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An algorithmic calibration approach to identify globally optimal parameters for constraining the DayCent model

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ABSTRACT

The accurate calibration of complex biogeochemical models is essential for the robust estimation of soil greenhouse gases (GHG) as well as other environmental conditions and parameters that are used in research and policy decisions. DayCent is a popular biogeochemical model used both nationally and internationally for this purpose. Despite DayCent's popularity, its complex parameter estimation is often based on experts' knowledge which is somewhat subjective. In this study we used the inverse modelling parameter estimation software (PEST), to calibrate the DayCent model based on sensitivity and identifiability analysis. Using previously published N_2O and crop yield data as a basis of our calibration approach, we found that half of the 140 parameters used in this study were the primary drivers of calibration differences (i.e. the most sensitive) and the remaining parameters could not be identified given the data set and parameter ranges we used in this study. The post calibration results showed improvement over the pre-calibration parameter set based on, a decrease in residual differences 79% for N_2O fluxes and 84% for crop yield, and an increase in coefficient of determination 63% for N_2O fluxes and 72% for corn yield. The results of our study suggest that future studies need to better characterize germination temperature, number of degree-days and temperature dependency of plant growth; these processes were highly sensitive and could not be adequately constrained by the data used in our study. Furthermore, the sensitivity and identifiability analysis was helpful in providing deeper insight for important processes and associated parameters that can lead to further improvement in calibration of DayCent model.

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1. Introduction

There is an increasing focus on carbon (C) credits for land management practices to encourage C storage, and a reduction in emissions of C and other greenhouse gases (GHG) (Copenhagen Accord, 2009) in Earth's atmosphere. The intent is to enhance removal of C from atmosphere and to reduce the adverse impact of C and other GHG on Earth's climate that also affects agricultural systems. Biogeochemical models are major tools for estimating the sources and sinks of GHG and soil C in both research and operational settings. Many of these models are highly complex and use a multitude of parameters, which are not directly measured due to their spatial and temporal variations, the complexity of simulated processes, as well as the model structure itself. Instead, these parameters are estimated by experts who develop and/or use these models, although there are some alternative approaches to expert model calibration (Lamers et al., 2007; Gao et al., 2011; Luo et al., 2009). The underlying assumptions and the way model parameters are formulated require a crucial step of model calibration for accurate interpretation of the simulated results.

The main purpose of model calibration is to test the model fidelity and performance based on the contributing parameters and key underlying processes that affect model results, and off course the availability of input data. However, applying these methods to models with a large number of parameters can become computationally intractable. To reduce the number of parameters actively considered in calibration process, a sensitivity analysis can be carried out to classify parameters that have significant impact on model outputs (Cibin et al., 2010). The equifinality of model parameters, where multiple combinations of parameter values yield the same model output, is another issue that further complicates this calibrations process as highlighted by Luo et al. (2009) and Wagener and Kollat (2007). Therefore, in addition to sensitivity

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analysis, the identifiability of parameters should also be evaluated prior to model calibration. To investigate the interactions among parameters and their impacts on the model output, all parameters under consideration should also be individually perturbed during parameter identification and sensitivity analysis (Doherty and Hunt, 2009).

DayCent is a biogeochemical model that is widely used to evaluate the impact of climate and land use changes on different ecosystems (Abdalla et al., 2010; Olander and Haugen-Kozyra, 2011; Cheng et al., 2013; Sansoulet et al., 2014). DayCent is characterized by a large number of parameters and processes; however, manual calibration through "trial and error" is still a common approach by users of this model. For example, the original DayCent parameters (Del Grosso and Halvorson, 2008) were calibrated to measured N_2O fluxes and corn yield data through "trial and error" for seven out of more than 140 parameters (Steve Del Grossos; personal communication). Although the simulated output matched observations reasonably well, this does not address the potential problem of over fitting, nor addresses the issue of local versus global convergence. These issues can be resolved to a large extent by using an algorithmic calibration supplemented by parameter sensitivity and identifiability analysis as suggested for other fields of environmental science (Doherty, 2010; Hunt et al., 2007).

Our aims in this study were to: (1) asses the sensitivity of model simulation results to input parameters, (2) identify which parameters were well constrained by the observed data, (3) test whether the initially proposed parameters were consistent with global optimal parameter set used in the DayCent model, and (4) suggest processes for future data-model integration based on our findings.

