## Chapter 9

# Computer simulations for the study of carbon and nitrogen dynamics and greenhouse gas emissions in agricultural production systems

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**Abstract:** Analytical methods and computer simulators are widely used to quantify the effects of agricultural management systems on soil stocks of carbon (C) and nitrogen (N) and on greenhouse gas (GHG) emission estimates. Century, RothC and EPIC simulators have been widely used in temperate climate regions and, to a lesser extent, in tropical regions, to analyze C and N stock trends in several agroecosystems, given the various scenarios they promote. Due to the complexity of data input, however, other simpler simulators are being tested, such as CQESTR. For example, in Brazil, simulations using Century and CQESTR are continuously growing, probably due to the high accuracy resulting from the validations performed. Applying these computing resources to scenarios for areas under various tillage systems, in the medium and long term, a C stock increase was observed in areas under no-tillage, compared to conventional tillage. There have been reports of successfully obtaining estimates of GHG emissions by agricultural management systems using DayCent, the daily time step version of Century and, especially, DNDC (the DeNitrification-DeComposition model). DNDC has shown reasonable applicability for estimating methane from flooded rice cultivation for sites studied in Brazil. In all these applications, simulators made it possible to identify management strategies having less impact among the scenarios to be investigated after being validated.

**Keywords:** simulator, greenhouse gases, carbon stock, Brazil, DNDC, Century, CQESTR, DayCent.

## Introduction

The study of agroecosystems having greater potential for greenhouse gas emissions may be accompanied by modeling activities based on system simulation. Identifying the main goal of scientific research is the key factor substantially guiding how these tools are used, in both the development phase, to support the decision-making process, and the phase of choosing and correctly using the simulators already available. Thus, the research goal, using mathematical modeling techniques and computer simulation, defines the level of complexity required for the expected response, and the information requirements, in terms of data input, are thus directly proportional to that complexity. There are several options for representing a given study subject, which is why there are generally various models and simulators proposed for representing it, each depending on the body of knowledge of the person who created it. Thus, a model is one of several possible descriptions of the real problem compatible with the goal of the study.

The amount of knowledge regarding the process being modeled or being evaluated by simulation directly influences the quality of the results provided by the tool. Thus, if basic information needed to correctly represent the actual system is lacking, this limits the model's development and further use and cause users to discredit it. Further details on mathematical modeling and computer simulation, including applications in agricultural research, can be found in Pessoa *et al.* (1997) and Pessoa & Scramin (2005).

Computational tools already available for use can be differentiated in terms of work scale and complexity. In this context, work scale is understood as whether the simulation is for a single site, a location, a region, or a broader scope (such as global). The work scale defines both the type of simulator to be used (depending on the detail needed) and the need to integrate these simulators with other computing resources, such as databases, specialized systems and Geographic Information System (GIS).

