carbon sequestration on net greenhouse gas emissions (Grant and Pattey, 2003; Kiese et al., 2005; Pathak et al., 2005; Plant, 1998), crop growth and yield (Britz and Leip, 2009; Qin, 2005; Tonitto et al., 2007b), residue decomposition (Li et al., 1992a, 1997,

Abbreviations: DNDC, denitrification and decomposition; SA, sensitivity analysis; GSA, global sensitivity analysis; BACCO, Bayesian analysis of computer code outputs; GEM-SA, Gaussian emulation machine for sensitivity analysis.

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2004a), and soil nitrogen leaching (Li et al., 2006, 2009; Nakagawa and Shinogi, 2006; Tonitto et al., 2007a). This model is currently being applied for greenhouse gas inventory or mitigation work in North America, Europe, Asia, and Oceania. In the International Workshop on Global Change for Asia Pacific Region in 2000, DNDC was designated as one of the biogeochemical models applicable for the Asia Pacific regions (Qiu et al., 2005).

Sensitivity analysis quantifies the impact of variation in input parameters on the variability of model outcomes. Input parameter uncertainty results from many sources including measurement error, absence of information, and incomplete mechanistic understanding. This uncertainty imposes a limit on our confidence in the response or output of a model. Sensitivity analysis allows us to determine the key parameters that have the greatest influence on the outputs, the necessary level of accuracy for a parameter to make the application valid, and the parameters which model outcomes are not sensitive to. It can also be used to verify and validate the model (Hamby, 1994) and to provide insight about the robustness of model results to assist decision making (Manheim, 1998; Phillips et al., 2000; Saltelli et al., 2000b). Without sensitivity analysis, one does not know which inputs contribute most to output values and their uncertainty. Moreover, without sensitivity analysis, parameters that are not well understood may be left unchanged even though they are sensitive or are adjusted to implausible values or resources are wasted to measure or evaluate non-sensitive parameters. Kolb, quoted by Rabitz (1989) indicated that without sensitivity analysis modelling is 'intellectually dishonest'.

Although SA was conducted on DNDC by several authors, many used a "local" approach (Li et al., 1992a, 2004b; Leip et al., 2008) instead of a "global" approach. Unlike global SA (GSA) (Nossent et al., 2011; Castaings et al., 2012; Borgonovo et al., 2012; Sun et al., 2012), local SA (Crick et al., 1987) allows only one parameter to vary at a time, which deals with only small perturbations of the reference model and is not able to take into consideration the interactions among parameters, their ranges of uncertainty, and non-linear responses to parameters. Recently, Monte Carlo-based GSA was introduced for DNDC (Hutchinson and Mosier, 1979; Li et al., 2004b, 2005; Werner et al., 2007). This method was embedded into the DNDC model, which was set to divide each parameter into eight intervals (Li et al., 2004b).

Most of the previous studies investigating SA of DNDC used only a single years simulation (Hutchinson et al., 2007; Li et al., 1992a, 2004b). Performing long-term (>10 yrs) SA is very important for evaluating ecosystem models, especially for the models used to predict soil organic carbon (SOC) and/or the impact of climate change. The objective of this study was to conduct a long-term GSA of the DNDC model for predicting annual change of SOC, N_2O emission and crop yield using a method based on Bayesian analysis of computer code outputs (BACCO; Kennedy and O'Hagan, 2001; Oakley and O'Hagan, 2004).

2. Materials and methods

2.1. The DNDC model

The DNDC model is a general model of Carbon (C) and Nitrogen (N) biogeochemistry in agricultural ecosystems, which consists of two components: (1) sub-models for soil environmental state, plant growth and decomposition which predict the dynamics of soil temperature, moisture, pH, Eh and substrate concentration profiles based on primary drivers (e.g., daily weather, soil properties, and crop management scenario); and (2) sub-models for nitrification, denitrification, and fermentation that track production, consumption and emission of N_2O, NO, N_2, ammonia (NH_3) and methane, based on soil environmental factors. The DNDC model is fundamentally designed around coupled C and N cycles. Soil organic carbon consists of four major pools: plant residues, microbial biomass, humads and passive humus. Each pool consists of sub-pools with different specific decomposition rates. The daily decomposition rate for each sub-pool is regulated by the pool size, specific decomposition rate, soil clay content, N availability, soil temperature and moisture. When SOC in a pool decomposes, the decomposed C is partially allocated to other SOC pools, and the remainder lost as CO_2. Dissolved organic C is produced as an intermediate during the decomposition process, and can be immediately consumed by the soil micro-organisms.

Soil aeration status is calculated based on oxygen diffusion and consumption in the soil profile in a kinematic module called an anaerobic balloon. Based on the predicted redox potential, the soil in each layer is divided into aerobic and anaerobic parts where nitrification and denitrification occur, respectively. When the anaerobic balloon is inflated, more substrates (e.g., dissolved organic C, NH_4^+ and N oxides) will be allocated to the anaerobic micro-sites to stimulate denitrification. When the anaerobic balloon is deflated, nitrification will be enhanced. Gases (NO and N_2O) are produced during both the nitrification and denitrification processes, and are subject to further transformation during their diffusion between the aerobic and anaerobic micro-sites.

Crop growth is calculated in a daily time-step based on solar radiation, temperature, N stress and water stress. Nitrogen demand of the crop is calculated based on the optimum daily crop growth and the plant C/N ratio. The actual crop N uptake is limited by N or water stress during the growing season. After harvesting the crop, all the roots are left in the soil profile and a user-defined fraction of the above-ground litter remains on the soil surface as stubble until a simulated tillage event incorporates the stubble into the soil profile. The crop litter incorporated into soil will be partitioned into different SOC pools based on the C/N ratio of the litter. The DNDC model has evolved into a comprehensive ecological model that can be used in most agricultural systems (Levy et al., 2007; Li et al., 1992a,b; 1994; Pattey et al., 2007; Saggar et al., 2007; Zhang et al., 2002).

2.2. Sensitivity analysis

Sensitivity analyses fall into two categories, local SA and global SA (Homma and Saltelli, 1996; Saltelli et al., 1999, 2000a; Shahsavani and Grimvall, 2011; Annoni et al., 2011). Local SA considers perturbations about local – or single point estimates – of model parameters. Parameters are varied one at a time to determine which parameters have the greatest effect on model output. Though widely used, local SAs often fail to produce meaningful results when the model under consideration is non-linear, when input variables are subject to different orders of uncertainty or they interact (Homma and Saltelli, 1996; Hunter et al., 2000; Saltelli et al., 1999), or model parameters are perturbed simultaneously but with different magnitudes (Mills et al., 1999). In contrast to local SA methods, global SAs (Saltelli et al., 1999) allow many parameters to vary simultaneously and consider variation in parameters throughout the parameter space. Hence, global SAs reflect the influence of each parameter averaged over all possible values of the other input parameters (Homma and Saltelli, 1996; Saltelli et al., 1999). In addition, they allow one to assess the importance of interactions among model parameters as they relate to model predictions. Several global SA methods have been introduced, such as regression analysis (Saltelli, 2004), the Morris method (Morris, 1991), regional SA (Hornberger and Spear, 1981), Sobol's variance decomposition (Sobol', 1993) and BACCO (Kennedy and O'Hagan, 2001). The method of BACCO was chosen for this study because of its advantages compared to other methods (Kennedy et al., 2006, 2009), which are described in the following paragraphs.