2. Methods

DayCent is a biogeochemical model that simulates C and nitrogen (N) dynamics among the atmosphere, plant, and soil (Parton et al., 1998; Del Grosso et al., 2001). The flow of C and N between different pools are controlled by the size of the pools, C/N ratio and lignin content of material as well as water/temperature controls. The primary model inputs are: daily maximum/minimum air temperature, precipitation, soil texture and land use data. The popular outputs include daily GHG fluxes, soil organic matter (SOM), and actual evapotranspiration (AET). A more detailed description of the model can be found in Del Grosso and Halvorson (2008).

The N_2O fluxes and corn yield data for this study was taken from a commonly cited paper for calibrating the DayCent model (Del Grosso and Halvorson, 2008). These data were obtained at the Agricultural Research Development and Education Centre (ARDEC) in North-eastern Colorado near Fort Collins, USA (40°39′ N; 104°59′ W). This region is characterized with a semiarid temperate climate with predominantly clay loam soil. The data was collected from continuous irrigated corn cropping under no-till (NT) systems with no N fertilization. On average, the N_2O emissions were sampled one to three times per week over the growing season. For further details on the experimental design and data collection, see Mosier et al. (2006).

DayCent was calibrated using a gradient-based optimization approach to linearize the nonlinear processes by computing the Jacobian matrix of sensitivities of the model observations to the parameters as implemented in PEST (Doherty, 2010). PEST interacts with DayCent by modifying the model's inputs as well as by running the model and assessing the model's outputs until they converge. For the numerical stability of the calibration process,