Simulators of C and N dynamics, in particular, have been used to estimate changes in soil C at a local, regional, national or global scale. The modeling of C, especially on a regional scale, ranges from extremely simple approximations, where empirical relationships are taken and applied to large areas, to complex approximations, where results obtained from evaluating dynamics using simulators are then integrated with georeferenced data, typically using geoprocessing, in order to consider spatial differences in climate, soil and land use. In particular, for approaching C dynamics at a regional scale, with simulators integrated with GISs, there are applications for assessing management systems in diverse environments. In the United States, results obtained by the Century simulator (PARTON *et al.*, 1987) were integrated with meteorological and soil databases generated in a GIS to estimate C sequestration potential for 44% of the country's land area. From this information, it was found that conservation tillage practices and the use of cover crops could be utilized to increase soil C storage for about 40 years (DONIGAN *et al.*, 1994). Applications of the RothC simulator (COLEMAN; JENKINSON, 1996), also associated with a GIS, in areas of natural ecosystems in New Zealand, showed that it is possible to assess impacts of climate change and land use on soil's organic C and $CO_2$ stocks. In this study, it was also estimated that the combined effect of ecosystem degradation and climate change can lead to a significant net release of $CO_2$ for over 40 years of soil cultivation (PARSHOTAM *et al.*, 1995). In Hungary, the C sequestration potential of various management practices was estimated using regression equations and RothC and Century simulators, associated with GIS, and it was found that there were differences between the methods, although estimates were on the same order of magnitude, and some management scenarios presented the same C mitigation potential as areas under reforestation (FALLOON *et al.*, 2002). In Brazil, there are still few studies integrating these simulators with a geographic information system (GIS) to estimate C sequestration or stocks. In Rio Grande do Sul (RS), Century associated with a GIS was used to assess changes in carbon stocks occurring in two municipalities since the adoption of agriculture in 1900, up until 2050. In this study, a significant reduction in C stocks was observed since the introduction of the conventional system of agriculture, and a recovery of these stocks was observed after adoption of conservation practices, such as no-tillage and a complex crop rotation system (TORNQUIST *et al.*, 2009). Soil C simulators, especially Century, EPIC (IZAURRALDE *et al.*, 2006; WILLIAM; RENARD, 1985; WILLIAMS *et al.*, 1989) and RothC, have also been used on a global scale to estimate the distribution of C and N in various land areas, as well as the effects of climate change (considering increases in temperature and $CO_2$) on global soil C stock. In this context, the potential use of DNDC is also noteworthy (LI, 2000; LI *et al.*, 1992) since this simulator represents processes involved in C and N dynamics in the soil, as well as in crop growth, thus making it possible to estimate both C sequestration and NO, $N_2O$, $CH_4$ and $NH_3$ greenhouse gas emissions for agricultural ecosystems (LI, 2007; LI *et al.*,1992, 1994). For this reason, several studies highlight the application of DNDC to environmental conditions observed in various countries, including Australia, Canada, China, India, United States, New Zealand and Japan (BABU *et al.*, 2006; BEHEYDT *et al.*, 2004; GRANT *et al.*, 2004; KIESE *et al.*, 2005; LI, 1996; LI; SAGGAR, 2004; LI *et al.*, 1996; MIEHLE *et al.*, 2006; SAGGAR *et al.*, 2003, 2007; SHIRATO, 2005; SMITH *et al.*, 2002; ZHUANG *et al.*, 2004).

The time scale of simulators is another factor to consider when choosing the tool for the intended application, as it can vary from hours to days, months and even several years. It should be noted, in particular, that the timescale for the application of C dynamics models ranges from short-term daily and seasonal estimates of the amount of C and N in soil (e.g., DNDC) to long-term quantification of soil organic matter stocks and C sequestration (e.g., Century). Two classes of soil C and N dynamics simulators have emerged with different goals but with similar technology: short-term simulators, which aim to predict soil C dynamics over a year or several years in a crop rotation system (e.g., Ceres) and long-term simulators, developed to estimate the status of C in soil throughout decades or centuries (e.g., Century). However, development of more advanced computers and demand for new technologies in agricultural and environmental sciences have enabled both types of simulators to be directed towards a common goal (e.g., DayCent simulator derived from Century) (DEL GROSSO *et al.*, 2001).

Depending on the complexity of the component models, simulators are usually classified as *screening* simulators (also known as reductive or summary simulators), *intermediate* simulators and *research* simulators. Screening simulators provide a preliminary view of the system's behavior, with little detail, as they only use information that is highly relevant for the model representation. However, despite limited output, they have the advantage of requiring a reduced amount of input information to use. Intermediate simulators are situated between screening and research type simulators. They do not present details as meticulously as research simulators, but they incorporate heuristics and empirical data to processes in search of more information than what is offered by screening simulators. In this case the input data is a bit more sophisticated, but on a smaller scale than what is required by models classified as research simulators. Those simulators present rich detailing of mathematically modeled real processes and, therefore, become extremely complex in terms of input data requirements. However, they usually offer the user the option to select specific routines for the intended scenarios, thus decreasing (the extremely demanding) data input requirements. Furthermore, they allow for a more thorough investigation and reliable representation of the real system. DNDC can be mentioned as one of the simulators using models of this type.

The increasing importance of multiple C pools in soil and in plant residue in the late 1970s and early 1980s represented a major change in the direction of research, resulting in a significant increase in the complexity of mathematical models and simulators. This complexity has developed in terms of the processes simulated, the rates estimated for each process, the role of soil microorganisms and the interaction between these processes (SHAFFER *et al.*, 2001). The development of simulators is still mostly done using the FORTRAN, Pascal, C and C++ programming languages, although the use of specific computational package languages, such as Stella, linked to Java language resources, will tend to increase in upcoming years, considering its ability to interact with the internet. Furthermore, the significant increase in computer efficiency has spurred the development of more complex simulators, with the challenge of making them increasingly useful for the needs of its users.