2.3. BACCO GEM-SA

The BACCO method is based on a Bayesian analysis which is able to address multiple sources of uncertainty affecting model performance (Oakley and O'Hagan, 2004; Kennedy et al., 2006). The theory related to the BACCO method of GSA is offered by Oakley and O'Hagan (2004), while the statistical theory and mathematical principles dominating the Gaussian process (GP) emulation are documented by Kennedy and O'Hagan (2001) and Kennedy (2004). Furthermore, a comprehensive introduction of the BACCO method could be found in a tutorial written by O'Hagan (2006). Recently, the BACCO approach has been implemented in the Gaussian emulation machine for sensitivity analysis software (GEM-SA, v1.1) (Kennedy, 2004, 2005), which can be downloaded for free.

The BACCO method has the ability to analyse the sensitivity of model outputs simulated by DNDC to all the important input variants over the full range of likely values adopted for the input parameters. In fact, the two major steps embedded in the BACCO method are: 1) building an emulator of the model from a set of training points generated from runs of the actual model under study, with these well designed to cover the multidimensional input space using a space-filling algorithm; 2) using the emulator built in the first step to compute the SA quantities of interest (Petropoulos et al., 2009).

Unlike LSA and other Monte Carlo based GSAs (Flores-Alsina et al., 2012), the BACCO is a comprehensive methodology. SA results are obtained directly from the emulator which could make the procedure very fast and efficient (O'Hagan, 2006). The results include the decomposition of output uncertainty into components due to uncertainty in single inputs or pairs of inputs, together with a measure of the additional uncertainty from emulation (the accuracy evaluation of the emulator) (Kennedy, 2004). Consequently, for the SA of comprehensive deterministic models like DNDC, the BACCO is a computational saving alternative because of the following advantages (O'Hagan, 2006): 1) the emulator is generated from a relatively small number of model runs covering a multidimensional input space, and is used to perform a computationally inexpensive and efficient analysis of all the SA computations found in the original model code; 2) as long as the emulator is built, is not necessary to run the actual model any more (Kennedy et al., 2009), regardless of how many analyses are required to assess the simulator's behaviour, which is a very distinct advantage compared to other GSA methods (Saltelli et al., 2000a), which typically require a new set of simulator runs for each analysis. Therefore, when BACCO is compared for instance with Monte Carlo based GSAs, the approach requires far fewer model runs since the original code is only run to develop the emulator; 3) the emulator provides a convenient way, in comparison to other GSA methods, to visualize the influence of varying individual parameter or pairs of parameters and to identify the inputs to which the output is most sensitive; and 4) last but not least, a self-test of the emulator's performance is embedded in matching the original model performance, thereby providing an accurate and reliable indication of the trustworthiness of its analysis.

The above mentioned emulator is based on Bayes' theorem, which is a statistical representation of the original model. For the emulator in BACCO, a prior belief based on a Gaussian processes model about the actual model is inferred. The theorem of Bayes' and a set of the model runs are considered together to refine the prior information to yield the posterior distribution of the output. The emulator is typically much faster, easier and more efficient to run across the entire multidimensional input space than is the actual model (Petropoulos et al., 2009).

One of the novel advantages of the BACCO GEM-SA is the self-test mechanism, i.e., accuracy assessment of the emulator (Bastos and O'Hagan, 2008). Several terms of it were involved, including a sigma-squared value, and a set of cross-validation statistical and roughness values. The sigma-squared value expresses the variance of the emulator after standardizing the output, and effectively provides a measure of the non-linearity in the emulator. Low sigma-squared values indicate these parameters exhibit only small or moderate deviations from linearity. Cross-validation statistical measures can be produced automatically when the emulator is built in order to check the accuracy of both types of output, including the cross-validation root mean squared error (CVRMSE) and cross-validation root mean squared standardized error (CVRMSSE). CVRMSE is simply the square root of the mean square error of the emulator predictions at the training points, and the CVRMSSE expresses the residual divided by an estimate of its standard deviation. The value of CVRMSSE should be close to 1.0 if the emulator variance is an accurate estimate of the actual error variance. In addition to cross-validation, the emulator provides estimates of the smoothness of each of the model inputs, so-called "roughness values", which is a unitless metric describing essentially how rapidly the output responds to changes in each input (Petropoulos et al., 2009). High roughness values are indicative of non-linear relationships of those inputs with regards to the output considered.

The primary SA output from GEM-SA includes the computation of the relative contributions of main and joint effects (pairwise interactions only) of the input parameters to the overall output variance, as well as the total effects. The computation theory of these results is based on a direct decomposition of the model output variance into factorial terms, named 'importance measures' (Ratto et al., 2001). The percentage variance contribution of each input's main effect to each output is reported, which provides a simple means of ranking the inputs in terms of their importance. The percentage variance component associated with each input measures the amount its main effect contributes to the total output variance, based on the uncertainty distributions for all inputs. Additionally, the total effect includes the main effect and interactions, so it can be used to determine the degree of pairwise or higher order interactions among parameters, and the sum of all inputs' total effects with respect to each model outcome will be greater than 100%.

There are two built-in sampling algorithms in GEM-SA software to assign training runs within the input space and build the emulator: LP-τ and Maximin Latin Hypercube (MLH). The LP-τ design (Saltelli et al., 2004) is based on the uniformly distributed sequences in space, providing a mechanism for generating a deterministic sequence of points in multidimensional space that is uniformly distributed (Saltelli et al., 2000a). The LP-τ method was considered to be an efficient, robust and sophisticated way to perform random sampling by Petropoulos et al. (2009). The Maximin Latin Hypercube design (MLH) is a particular case of stratified sampling (Saltelli et al., 2004), which ensures that each input factor is represented in a fully stratified manner. The maximin criterion maximizes the minimum distance amongst all pairs of points (Morris and Mitchell, 1995) and is frequently used to obtain good space-filling properties (Daneshkhah and Bedford, 2008; Kennedy et al., 2006; Van Dam et al., 2005; Voyer et al., 2009; White et al., 2008).

2.4. Sensitivity analysis of DNDC

A global sensitivity analysis was conducted on a continuous spring wheat system because continuous cropping appears to be one of the most effective dryland cropping systems to increase soil organic carbon (Liebig and Gollany, 2004). Among more than 50 inputs for DNDC (v 93), 27 parameters with wide ranges (minimum and maximum values) were selected for SA, based on experts' experience, literature review as well as the model recommendations (Table 1). Weather conditions, such as precipitation and air temperature are already well-known to be sensitive factors affecting DNDC model outputs (Li et al., 1992a, 1996, 2004b; Giltrap et al., 2010) and are beyond the control of the user, and thus, were not selected for this study. We used weather data (daily precipitation, minimum and maximum temperature) collected from 1921 to 2006 from a site near Three Hills, Alberta, Canada (51°42′ N, 113°13′ W, and 907 m). We use this weather data in order to simulate the continuous spring wheat experiment (the site and experiment is described in detail in "3.4 Model calibration and validation") under no-till or conventional till management during the period of 1991–2006 (Wang et al., 2007). Corresponding cropping system observation data, including annual change in surface horizon SOC, N_2O flux and yield, were available for comparison against DNDC outcomes. Results of this SA study will be used for testing the DNDC model on simulations of this site. Results could also be used for much broader environments because wide ranges of parameter values were selected for SA. In addition, the 86 year simulation was examined for ten snapshot years (the year of 0, 10, 20, 30, 40, 50, 60, 70, 80 and 86 from 1921) to examine the long-term sensitivity of input parameters.