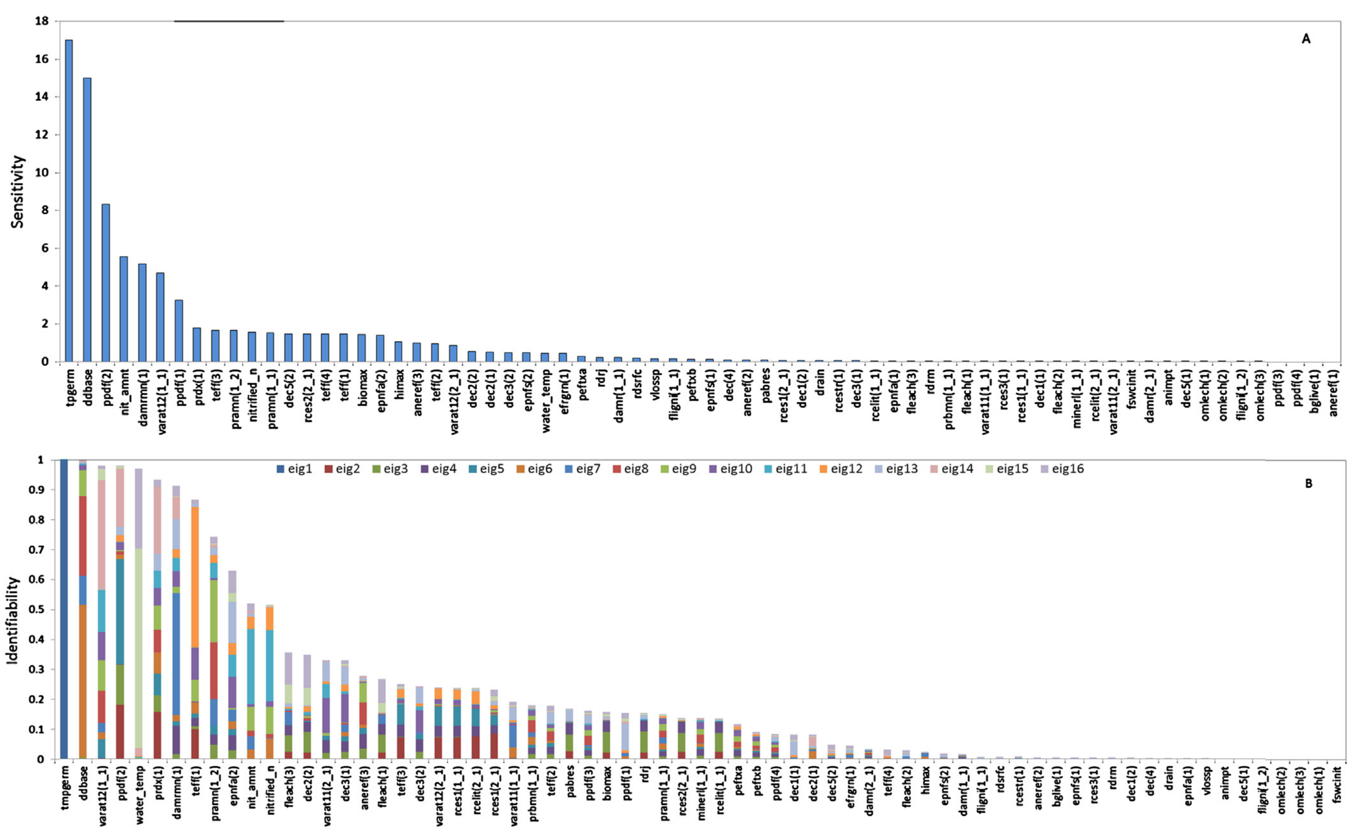

Fig. 1. (A) Sensitivity analysis of the parameters controlling the N_2O emissions and corn yield production in DayCent model. (B) Identifiability analysis of the parameters controlling the N_2O emissions and corn yield production in DayCent model. Colour codes in each bar of identifiable parameters represent the contribution of different Eigen components. (For interpretation of the references to color in this text, the reader is referred to the web version of the article.)

singular value decomposition (SVD) was applied in PEST. Parameters which were identified as strongly affecting N_2O fluxes and yield in the sensitivity and identifiability analysis were prioritized in the parameter exploration process.

The parameter sensitivity in PEST is estimated using a finite difference approximation.

$$\frac{\partial y}{\partial p} = \frac{y(p+\nabla p) - y(p)}{\nabla p} \quad (1)$$

where $\partial y/\partial p$ is the sensitivity of the modelled output (y) to a parameter (p). The combination of parameters and observations result in an NPAR × NOBS Jacobean sensitivity matrix which is used in Gauss-Marquardt-Levenberg (GLM) algorithm for regressions calculations (Doherty, 2010).

$$J_{ij} = \frac{\partial_{yi}}{\partial_{pj}} \quad (2)$$

where $i = 1$ to NOBS and $J = 1$ to NPAR. NOBS is the number of observations and NPAR is the number of parameters. The diagnostic values in Jacobean matrix represent the importance of parameters. The lower sensitive parameter values indicate that those parameters can be changed arbitrarily without significantly impacting the match between modelled and observed values. Therefore, it is important to address the composite sensitivity over each column for all observations. These sensitivities can also be scaled up by multiplying with the parameter values.

The identifiability *fi* of a parameter *i* can be estimated as:

$$fi = (V_1 V_1^t)ii = i^t(V_1 V_1^t)i \quad (3)$$

where, V_1 is a matrix with columns of orthogonal unit vectors that span the calibration solution space and i is a unit vector with all zero elements except for the parameter in demand. The value of *fi* can vary between zero to one. Zero indicates complete non-identifiability of parameter due to its existence within the calibration null space, whereas, one shows the complete identifiability of parameter due to its presence in calibration space. The non-identifiability (*ni*) is defined as:

$$ni = 1 - fi \quad (4)$$

Identifiability is a metric relating the information content from the calibration observations to the parameters when using SVD. When SVD information from observations (as described by the Jacobian matrix) is picked up, the singular value spectrum is truncated at a point often defined by stability. Information from the observations can then be projected either into parameters (solution space) or into uninformative noise (null space), based on the truncation level using the PEST utility IDENTPAR (a software utility used to compute parameter identifiability) (Doherty and Hunt, 2009). Since this analysis is performed on the Jacobian matrix, some similarity to composite sensitivities can be observed.

A total of 140 parameters, with model developer-recommended default values, were used to perform the sensitivity and identifiability analysis. The sensitive parameters were used to run the DayCent/PEST in calibration mode. The results obtained from calibration mode, referred to as "PEST-Calibrated", were compared with the results published in Del Grosso and Halvorson (2008), referred to as "Expert-Calibrated". We used the well-established statistical criteria of the sum of weighted squared residuals (SWSR) and the coefficient of determination to evaluate the performance of our proposed calibration approach.