However, depending on the goal of the study, information available from databases or previously conducted research is not always usable in simulators producing estimates on greenhouse gas emissions, since there are environmental conditions (ecological, economic and social) that dramatically impact the management system locally used, and consequently, the results obtained. Additionally, the conditions under which such information was obtained must also be taken into account, as they do not always allow extrapolation for use in other areas or situations, as already pointed out. As an example, there are conditions involving the physical-chemical nature of the soil, where, for example, organic matter content and density may vary for the same type of soil.

Thus, the development of databases – in particular databases that are able to effectively bring together essential information currently scattered throughout Brazil in order to simulate scenarios to estimate greenhouse gas emission – should focus on providing local aspects which have low variability and which are related to specific features of crop varieties (development time in degree days, maximum grain yield, quantity of dry matter, (harvested) grain fraction of total biomass, N fixation index, quantity of C present in various parts of the plant, and grain C/N ratio) and animal breeds (digestibility rates as a function of feed supplied and development stage), as well as daily climate information (maximum and minimum temperature, rainfall, solar radiation, relative humidity and wind speed).

The following is a presentation of more detailed considerations on some of the main simulators for evaluating carbon and nitrogen dynamics applied to the study of greenhouse gases.

# Simulators for the study of C and N dynamics

## Contribution to understanding environmental aspects

Simulators modeling C and N dynamics are important components of ecosystem simulators, which have been intensively used to expand knowledge about the impacts of land use on environmental quality.

### Carbon sequestration and soil quality

Long-term stabilization of soil organic carbon (SOC) content has important implications for sequestration of atmospheric $CO_2$ and maintenance of soil quality. Effects of land use on carbon stabilization can be estimated from changes in SOC content under various management systems and specific soil and climate conditions. Those estimates require data from long-term experiments and are thus restricted to a limited number of locations. Observations obtained from these experiments can be extrapolated to a wider variety of conditions through the use of ecosystem simulators that include transformations of C and N in the soil and in the plant. These simulators, such as Century or RothC, have been used to estimate changes in SOC in areas of pasture, organic and mineral fertilization and crops and tillage systems. Recently, simulators are being used to estimate changes in SOC in management practices as part of regional and national $CO_2$ emission studies.

As a result of changes in SOC representing differences between C inputs due to net primary productivity (NPP) and C losses due to heterotrophic respiration (HR), ecosystem simulators used for estimating C sequestration should be able to estimate the effects of land use on NPP and HR. Simulation of NPP must be clearly distinguished from simulations of phytomass growth, where NPP is represented using various models. NPP is the difference between gross primary production and autotrophic respiration spent on maintenance and growth of phytomass. NPP includes above-ground phytomass – and litter, which is largely in the roots. Accurate simulation of the dynamics of residues above and below ground is thus extremely important in order for a simulator to quantify changes in SOC.

An essential aspect of HR modeling is the rate at which labile C from litter becomes protected from rapid decomposition, thus reducing HR. This rate is typically dependent on the soil's clay content (VEEN; KUIKMAN, 1990) and lignin content (PAUSTIAN *et al.*, 1997), which determine the soil's ability to protect labile C. Therefore, clayey soils show less HR than sandy soils with the same C input. Accurate simulation of the rate at which labile C is protected is essential, as this rate determines soil C sequestration in the medium and long term.

## Greenhouse gas emissions and air quality

As a result of $N_2O$ and $CH_4$ being radiatively active in the atmosphere, there is major interest in estimating the net exchange of these gases between terrestrial ecosystems and the atmosphere as part of climate change studies. Those estimates are important for evaluating management options to reduce emissions of these greenhouse gases, mainly due to national and international agreements to minimize their release into the atmosphere.