Table 1
DNDC input parameters tested for long-term sensitivity analysis using the BACCO GEM-SA method. The table includes parameters definitions and the minimum and maximum parameter values.

Brief name of model input	Actual name of the model input	Unit	Minimum	Maximum
NRAIN	Atmosphere N deposition concentration in rainfall	ppm	1.3	1.9
NATM	Atmosphere background NH_3 concentration	$\mu g\ N\ m^{-3}$	0.01	0.1
CO_2	Atmosphere CO_2 concentration	ppm	320	450
BD	Soil bulk density	$g\ cm^{-3}$	0.5	2.25
PH	Soil pH	Unitless	4.5	9.1
ISOC	Initial SOC (Soil organic carbon at surface 0–5 cm)	$kg\ C\ kg^{-1}$	0	0.5
CLAY	Soil clay content	Unitless[a]	0	1
LITSOC	Litter SOC	$kg\ C\ kg^{-1}$	0.005	0.02
NO_3	Soil NO_3^-–N density	$mg\ N\ kg^{-1}$	8.5	15.5
NH_4	Soil NH_4^+–N density	$mg\ N\ kg^{-1}$	0.85	1.5
MOI	Soil moisture	Unitless[a]	0.27	0.65
TEM	Soil temperature	Degree Celsius	−10.5	10.5
FC	Field capacity	unitless[a]	0	1
WILP	Wilting point	Unitless[a]	0	1
HYDC	Hydro-conductivity	$m\ h^{-1}$	0.01	0.025
PORO	Soil porosity	Unitless[a]	0.2	0.8
SOCPA	Depth of soil profile with uniform SOC content	m	0.04	0.15
SOCPB	SOC decrease rate below top soil	%	0.5	5
GRESD	Ground residue	Unitless[a]	0	1
MYD	Maximum yield	$kg\ C\ ha^{-1}$	1000	2000
CNG	Grain C/N ratio	Unitless[b]	20	35
CNS	Shoot C/N ratio	Unitless[b]	45	55
CNR	Root C/N ratio	Unitless[b]	55	65
WTREQ	Water requirement demand	g water g^{-1} DM	100	250
DTILL	Tillage depth	Method[c]	1	4
DFERTI	Fertilization depth	cm	0	20
UREA	Urea application amount	$kg\ N\ ha^{-1}$	0	180

[a] A value between 0 and 1.
[b] A ratio between carbon content and nitrogen content.
[c] The method of DTILL in the interface of the DNDC model include four alternative depths of tillage, i.e., 1 represents "only mulching 0 cm", 2 represents "ploughing slightly 5 cm", 3 represents "ploughing with disk or chisel 10 cm" and 4 represents "ploughing with moldboard 20 cm".

Given the GEM-SA software constraint limiting a maximum number of training points to 400, a two-step GSA was carried out to improve the efficiency of SA (Kennedy et al., 2009). Firstly, a preliminary BACCO GEM-SA was conducted with 400 code runs for the 27 input parameters using the two sampling methods. The purpose was 1) to identify a suitable sampling method for GEM-SA of the DNDC model which produced relatively low roughness values, sigma-squared values, and CVRMSSE and 2) to select input parameters that may have significant influence on the outputs (defined here as parameters which have an average total effects of >5%). Using these preliminary results a second SA was subsequently conducted with BACCO GEM-SA. The second run of BACCO GEM-SA with fewer input parameters allowed more training points for each parameter, which improves the accuracy of SA (Kennedy et al., 2009). In this step, means and dynamics of change over 10 snapshot years in main effect and total effects (main effect plus interactions) on predictions of the three outputs were compared among these input parameters.

2.5. Model calibration and validation

Model calibration and validation were conducted using the data collected from a long-term cropping systems experiment near Three Hills, Alberta, Canada. The details of the experiment were described by Wang et al. (2007). Briefly, the experiment was initiated in 1991 with the whole area seeded to canola, then nine different crop rotation treatments began in 1992 and continued to 2006 [continuous wheat (CW), wheat-fallow (WF), wheat–wheat-fallow (WWF), peas–wheat-fallow (PWF), canola–barley–peas–wheat (CBPW), wheat-green manure (peas) (WP), wheat–peas–oat silage-fall rye, grass, and the mixture of alfalfa and grass]. All phases of each rotation were present each year. The experimental design was a randomized complete block with three replications. Since the fall of 1994 each treatment was split into two tillage methods: conventional and no-till. The conventional system usually received pre-seed and post-harvest tillage operations during the cropping year and some tillage operations during the fallow year.

Firstly, we conducted a spin-up run (perennial grass, 1400 years) to achieve a near-steady state in SOC pools before the start of cultivation (1905) in order to reduce the effects on simulation results from uncertainties in the initial conditions, such as the composition of SOC (Fumoto et al., 2008; Leip et al., 2008; Peltoniemi et al., 2007; Foster et al., 2003). Additionally, the spin-up run may also minimize the effects of other erroneous initial conditions, such as soil moisture (David et al., 2009).

Secondly, model calibration was conducted with the real observed data, but because of data limitations we only used in the calibration the simulated and measured N_2O flux from the WF rotation of Three Hills. Parameters to be calibrated were those with 'important' impacts on the N_2O emissions of DNDC prediction (i.e., dSOC and yield) based on the results of BACCO GSA. The calibrated values of the selected parameters were given and ranges with $\pm 10\%$ of the calibrated data were also showed.

Finally, after the calibration, model validation was executed by using another part of the real measured data of Three Hills. In this study we focus on validation of the results of SA instead of the overall prediction performance of DNDC, which will be conducted in further studies. Also, because of the design of the experiment we are only able to validate the sensitivity of tillage on the prediction of yield, N_2O flux and soil carbon. We used the CW, CBPW and WF treatments for model validation.

3. Results and discussion

3.1. Emulation accuracy

Generally speaking, some statements considering emulation accuracy should be made before any analysis of the SA results. Assessment of the emulator performance used the self-test mechanism of the BACCO approach (see Section 2.3), with these criterion based upon the quantitative evaluation of the series of statistical measures calculated by GEM-SA. The following summarises the sigma-squared value and a set of "cross-validation" self-explanatory statistical parameters for the two sampling methods.

Firstly, most of the sigma-squared values for all the conducted SA tests are low, while the data of input parameters in the MLH sampling ranged from 0.6 to 1.73 whereas it is 0.9–2.1 in the LP-τ sampling, indicating that these parameters exhibit only mild bias from linearity. And by Fig. 1, we can see most sigma-squared value of inputs in MLH sampling are less than that of LP-τ sampling, reflecting that the MLH should be a suitable measurement of the non-linearity in the emulator.

Fig. 1 also shows the statistics related to the cross-validation outcomes of the emulator. Most of the CVRMSE generated by the MLH design is less than that of LP-τ design, especially for dSOC and N_2O flux in most of the snapshot years. Additionally, the CVRMSSE for two designs are also very close to 1.0 in all the SA experiments, with values varying between 0.95 and 1.06 for the MLH design and 0.1 to 1.08 for the LP-τ sampling, respectively (Fig. 1). The deviation from 1.0 of CVRMSSE for MLH design in the 10 snapshot years for dSOC, N_2O flux and yield is 0.05, 0.13 and 0.24, respectively, while the value for LP-τ design is 0.23, 0.94 and 0.21, respectively. This indicates that most of the CVRMSSRE values of MLH design are closer to 1.0 than that of the LP-τ sampling, which means that the emulator variance generated by MLH was a more accurate estimate of the actual error variance.