3. Results and discussion

The sensitivity analysis proved to be an important step in determining the key parameters influencing the N_2O fluxes and crop yield. Out of 140 parameters, 70 parameters were found to be most sensitive to N_2O fluxes and corn yield while the remaining ones displayed little or no response to the calibration process. The most sensitive parameters influencing N_2O fluxes and yield include germination temperature (*tpgerm*), number of degree days required to trigger a senescence event (*ddbase*), and the maximum temperature dependency of plant growth (*ppdf(2)*), all of which showed sensitivity greater than 8.0 (Fig. 1A). Out of the remaining parameters, only four parameters showed sensitivity greater than 2.0, indicating moderate contribution to calibration process.

Although sensitivity analysis was useful in identifying important parameters, several previous studies (Doherty and Hunt, 2009) have shown that the sensitivity analysis alone does not fully explain the correlation coefficient of sensitivity parameters. Therefore, it was essential that indentifiability, which is defined as the capability of model calibration to constrain parameters, to be carried out in order to explain the parameters correlation and model behaviour. Parameter identifiability for these parameters is presented in Fig. 1B showing a large variation ranging from zero to one. The total height of each bar in this figure indicates the identifiability of specific parameter. The colour associated with each bar represents the contribution of different Eigen components spreading over the calibration solution space. The identifiability of 0.4 was chosen (arbitrarily) to mark the cut-off between most identifiable and less identifiable parameters. Based on this criteria and conditions suggested by Doherty and Hunt (2009), we found 12 parameters to be identifiable out of total 70 parameters considered.

The identifiability analysis was very useful in both charactcterizing the parameters and the important interactions among them. The germination temperature (*tpgerm*) parameter was the most identifiable followed by number of degree days required to

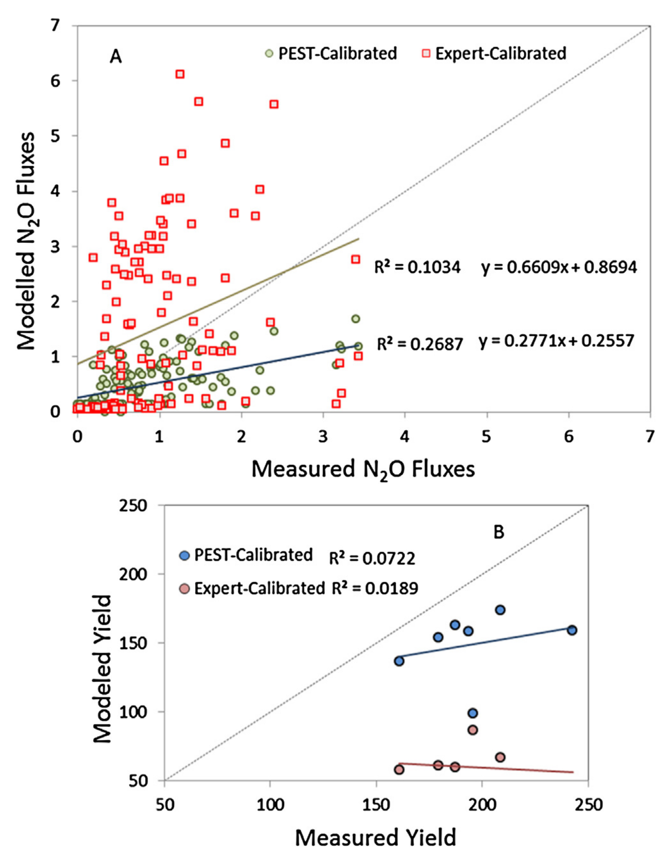

Fig. 2. (A) Scatter plot between measured and simulated N_2O fluxes obtained from Expert-calibrated and PEST-calibrated runs. (B) Scatter plot between measured and simulated corn yield production obtained from Expert-calibrated and PEST-calibrated runs.

trigger a senescence event (*ddbase*), maximum C/N ratio of SOM pool, (*varat12(1_1)*), maximum temperature dependency of plant growth (ppdf(2)) and the water and temperature limitation on nitrification process (*water_temp*). Smaller identifiability values (<0.2) indicate less identifiable and insensitive parameters and vice versa (Doherty, 2010). For comparison, sensitivity analysis showed that all of the 70 parameters are estimable based on the conditions provided. However, the differences between identifiability and sensitivity illustrated in Fig. 1 are mostly due to the parameter correlations (Doherty, 2010). Furthermore, the results of this study indicate that the suggested initial values for most of globally optimal parameters in DayCent were not consistent with their initially proposed values (see Appendix). Among the highly sensitive parameters, most of them showed a large shift from initial suggested values. This convergence of global optimal parameters indicates that the algorithmic calibration proposed here was useful in understanding the behaviour of parameters and interactions among them.