Emissions of NO, $N_2O$ and $CH_4$ are highly variable in space and time. Using system simulation techniques to research the environmental impact of greenhouse gases generation and emission processes by agroecosystems involves three main challenges: 1) some of the gases (e.g., NO and $N_2O$) have multiple sources or origins, such as nitrification, denitrification and methanogenesis; 2) all gases are produced and consumed simultaneously in soils, controlled by the kinetics of a series of geochemical and biochemical reactions; and 3) there are a large number of environmental variables controlling biochemical reactions. Therefore, to simulate agroecosystems with potential to generate greenhouse gases, all factors must be considered, including ecological aspects, soil environment variables and biogeochemical reactions (Figure 1).

| CHAP 9 - FIGURE 1 | |
|---|---|
| Reações bioquímicas/geoquímicas | Biochemical/geochemical reactions |
| Fatores ambientais | Environmental factors |
| Variáveis de controle ecológicas | Ecological control variables |
| Produção e consumo de gases-traços no sistema solo-planta | Trace gas production and consumption in the soil-plant system |
| Movimento mecânico | Mechanical movement |
| Dissolução/cristalização | Dissolution/crystallization |
| Combinação/decomposição | Combination/decomposition |
| Oxidação/redução | Oxidation/reduction |
| Adsorção/dessorção | Adsorption/desorption |
| Complexação/decomplexação | Complexation/decomplexation |
| Assimilação/dissimilação | Assimilation/dissimilation |
| Gravidade | Gravity |
| Radiação | Radiation |
| Temperatura | Temperature |

| | |
|---|---|
| Umidade | Humidity |
| Substrato | Substrate |
| Clima | Climate |
| Propriedade do solo | Soil properties |
| Vegetação | Vegetation |
| Atividades antropogénicas | Anthropogenic activities |

**Figure 1.** Variables, factors and reactions involved in production and consumption of trace gases in the soil-plant system contemplated by the DNDC simulator.

Source: Adapted from Li (2000).

The important soil environment variables for simulation are especially associated with temperature, $O_2$ concentration and water content at depth, in addition to readily available C resulting from NPP. Those variables must be related to conditions of the specific site under study, as temporal and spatial emission patterns are highly variable and complex (GRANT, 2001). Consequently, the predictive value of short-term flux measurements for long-term estimates is limited to locations having similar soil and climate conditions.

## Soil management

Land use practices involving soil changes and vegetation removal have caused releases of C into atmosphere. Those releases account for about 1/3 of atmospheric $CO_2$ accumulated since the pre-industrial period and indicate an intense degradation process. Certain practices such as no-tillage, crop rotation, use of legumes and use of mineral and organic fertilizers have been adopted in order to increase C stocks and sequester atmospheric $CO_2$.

Ecosystem simulators have been used to estimate changes in SOC under various management practices and must be able to adequately represent the processes by which these practices affect the SOC. For example, the effect of tillage systems on SOC must be quantified using simulations that take into account the residue on the soil surface with its own microbial population and microclimate (temperature and water content), as contemplated in the Century simulator. These residues must also affect the energy balance on the soil surface and, consequently, the temperature fluxes and subsurface heat. Tillage practices available in simulators must influence the intensity and the depth at which surface residues are incorporated throughout the soil profile. This incorporation increases contact between the residue and the soil's microbial population and microclimate, thus increasing its decomposition rate. Incorporation also reduces the heat flux from the residue, promoting faster heating and cooling processes.

Soil tillage has an additional effect on release of $CO_2$ due to increased contact between soil C and the microbial population, which also eed to be considered in simulators. In some of these tools (LI *et al.*, 1992; MOLINA *et al.*, 1983; PARTON *et al.*, 1987) this effect can be simulated by redistributing part of the C from recalcitrant pools to labile pools (e.g., passive and active pool, respectively, in the Century model). Tillage alters the properties of the soil surface, such as roughness and residue coverage, and also of the subsurface, such as soil density. Such changes are also included in some available simulators (RICKMAN *et al.*, 2001; SHAFFER; LARSON, 1987; WILLIAMS *et al.*, 1989).

To simulate the effects of grasses and perennial legumes versus annual crops on SOC it is necessary to establish differences in C allocation between shoot and root. This allocation is heavily influenced by climate, including radiation, temperature and atmospheric $CO_2$ concentration, and by soil properties, such as water and nitrogen. Ecosystem simulators must therefore estimate the root system's NPP, including root recycling and rhizodeposition, separately from above-ground NPP, in a way that represents local effects on NPP and on allocation of C in roots without the need to calibrate them for a specific location (GRANT, 2001).