Notably, roughness values for most of the input parameters were very low for both sampling methods (data not show) indicating that the emulator is a strong approximation to the true model (Petropoulos et al., 2009). Higher roughness values are indicative of non-linear relationships between parameter and model outcomes

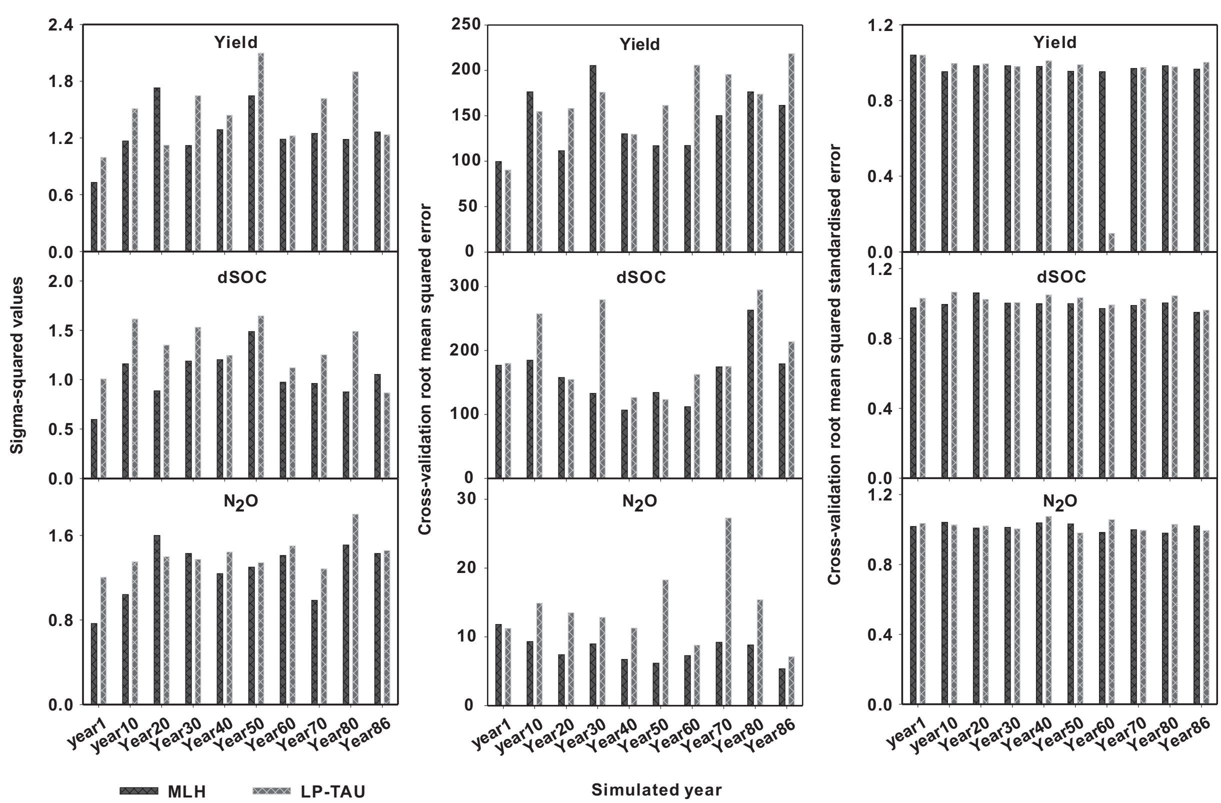

Fig. 1. Variation of long-term contribution of most important factors with respect to total DNDC output variance. The year 1 to year 86 is the ten snapshot year selected from the long-term simulation.

(Petropoulos et al., 2009). We found that parameter roughness values obtained by the MLH method were generally lower than that obtained by the LP-τ method, which partially proved the MLH design provided a superior emulation compared to LP-τ sampling.

In conclusion, the emulator fit of GEM-SA is a good representation of the DNDC model. Data analysis indicates the MLH sampling method is more efficient than Lp-τ design when conducting the emulation and it was better suited for use in the second step of the BACCO GEM-SA of the DNDC model.

3.2. Preliminary BACCO GEM-SA

According to the preliminary BACCO GEM-SA with the MLH method, the total effects of each input parameter contributed to the total variances of DNDC outputs differently (Table 2). Most of the input parameters have little total effects on the output of dSOC. Only 10 parameters had >5% contributions to the total effect on dSOC. The most influential parameters on the output of dSOC were the cumulative effects of ISOC (26.9%), PORO (18.0%), GRESD (ground residue) (16.6%) and WILP (16.3%) (see Table 1 for parameter definitions). Furthermore, for the prediction of N_2O, there were only 8 parameters that had >5% contribution to the total effects. The most influential parameters were DFERTI (fertilization depth) (25.0%), PH (soil pH) (15.4%), ISOC (13.8%) and PORO (13.6%). Similarly, eight of the 27 input parameters contributed >5% of the total effects on simulated grain yield. WILP was the most influential parameter (28.3%), followed by PORO (25.0%), WTREQ (water requirement demand) (22.7%) and ISOC (20.5%). Some parameters, such as ISOC, CLAY, PORO and SOCPA had significant contributions (>5%) to the predictions of all three outputs, while some only had significant contribution for a single output, such as GRESD for dSOC, and DFERTI and PH for N_2O (Table 2). In total, there were 14 parameters that had averaged total effects over the ten snapshot years greater than 5% for at least for one prediction output (Table 2), which were selected for the next step of SA.

Table 2
The long-term average value of total effects (%) of each parameter with respect to the output variance of annual change of soil organic carbon (dSOC), nitrous oxide flux (N_2O) and yield predicted by DNDC over 10 snapshot years in the first step of BACCO GEM-SA.

Input parameters[c]	Total effects (%)[a]		
	dSOC	N_2O	Yield
BD	**6.5**[b]	4.1	1.9
CLAY	**8.3**	**9.6**	**10.6**
DFERTI	1.0	**24.9**	1.6
DTILL	**5.7**	**9.9**	0.8
FC	**6.1**	3.0	**11.7**
GRESD	**16.6**	1.5	1.3
ISOC	**26.9**	**13.8**	**20.5**
MYD	**7.8**	2.1	**13.7**
PH	1.0	**15.4**	2.0
PORO	**18.0**	**13.6**	**25.0**
SOCPA	**6.9**	**6.2**	**9.5**
UREA	2.1	**6.5**	2.6
WILP	**16.3**	3.4	**28.3**
WTREQ	**6.3**	3.6	**22.7**
HYDC	1.3	4.3	1.4
LITSOC	0.6	0.9	1.0
MOI	0.7	0.8	3.5
NATM	0.9	2.0	0.7
NH_4	0.3	0.5	0.6
NO_3	0.7	2.4	1.0
NRAIN	0.5	0.8	1.4
SOCPB	3.5	4.8	2.3
TEM	1.1	1.2	1.6

[a] Total effects includes main effect and all of the interactions between each input.
[b] Bolded values are greater than 5% in form of total effects.
[c] Definition of each input parameter is described in Table 1.