Supplementary material related to this article can be found, in the online version, at http://dx.doi.org/10.1016/j.ecolmodel.2014.11.022.

The algorithmic calibration improved the model's performance (Fig. 2) largely due to the important role of sensitivity and identifiability analysis, consistent with findings of similar studies in hydrology, remote sensing, etc. (Doherty and Hunt, 2009; Hunt et al., 2007). This is also consistent with earlier findings that as PEST integrates the measured data with DayCent and then runs the model iteratively, until minimum residual differences between the observed and estimated values are achieved (Rafique et al., 2013). The optimized values of all parameters along with their initial, and upper and lower bounds are given in appendix to this paper. In general, the modelled N_2O fluxes and corn yield were comparable to the measured data, but on certain occasions tended to over or underestimate the measured values. However, the Expert-Calibrated simulations displayed larger differences between the measured and modelled N_2O fluxes compared to the PEST-Calibrated simulations. After calibration, the SWSR reduced by 79% for N_2O fluxes and 84% (*this is only squared residual as the standard deviation data was not available*) for corn yield production. Similarly, the coefficient of determination was improved by 63% for N_2O fluxes and 72% for corn yield production (Fig. 2). The DayCent model has already been evaluated in several previous studies using manual calibration approaches e.g. Parton et al. (2001) and Jarecki et al. (2008), but in comparison to these and other studies our results proved to be more promising and reproducible based on the statistical criteria/analysis.

The N_2O fluxes displayed an episodic nature with small pulses throughout the year (Fig. 3A). The mean daily N_2O fluxes observed from Expert-Calibrated and PEST-Calibrated simulations were 0.84 and 0.37 g N ha^{-1} d^{-1}, respectively. Expert-Calibrated approach overestimated the total sum of N_2O fluxes by 85% compared to the observed value. In contrast, PEST-Calibrated approach underestimated the total N_2O fluxes by 12%, compared to the observed values, and these were closer to the observed data. The N_2O peaks were more pronounced in Expert-Calibrated simulations as compared to those in PEST-Calibrated results. This pattern was more prominent mostly during the summer. The same trend was also observed for corn yield data. PEST-calibrated results matched better to measured corn yield data compared to the Expert-Calibrated data (Fig. 3B).

The discrepancies between DayCent simulated and observed data have been reported in numerous other studies