## Biogeochemical processes in C and N dynamics simulation

Several tools are used to understand alterations to an ecosystem resulting from land use changes. In this sense, it has been observed that understanding C and N dynamics is essential to improve the quality of simulators in performing accurate predictions of the effects of land use changes and responses to global climate change. Modeling of biogeochemical processes emerged in the 1930s and currently it is systematically addressed by an extensive list of simulators, whether empirical or mechanistic. There are, however, variations in terms of the complexity and mathematical description of the various biological and geochemical processes involved, which are represented in most simulators by primary productivity, mineralization, immobilization and humification. Currently, with the introduction of simulators of greenhouse gas emission dynamics – especially nitrous oxide and methane – nitrification and denitrification processes are also incorporated.

### Primary productivity

Correct representation of processes related to NPP above and below the soil is essential for any simulator aiming to estimate effects of land use and climate change on SOC. NPP is represented at various levels of complexity in various simulators.

Below-ground NPP is a determinant of SOC stocks, as, under certain conditions, up to 40% of the shoot's C can be transferred to the roots (GRANT, 2001). In most simulators, below-ground NPP is represented as a fraction of above-ground NPP, which can be constant (PARTON; RASMUSSEN, 1994) or dependent on phenology (HANSEN *et al.*, 1990). Spatial distribution of below-ground is sometimes represented in these computational tools using a logarithmic function of the soil's depth. This NPP, however, is the largest fraction of above-ground NPP, and its spatial distribution is modified depending on species, perennial or annual, as well on water and nutrient content. In deeper root systems, there are higher rates of C accumulation, often measured in areas under forages and annual crops (BREMER *et al.*, 1994; GRANT, 2001). Therefore, changes in the allocation of C between root and shoot caused by growth habit or soil conditions need to be represented in C dynamics simulators used to estimate changes in SOC (PARTON; RASMUSSEN, 1994). One approach to simulating allocation of C between root and shoot is by using the functional balance hypothesis proposed by Thornley (1995), where transport of C and N occurs as a function of a concentration gradient generated in the plant by C fixation and N uptake versus consumption of C and N in the root and shoot. This hypothesis allows root growth versus shoot growth to adapt to changes in environmental conditions and to be parameterized independently of location-specific root growth data (GRANT, 2001).

### Mineralization and immobilization

Several models use the same approach for HR simulation, i.e., the inclusion of first-order kinetics where metabolic demand of the soil biomass exceeds supply from the substrate. This assumption, however, becomes invalid when the supply from the substrate exceeds the metabolic demand from the biomass. This indicates that, in future development of simulators, a more mechanistic approach to soil microorganisms is essential. The role of these microorganisms is extremely important for C and N dynamics. They respond to environmental changes so dynamically that most simulators cannot produce adequate estimates. Not only do microorganisms compose C and N pools, they also catalyze most processes. It is, therefore, essential to properly simulate their role in the soil environment.

These differences in approaches to microbial decomposition are necessary because C and N transformation rates may be inadequate to the first-order kinetics equation commonly used. An alternative to this equation is one where microbial activity is represented as a C and N transformation agent, using Monod's kinetics (SMITH, 1982):

$$r_i = \mu_m C_i / K_s + C_i * B$$

where $r_i$ is the decomposition rate; $C_i$ is the C content in the pool; $B$ is the size of the microbial biomass; $\mu_m$ is the maximum mineralization rate; and $K_s$ is a constant. For simulators that do not take into account the role of microorganisms, maximum mineralization rate and size of microbial biomass can be combined to adjust to Michaelis-Menten's kinetics. The above equation can be simplified as first-order kinetics ($r_i = k_1 C_i$) or as zero-order kinetics ($r_i = k_0$), in which $k_1$ and $k_0$ are the first- and zero-order coefficients, respectively, which can be modified by temperature, pH, $O_2$ and microbial effects.