3.3. Second step of BACCO GEM-SA

The second run of BACCO GEM-SA with fewer input parameters (which have the average total effects greater than 5% to each of the DNDC output over 10 snapshot years in the first step of BACCO GEM-SA) was conducted. In this step, means and the long-term trend of change over 10 snapshot years in the main effect and total effects (main effect plus interactions) on predictions of the three outputs were compared among these input parameters. According to the results of step 2, the main effect on variance of dSOC outcomes resulting from each input parameter ranged widely (0–35.6%) (Table 3). The parameter with the most significant individual effect was ISOC (initial shallow soil organic carbon) (35.6%), followed by CLAY (soil clay content) (16.1%) and BD (soil bulk density) (15.3%), with the other parameters having insignificant contributions to dSOC. Some parameters had noticeably higher total effects compared to their corresponding main effects indicating strong interaction effects (Table 3). Input errors of these parameters can lead to significant errors in simulations of dSOC. The main effect alone accounted for 73.7% of the total dSOC variance, while the first order interactions accounted for 18.3% and the remaining effect (8%) was owed to the second or higher order interactions. It seems that parameters with high main effects, such as ISOC, CLAY and BD, also tended to have high interaction effects and resulted in high total effects on dSOC, and vice versa. These three parameters also showed high contributions to variance of dSOC in the preliminary selection of step 1, but CLAY and BD were only the fifth and eighth most relevant parameters (Table 3), indicating that the two-step approach could improve the accuracy of SA. Previous studies also found that CLAY (Leip et al., 2008), ISOC (Li et al., 1994) and BD (Liu et al., 2006) sensitively affected the modelled dSOC, but no study was conducted to investigate the changes of their sensitivities to dSOC over time. Contributions of ISOC and BD over the ten snapshot years were relatively consistent, but the main and total effects of CLAY with respect to the total variance of dSOC changed dramatically over the years (Fig. 2). It was very high in the first year of simulation, and then it continually declined until simulation-year 80. It seems that the importance of clay content in the dSOC is described by the DNDC model, but its effect was later

Table 3
The long-term average value of the main effect and total effects (%) of each parameter with respect to dSOC, N_2O and yield predicted by DNDC over 10 snapshot years in the second step of BACCO GEM-SA.

Input parameters[b]	dSOC		N_2O		Yield	
	Main effect	Total effects	Main effect	Total effects	Main effect	Total effects
BD	**15.3**[a]	**25.7**	1.1	**9.0**	0.2	2.8
CLAY	**16.1**	**30.1**	**11.1**	**32.2**	**8.4**	**19.7**
DFERTI	0.03	0.6	2.0	**19.6**	0.1	1.3
DTILL	0.1	1.4	0.5	**8.7**	0.1	2.0
FC	0.6	2.8	0.7	2.7	4.1	**16.6**
GRESD	1.1	2.8	0.3	3.4	0.1	1.4
ISOC	**35.6**	**52.1**	1.1	**22.6**	2.0	**23.4**
MYD	0.3	1.7	0.2	3.2	1.4	**6.7**
PH	0.03	0.2	**10.0**	**33.8**	0.1	0.2
PORO	1.0	4.2	1.3	**18.7**	**6.0**	**22.1**
SOCPA	1.6	4.8	0.1	1.9	0.1	2.0
UREA	0.03	0.8	**14.1**	**33.4**	0.3	4.0
WILP	1.6	**7.4**	0.3	**6.1**	**27.5**	**51.1**
WTREQ	0.3	2.1	0.7	**5.6**	**9.0**	**18.0**
Total % variance	73.7		43.3		59.3	
First order interactions	18.3		27.1		19.5	
2nd or higher order interactions	8.0		29.6		21.2	

[a] Bolded values are greater than 5%.
[b] Definition of each input parameter is described in Table 1.

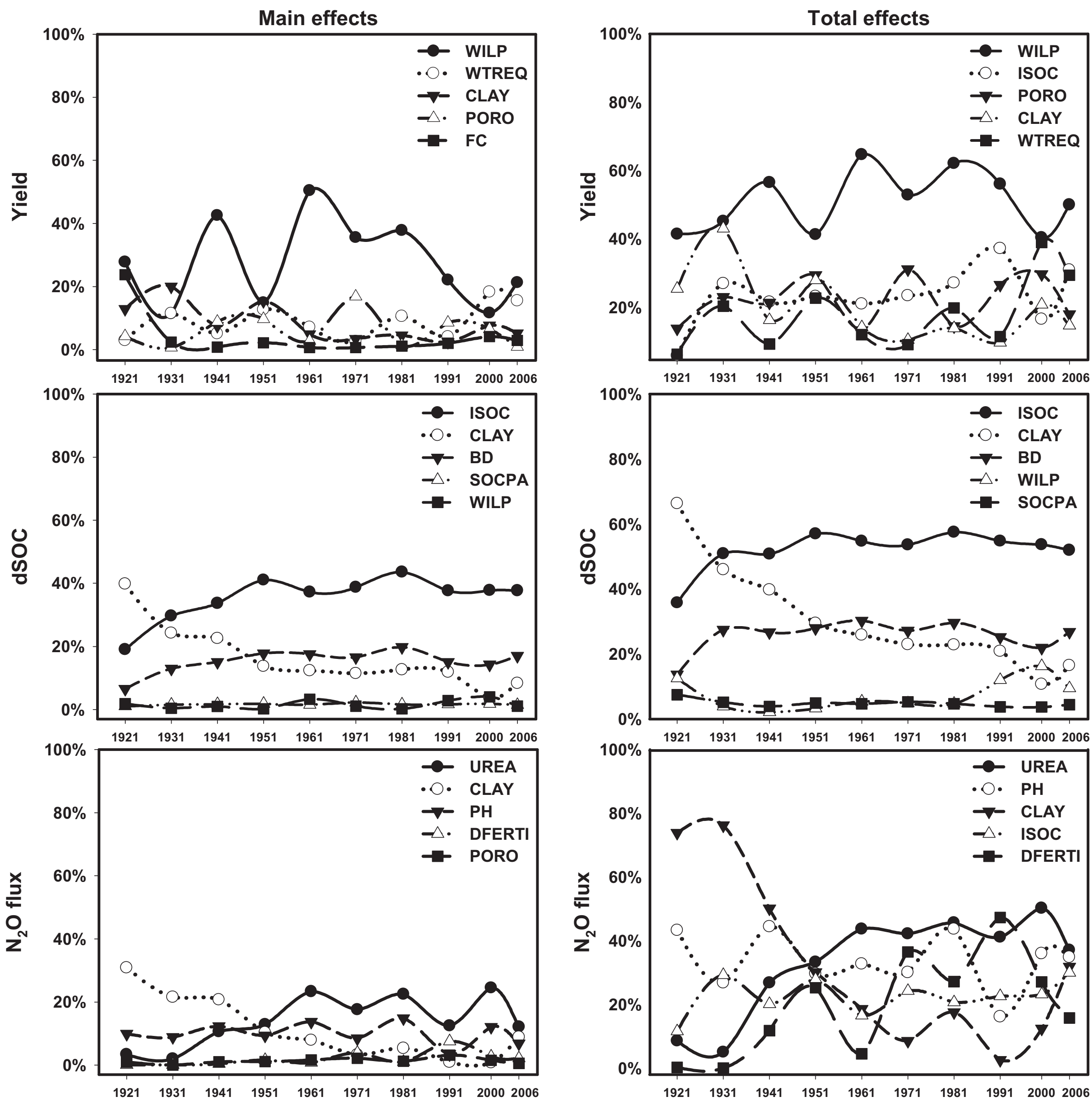

Fig. 2. Long-term variation of main effect and total effects of five most sensitive parameters with respect to total DNDC output's variance according to the second step of BACCO GEM-SA. Annual change of SOC, N_2O and yield is the model output. Definition of the parameters is described in Table 1.

partially replaced or concealed by other factors that might be closely associated with clay content. Even so, clay content was always an important factor for dSOC in the model compared with most of the parameters (>5% of total effects to the total output variances of dSOC).