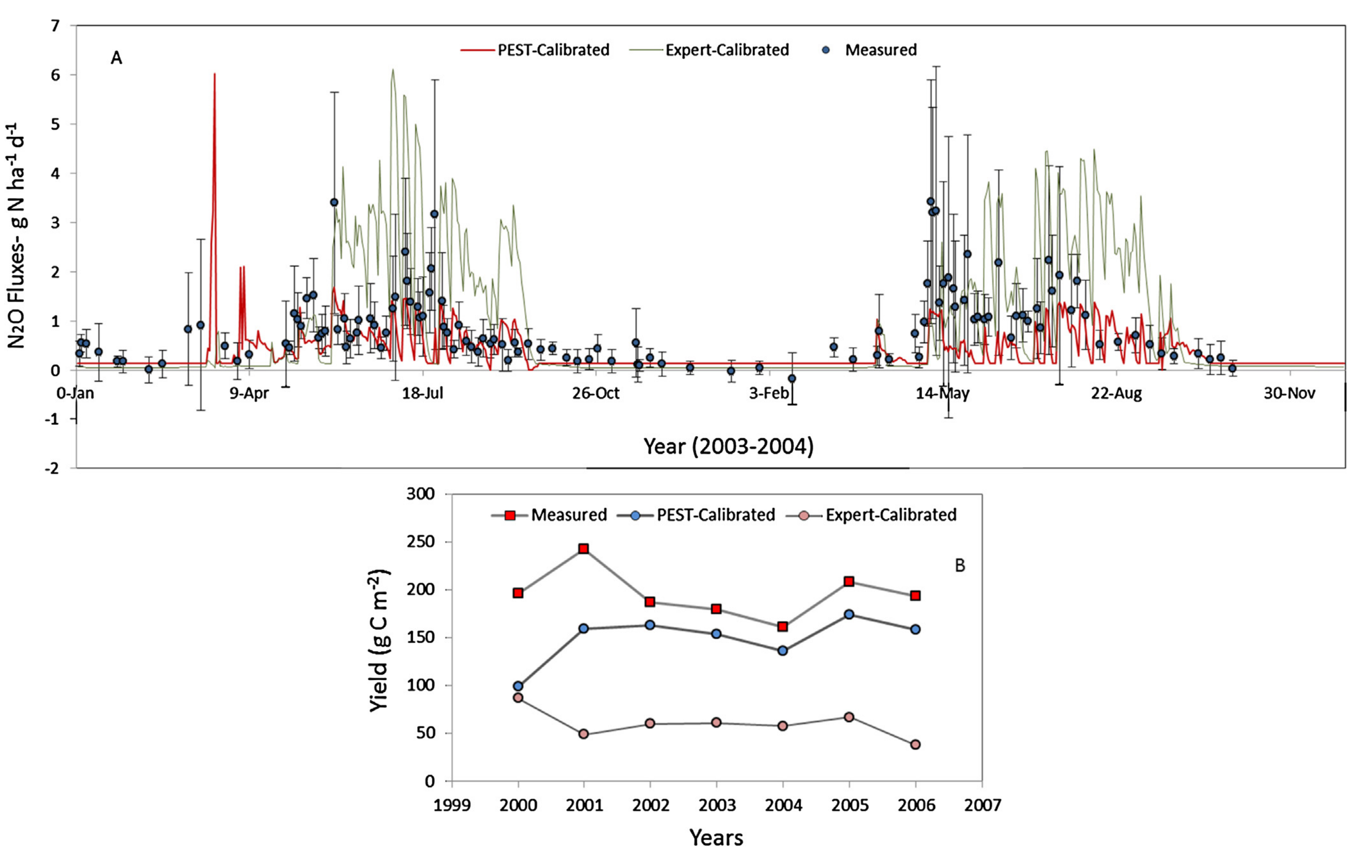

Fig. 3. (A) N_2O flux time series obtained from measured, Expert-calibrated and PEST-calibrated simulation results. (B) Corn yield production time series from measured, Expert-calibrated and PEST-calibrated simulation results.

(Rafique et al., 2014, 2011; Lamers et al., 2007). The variations in the N_2O fluxes can be partially attributed to the inherent temporal and spatial variability caused by the heterogeneous soil properties and spatial distribution of N hot spots (Rafique et al., 2012; Li et al., 2013). The N transformation processes such as nitrification and denitrification in DayCent, have also been criticized because of their over or under estimation of N rates to N_2O fluxes (Del Grosso and Halvorson, 2008). Other factors due to interaction of land management and soil properties can also affect the episodic behaviour of N_2O fluxes (Rafique et al., 2012). These factors have not been accurately presented in DayCent (Rafique et al., 2014). Overall, this study has addressed the importance of algorithmic calibration and provided a better insight to the model and its sensitivity to input parameters, which will be helpful for future modelling studies. The identifiability and sensitivity analysis explain the simulated parameter(s) relationship with the observed data as well as provide further insight for model improvement and calibration.

4. Conclusion

Biogeochemical models are increasingly becoming more complex, due to inclusion of different processes as well as a multitude of parameters describing them. Accurate representation of parameter values is critically important for the robust estimation of model results that are used both for research and ecosystem management purposes. DayCent, is a popular biogeochemical model that is normally calibrated manually by its developers and users, which is quite subjective and depends on expert's knowledge about the model and underlying processes that it represents. In this process often implementation of the algorithmic parameter estimation is usually overlooked. This study indicates that algorithmic calibration improved the performance of DayCent. Based on our proposed algorithmic calibration, the residual differences between simulated and observed values were reduced by 79% in N_2O fluxes and 84% in corn yield production. Similarly, the coefficient of determination between observed and simulated values was improved by 63% in N_2O fluxes and 72% in corn yield. Our study also suggests that the manual calibration results in over estimation of N_2O fluxes and corn yield, hence leads to their inaccurate estimates. The global optimal parameters identified based on our proposed method were largely different compared to their initially proposed values. Furthermore, this study revealed that the germination temperature, degree days and temperature dependency of plant growth parameters could not be well constrained based on given conditions and they need be studied in future.

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