The NLEAP simulator (SHAFFER *et al.*, 1991), used to quantify nitrate leaching, takes a relatively simple approach for immobilization and mineralization processes. The net mineralization of N in the plant residues pool depends on its C/N ratio and decomposition rate: $M_r = r_r\,(1 / (C/N)\,r - 1/30)$, where $M_r$ is the net nitrogen mineralization rate in the residues pool; *C/N* is the C-to-N ratio in the residues pool; and $r_r$ is the residues decomposition rate. Once the C/N ratio reaches between 6.5 and 12, depending on the type of residues, the C and N remaining in the residues are transferred to the fast cycling SOC pool. The decomposition rate is calculated by first-order kinetics: $r_r = k_r T_f W_f C_r$, where $k_r$ is the constant rate and can be adjusted based on the C/N ratio; $C_r$ is the C content in the residues; and $T_f$ and $W_f$, are coefficients associated with water and temperature. In RZWQM (AHUJA *et al.*, 2000), which simulates soil water, plant growth and C and N dynamics in the soil, mineralization and immobilization processes are determined by the decomposition of organic pools and the growth of microorganism. There isn't a previously defined C/N ratio to control net mineralization and immobilization, as is the case with the NLEAP simulator. Decomposition of organic matter in each pool is simulated by the first-order equation and modified by the effects of soil temperature, oxygen, heterotrophic aerobic microbial population, aerobic condition and ionic strength.

In Century, surface residues are divided into metabolic and structural pools. The structural pool is subdivided into cellulose and lignin components. The metabolic C and cellulose pools are transferred to the fast cycling C pool (microbial biomass), whereas C bonded to lignin is directly allocated to the slow C pool (PARTON *et al.*, 1994). The fast cycling (active) microbial pool has four destinations during the decomposition process: 1) slow C pool; 2) passive C pool; 3) pool of soluble C which can be leached; and 4) $CO_2$. Decomposition of all pools occurs through first-order kinetics.

The decomposition rate is specific for each pool. For the structural pool, it is expressed by the equation: $k = k_c e^{-3Ls} A_t A_w$, where *Ls* is the lignin content in the structural C pool, $K_c$ is the constant rate, and $A_t$ and $A_W$ are factors related to temperature and water. For the active C pool, the decomposition rate is influenced by soil texture ($T_m$) in the equation $k = kc\, A_W\, A_t\, T_m$, where $Tm = 1 - 0.75\ (F_{silt}+F_{cla})$. For the remaining C pools (metabolic, slow C and passive C), decomposition rates are functions of just $A_t$ and $A_{W.}$

## Humification

Greater C stabilization in soils with high clay content was demonstrated by Sorenson (1981). Since then, soil clay content has been increasingly used in ecosystem simulators to reduce C decomposition and allocate products of that decomposition between pools with different decomposition rates. Verberne *et al.* (1990) divided the products of microbial decomposition into non-protected and protected organic fractions, using, in the case of the latter, coefficients ranging from 0.3 for sandy soils to 0.7 for clayey soils. Veen and Kuikman (1990) and Whitmore *et al.* (1991) suggested that efficiency of substrate use increases with clay stabilization. However, some studies concerning the effect of clay on substrate use have not endorsed this hypothesis (VEEN *et al.*, 1985). Li *et al.* (1992) proposed that decomposition rates of organic substrates, using first-order kinetics, were reduced according to clay content. On the other hand, this hypothesis does not explain the marked increase in recovery of C as amino acid or microbial biomass, in soils with high clay content. It is more likely that microbial products and metabolites, as well as lignin degradation products, are stabilized by clay surfaces. Parton *et al.* (1987) thus adopt lignin content to allocate the products of decomposition of slow and active pools of the model incorporated into Century. Grant (2001) combined some of the products from lignin and protein hydrolysis and carbohydrates, following the stoichiometry proposed by Shulten and Schnitzer (1997), and allocated the resulting compounds in a complex of particulate organic matter, according to soil's clay content. The rates of particulate organic matter formation were therefore a function of the lignin content in the residues, clay and heterotrophic microbial activity. Those rates contributed to long-term changes in the C of the simulated soil, under various management practices, which were corroborated by field measurements (GRANT, 2001).

## Nitrification and denitrification

Nitrification is an important process for controlling N transformations between less ($NH_4^+$) and more ($NH_3$) mobile forms. Accurate representation of nitrification in ecosystem simulators is therefore necessary to simulate losses of N through leaching and denitrification. Nitrification has currently been incorporated into simulators because it is an important cause of $N_2O$ emissions following fertilization. It is influenced, however, by several environmental factors, including substrate concentration ($NH_4^+$ and $CO_2$), aeration, temperature and pH.