For N_2O, UREA (urea application amount) (14.1%) had the highest main effect, followed by CLAY (11.1%) and PH (10.0%) (Table 3). The main effects of the other parameters were quite small (≤2%). Some input parameters, however, had high total effects on the simulation of N_2O by DNDC compared to main effects indicating significant interactions (Table 3). This also suggests that the influence of the characteristics of the soil-crop-climate system on emissions of N_2O is very complicated, and the synthetic effect of all the factors should be considered. The total main effect of all 14 parameters was only 43.3% which means effects were mainly contributed by interactions, where first order and higher order interactions contribute by 27.1% and 29.6%, respectively. Seven of the inputs exhibited ≥9% of the total effects with respect to variation of N_2O emissions by DNDC, with PH being highest (33.8%), followed by the almost equally high UREA (33.4%) and CLAY (32.2%) (Table 3). Other high-contribution factors were ISOC (22.6%), DFERTI (19.6%), PORO (18.7%) and BD (9.0%). Although the selected parameters with high contributions to the simulation of N_2O were similar between the two steps, the orders of value were quite different. For example, UREA (33.4%) and CLAY (32.2%) had the second and third largest total effects, respectively, according to step 2, while the corresponding total effects calculated by step 1 were only the seventh (6.5%) and sixth (9.6%) largest, respectively (Table 2). Some previous studies also found PH (Li et al., 1992a), UREA (Brown et al., 2002), CLAY (Li et al., 1992a; Villa-Vialaneix et al., 2012) and ISOC (Li et al., 1996; Villa-Vialaneix et al., 2012) to be important parameters influencing the prediction of N_2O by DNDC. Similar to dSOC, clay content had very high total effects on simulated variance of N_2O emissions from the beginning of the run (Fig. 2). It then reduced linearly until simulation-year 50. Oppositely, the total effects of urea application were relatively low in the beginning of the run. It increased from simulation-year 20 until simulation-year 40,then was relatively stable. Dynamic changes of other parameters were either relatively small or no clear trend could be revealed.

To our knowledge, no previous SA has been conducted on yield simulation by DNDC. According to the second step of BACCO GEM-SA, WILP (wilting point) had the highest main effect on the output variance of grain yield (27.5%), which was much higher than other parameters (Table 3), indicating the importance of soil water status on crop growth. The second and third highest parameters with respect to the main effect were WTREQ (9%) and CLAY (8.4%), respectively. Similar to the prediction of N_2O, some parameters had high total effects that were mainly associated with their high interaction effects on yield prediction (Table 3). Consequently, the sum of the main effects was able to explain only 59.3% of the yield variance. First order and higher order interactions explained 19.5% and 21.2% of the total yield variance, respectively. There were six parameters that greatly affect the prediction of yield by DNDC with WILP being extremely high (51.1%), followed by ISOC (23.4%), PORO (22.1%), CLAY (19.7%), WTREQ (18.0%) and FC (field capacity) (16.6%) (Table 3). The most relevant parameters calculated by step 2 were quite consistent to those selected by step 1 (Table 2). Again, the total effects of clay content were very high from the start of simulation (Fig. 2). It continuously reduced after simulation-year 10 until simulation-year 70. Other parameters did not have dramatic variations in their total effects on the output variance of yield over the near 90 year simulations.

There are a number of implications of these SA results. First, both of ISOC and CLAY were among the five most sensitive parameters for all the three DNDC outputs simultaneously. In practice, initial soil organic carbon and clay content are very important soil characteristics, they have a primary effect on soil carbon decomposition and the composition of soil texture, which will influence the physiochemical processes in soil and crop production, respectively, and our results reflect that the DNDC model adequately captured the response of dSOC, N_2O flux and yield to the changes in ISOC and CLAY, especially during the long-term simulation.

CLAY content dominates the composition of soil texture, which controls the soil type, and affects all of the physiochemical procedures during soil substrate decomposition. This decomposition process influences the evolution of SOC, the production of N_2O and the formation of crop yield. Furthermore, sensitive effects of some input parameters changed dramatically during the long-term GEM-SA, such as CLAY, for which the SA curve decreased during the simulation, while oppositely, the ISOC and WILP as well as BD increased through time (Fig. 2). This phenomenon was partially due to the long-term weather data we used during this study, which has been emphasized was the most influential factor affecting the behaviour of DNDC simulation (Li et al., 1992a, 1996, 2004b; Giltrap et al., 2010). Our GSA was initiated with the long-term simulation based on 86-year weather data set from Three Hills, soil properties like SOC, clay content and bulk density had responded differently under the various weather conditions, and the simulated DNDC outputs varied during the long-term emulation. Consequently, the SA results of the most important input parameters changed dramatically with the analysed years as they were involved in most of the procedures in DNDC that influence the model outputs (their total effects are the indication). In addition, the two-step BACCO GEM-SA of the DNDC model indicates that the screening (Makler-Pick et al., 2011) of the most influential input parameters is necessary for GSA of a complicated stochastic model to reduce the number of important inputs, which allows a more effective coverage of the reduced input space. Secondly, the discrepancy between step 1 and 2 (the important sequence of some parameters with respect to DNDC outputs, Tables 2 and 3) is partially due to the emulator approximation errors, because the emulator is built based on the Gaussian process hypothetic prior belief of the DNDC model, which is just a statistical approximation of the model input and output. The difference between the two steps are also due to the different proportions each parameter contributed during the variance decomposition of model outputs in the two steps based on a distinct number of input parameters (i.e., 27 and 14). Last but not least, the results of our study could be applied in a wider environment of DNDC simulation. Firstly, the range of selected input parameters was wide enough (Table 1) to cover almost all the land use types, especially for the north temperate zone, and secondly the long-term trend of SA results was also sufficient to catch the most important parameters with respect to the DNDC outputs, which could be focused in the future validation and parameterization of the DNDC model.

Table 4
Site and field management characteristics of Three Hills, Alberta, Canada.

Items	Three Hills' information
Pre-cultivation history	Semiarid grassland vegetation-fescue prairie-primarily rough fescue
Land first cultivated	1905 (1900–1910)
From 1905 to 1975	Cereal-fallow 2 year rotation with the cereal phase mostly wheat with barley about every third rotation
From 1976 to 1985	Canola-cereal-fallow 3 year rotation with the cereal phase mostly wheat with barley about every third rotation
From 1986 to 1991	Cereal-canola–cereal-fallow 4 year rotation with the rotation probably wheat-canola–barley-fallow
Research site opened	1991
Experiment initiated	1992 (continuous wheat, wheat fallow, canola-barley-pea-wheat, etc.)
Location, and elevation	51°42′ N, 113°13′ W, 923 m
Ecoregion name	Moist mixed grassland
Soil landscape of Canada (SLC)	546
Initial carbon Ap horizon (%)	3.65
Soil classification	Solonetic Black Chernozem
Landscape	Undulating
Growing degree days (>0 °C)	2519
Growing degree days (>5 °C)	1489
Frost free period	113
Growing season precipitation (mm)	232 (mean), 98 (min), 378 (max)
Growing season temperature (°C)	15 (mean), 7 (min), 22 (max)

3.4. Model calibration and validation

A series of 102-year (1905–2006) runs of the DNDC model was conducted using the management data of Three Hills, Alberta (Table 4), and the annual N_2O flux of wheat-fallow treatment from 2000 to 2006 was compared to the value of DNDC predicted. DNDC simulations were carried out by varying four important parameters ($\pm$10%) to N_2O emissions according to the two-step GSA (Table 5),

Table 5
Calibration of some important parameters for N_2O of DNDC prediction.

	Calibrated	+10%[c]	−10%[c]
ISOC (kg C kg^{-1})[a]	0.04[b]	0.044	0.036
BD (g cm^{-3})	1.26	1.38	1.13
CLAY (Unitless)	0.41	0.45	0.37
DTILL (cm)	10	11	9

[a] Definition of each input parameter is described in Table 1.
[b] The calibrated value of each parameter, which induced comparable N_2O flux with the real observed data.
[c] Values in the third and fourth column are the data plus and minus 10% by the calibrated value.

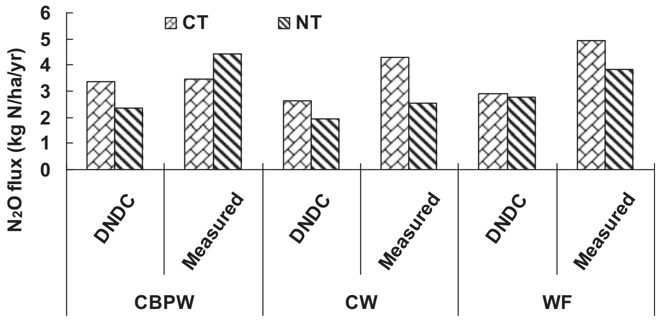

Fig. 3. Measured and DNDC simulated Nitrous oxide flux of each crop system based on till and no-till management of Three Hills, Alberta from 2000 to 2006. CT, conventional tillage, NT, no-till, CW, continuous wheat, CBPW, canalo–barley–pea–wheat, WF, wheat-fallow.

while the values of other less-important parameters were fixed. Results confirmed that among many input parameters, only several of them have the important influence on the output variation of N_2O flux. This indicated that a number of inputs should be ignored in the future parameterization of DNDC. However, for the data limitation, calibration only employed for N_2O flux instead of dSOC and yield. Further validation of the model with real observed data is described in the following part.

Measured N_2O flux of the Three Hills site were used to validate the DNDC model simulated N_2O emissions from 2000 to 2006. For this site, a number of "tillage*crop-rotation" treatment combinations were established in 1994. Four of these combinations are considered in the current work, including continuous wheat (CW), a wheat-fallow rotation (WF), as well as canola–barley–pea–wheat rotation (CBPW), all under No-till (NT) and Conventional Till (CT) management. All wheat phases receive 67 kg N ha^{-1}; no N is applied to the pea phase. Grain yield, seven-year results (2000–2006) of N_2O and the change of soil carbon over time were made available for use for validation. In this study we focus our validation of the results of SA instead of the overall prediction performance of DNDC which will be conducted in further studies. Also, because of the design of the experiment we are only able to validate the sensitivity of tillage on the prediction of yield, N_2O flux and soil carbon.

As discussed above, the depth of tillage (DTILL) (0–20 cm) is the fifth (step 1) and eighth (step 2) most sensitive factor for N_2O emissions by its total effects, as tillage is an important management factor affecting the soil air permeability, which is a dominant factor of N_2O production and emissions.

Previous studies found no-till (NT) is a practice that could inhibit (Elder and Lal, 2008; Gregorich et al., 2008) or enhance (Ball et al., 2008) N_2O emissions from soil, while Rochette (2008) pointed out that NT only increases N_2O emissions in poorly-aerated soils, while other research indicates that NT systems only reduce measurable soil N_2O flux when practiced in the long term (Six et al., 2004). So, high uncertainties still exist in the research of N_2O production and emissions from soil. More field experiments and model simulation should be conducted to minimize the uncertainties. Our field experiment resulted in the NT treatment having reduced N_2O emissions compared with the tillage treatment from Three Hills (except the CBPW rotation) ($p < 0.05$), and the DNDC model captured the same information (Fig. 3). Although the simulated N_2O flux by DNDC was less than that measured, experiment error may account for this, thus, Fig. 4 illustrated that most of the DNDC simulated annual average N_2O flux fell into the ±95% confidence interval of the measured data. This indicated that DNDC simulated N_2O emissions was well fitted with the observed data. Due to the data limitations, our validation needs to be continued after more field trials have been performed.

As one of the most important inputs for the DNDC model, the initial value of soil organic carbon in the soil surface layer was also focused upon to validate the field observation with that of the model simulation to see the response of the DNDC model to field management (ISOC, Table 5). The studied time span was 1992–1997, the first five years after the research site was opened. By comparing measured and DNDC modelled value of SOC, we found the treatments based on NT sequestered more C than conventional tillage (CT) rotations (Fig. 5A). By the measured data, the treatments with NT, the CW and CBPW caused an increase of SOC sequestration during the 6 years while the WF led decreased SOC. However, significant differences between rotations were not apparent in this

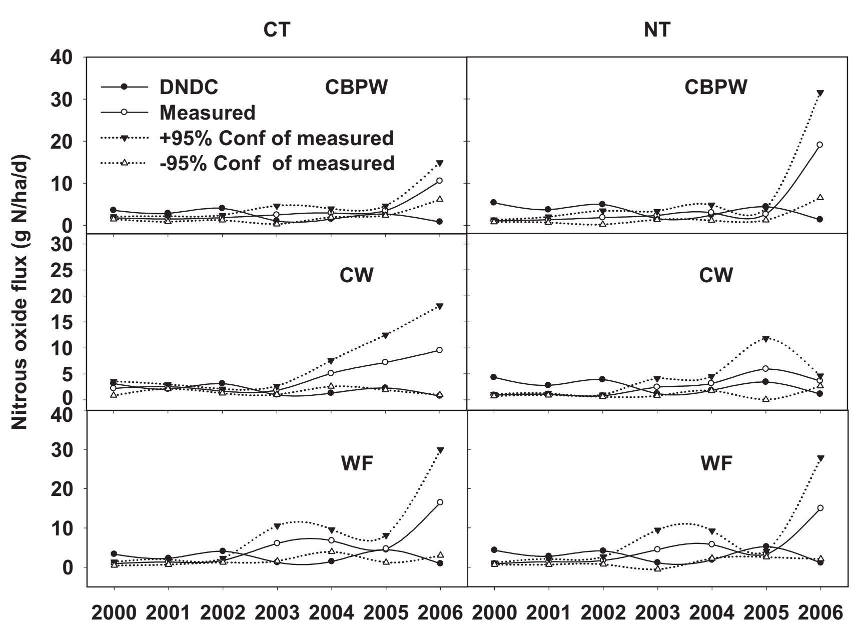

Fig. 4. Validation of DNDC model with real measured N_2O flux from Three Hills crop systems 2000–2006. ±95% Conf represent the measured data ±95% confidence interval. CT, conventional tillage, NT, no-till, CW, continuous wheat, CBPW, canola–barley–pea–wheat, WF, wheat-fallow.

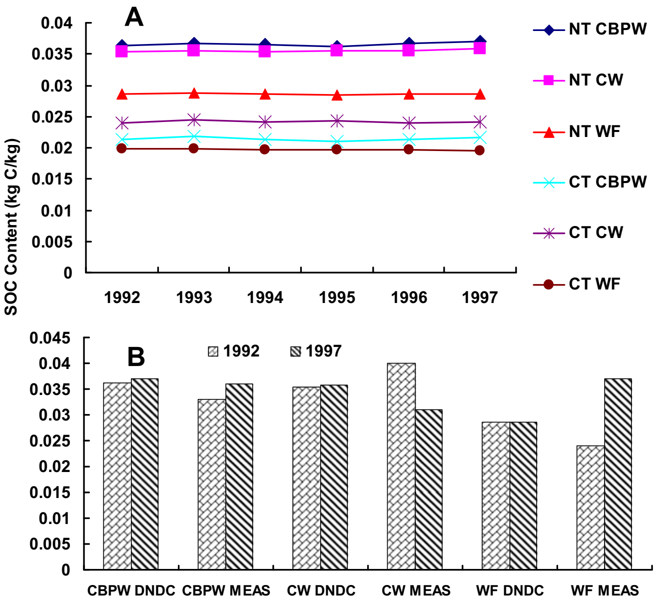

Fig. 5. Soil organic carbon content of Three Hills (1992–1997) by simulation of DNDC model (A) and the soil organic carbon content of the year 1992 and 1997 based on no-till (B). CT, conventional tillage, NT, no-till, CW, continuous wheat, CBPW, canola–barley–pea–wheat, WF, wheat-fallow. MEAS means measured value.

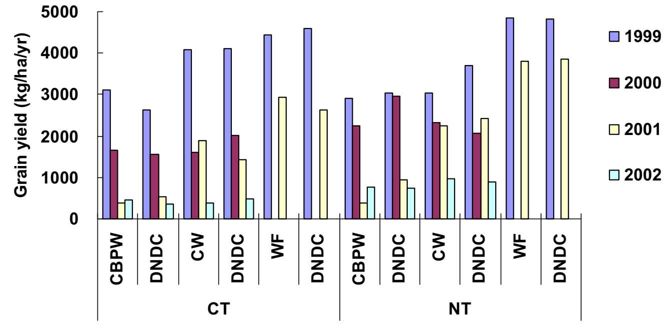

Fig. 6. The measured and DNDC modelled grain yield of Three Hills' rotation systems from 1999 to 2002. CT, conventional tillage, NT, no-till, CW, continuous wheat, CBPW, canola–barley–pea–wheat, WF, wheat-fallow.

study and may be due to the unseasonably dry growing season and the natural variability at the site. The continuous crop rotations appeared to sequester more C than the rotations with fallow. For the SOC simulated by DNDC, it increased from 1992 to 1997 except for the CW treatment (Fig. 5B). This suggested that DNDC captured the correct evolutions of soil carbon, as different tillage strategies controlled the change of initial SOC input, which has been fixed to 0.035 kg C kg^{-1} in this validation procedure, though this still proved that DNDC corresponded correctly to the variation of ISOC. We did not find DTILL to be one of the most important factors for dSOC in this two-step BACCO GEM-SA, mainly because the tillage is just an indirect factor that influences the evolution of the ISOC during the crop growing stage, and thus the annual change of SOC. Actually, no-till management is one of the most efficient practices for carbon sequestration in cropland if it is combined with the management of crop residues, proper crop rotations, fertilization regimes and manure applications. However, the conversion of CT to NT will increase SOC if it: 1) decreases the rate of SOC decomposition; or 2) increases carbon inputs and thus crop yield, which is often observed in some regions of the prairies (Desjardins et al., 2002).

There are a number of factors contributing to grain yield, and climate is the most important. So uncertainties in grain yield calculation exist both during the field experiment and the model simulation. According to our GSA of the DNDC model, we did not find great sensitivity of grain yield of spring wheat to the depth of tillage. But as discussed above, NT will increase crop yield in specific areas due to its greater water conservation ability than CT. In another study, Wang et al. (2007) observed that NT could mitigate heat stress of wheat and improved biomass and yield. The surface residue and standing stubble in NT act as insulation and impede the exchange rate of thermal energy between the soil and atmosphere. The higher near-surface soil moisture under this system can also help buffer the extremes in daily soil temperatures and reduce root heat stress (Wang et al., 2012). While DNDC does not simulate this physiological process, this should be included in future versions of the model, which could greatly improve it. Our validation was carried out by comparison of observed grain yield with the DNDC simulated data. We found the yield of NT-based rotations were greater than CT-based rotations, indicated by the field experiment as well as the DNDC simulation (Fig. 6). This indicates that the DNDC model performed well simulating grain yield for the cropping systems of Three Hills, Alberta. DTILL was not one of the most sensitive inputs of grain yield, mainly because it was just an indirect factor that affects the productivity of crops. The total effects of DTILL with respect to total output variance of yield were much greater than its main effect (Table 3). From Fig. 6, it also can be seen that there is only 4 years yield data that were validated. Further validation should be conducted based on longer-term field trials.

In conclusion, the results of the two-step of BACCO GEM-SA indicated that initial soil organic carbon in soil surface and soil clay content are the most important parameters for the main outputs of DNDC model, while most of the input parameters contribute little to the total output variance of DNDC outcomes. This suggested to us that, in the future parameterization of DNDC model, we should use fixed values for the less-important parameters, and calibrate the important variants with the field trials.

4. Conclusions

The selection procedure included two steps which ensured a more accurate sampling method (MLH) and increased training points for each pre-screened parameter and resulted in improved efficiency of the sensitivity analysis. Our study indicated that most of the 27 input parameters contributed little to the three model outputs. There were only three and six inputs that contributed to greater than 10% of the total output variances of dSOC and N_2O by their total effects, respectively. And six parameters contributed greater than 10% of the total output variance of grain yield simulated by DNDC. Among the selected parameters, both the ISOC and CLAY were included amongst the five most important input parameters with respect to the three outputs. Results also indicated that sensitivities of some parameters were time-dependent, which changed dramatically over the years. Therefore, it is necessary to conduct long-term global sensitivity analysis instead of only one year's simulation as previous studies did (Li et al., 1992a, 2004b). Otherwise, the impact of a parameter on the long-term prediction might be overestimated (in the case of CLAY) or underestimated (in the case of UREA for N_2O).

Some cautionary notes for future applications of GEM-SA should be considered, as no statistical method is perfect. Uncertainties in the estimation of the computation of main and total effects exist. With regards to this point, we know that, overall, emulator performance of MLH was found to be satisfactory as was documented by the overall range of values of the 27 input roughness measures (which varied from 0.0 to 7.9) as well as from the overall emulator statistics of sigma square (which varied from 0.6 to 1.7) and the

CVRMSSE results (which varied from 0.95 to 1.06). Noticeably, a number of the most sensitive model inputs (such as PORO for dSOC, PH for N_2O emissions and WILP and ISOC for yield) were often those that had the highest roughness values. This is easily understood because the effects of these factors on the DNDC outputs are highly non-linear, something that is also verified from the presence of the high order interaction effects and from studying the relationship between these model inputs and the outputs from the model. Although the site-specific values from Three Hills, Alberta were used for the GSA, incorporating their variation in the training data used with GEM-SA was impractical. Results from the present study are not expected to be site-specific, as all other model input parameters were varied in their whole theoretical range that can be used in the DNDC model. However, in order to quantify the influence of the parameters in this study which were adopted from the Three Hills site, the same work could be implemented for different sets of these fixed inputs. In order to furnish a fully inclusive evaluation of DNDC, the SA study performed here should ideally be followed by comparisons of DNDC simulations with more real field measurements from other sites.

Validation of real field data with the DNDC model outputs suggested that the model responded well to the ISOC and DTILL, and detailed validation based on long-term field trials should be considered. Furthermore, future parameterization of the DNDC model should focus on the most important input parameters to yield a highly efficient model calibration.

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