In simpler simulators, nitrification rates have been represented by functions of variable orders (zero- and first-order) based on the rates of $NO_3^-$ formation observed in field trials. In more complex simulators, first-order functions based on Michaelis-Mentem kinetics are associated to nitrifying biomass and specific activity. In most simulators, these functions can be modified by those associated with temperature, pH and porosity, which may be dependent upon soil texture.

Some simulators consider that mineralization occurs at a much lower rate than nitrification, so the first inorganic N to be formed is nitrate ($NO_3^-$), instead of ammonium ($NH_4^+$). In addition, they assume that the ammonium fertilizer applied is converted into nitrate immediately, not in the course of several days or weeks, as observed in the field (HANSEN *et al.*, 1995). Century incorporates this assumption. Because it uses a monthly time-step, nitrification does not become important. In fact, the simulator does not differentiate ammonium from nitrate in the soil. DayCent (the daily version of Century) considers nitrification to be proportional to the soil N cycling rate (PARTON *et al.*, 1996). In this simulator, $N_2O$ production resulting from nitrification is calculated both by the N cycling rate and by the excess of $NH_4^+$ in the soil (> 3 µg N $g^{-1}$) as $R_{N2O} = N_{H2O}N_{pH}N_t\ (k_{mx}+N_{mx}N_{NH4})$, in which $R_{N2O}$ is the flux of $N_2O$; $N_{H2O}$, $N_{pH}$ and $N_t$ are factors related to water, pH and temperature, respectively; $k_{mx}$ is the N recycling coefficient; $N_{mx}$ is the maximum flux of $N_2O$ based on the excess of $H_4^+$; and $N_{NH4}$ is the effect of the soil's $NH_4^+$ on nitrification.

Denitrification is an important cause of N loss by gaseous emission, especially $N_2O$. Simulating denitrification is extremely empirical, not only because of the relatively unknown nature of the process itself, but also due to the spatial and temporal variability of the soil's anaerobic conditions. Mathematical simulation of denitrification can also use zero-order kinetics, first-order kinetics or Michaelis-Mentem kinetics. In the DayCent simulator, denitrification is simulated to calculate emissions of $N_2$ and $N_2O$. The total flux of N ($N_2 + N_2O$) is estimated by the following equation: $D_t = \min (F_d\ (NO_3), F_d\ (CO_2))\ F_d(WFP)$, in which $D_t$ is the total gas flux; $F_d(NO_3)$ and $F_d(CO_2)$ are the maximum flux of gaseous N for a given $NO_3^-$ and the soil respiration rate, respectively; and $F_d(WFP)$ is the effect of water on denitrification.

## Simulators for studying C and N dynamics and greenhouse gases

There is a large collection of simulators created by the agriculture and forestry sector to assess the dynamics of C and N and to study greenhouse gas emission (Table 1). Simulators like RothC, Century or EPIC have been widely used to estimate C sequestration in various agroecosystems, mostly in temperate regions, with few studies in tropical environments. However, due to the complexity of the models incorporated into these simulators, several researchers have been motivated to develop simpler models, such as the one available in the CQESTR simulator. Furthermore, the models incorporated into the DNDC and DayCent simulators are capable of estimating $N_2O$ and $CH_4$ emissions for wetlands and flooded rice crops as well.

**Table 1.** Simulators for C and N dynamics and greenhouse gases.

| | **Simulators** | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | **DNDC crop**(1) | **Ceres**(2) | **GePSI**(3) | **RothC**(4) | **Century**(5) | **Ecosys**(6) | **DayCent**(7) | **EPIC**(8) |

| **General Resources** | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Time step | Daily | Daily | Hourly | Monthly | Monthly | Hourly | Daily | Daily |
| Simulation period (years) | 1–102 | 1–10 | 1–10 | 1–102 | 1–102 | 10-1–10 | 1–102 | 1–102 |
| Plant pool | 4 | 4 | 5 | 0 | 3 | >50 | 5 | 3 |
| Organic C pool in the soil | 8 | 4 | 0 | 5 | 8 | ~ 40 | 8 | 8 |
| Inorganic N pool in the soil | 7 | 2 | 2 | 0 | 2 | 1 | 2 | 2 |
| **Processes simulated** | | | | | | | | |
| Soil temperature | X | X | X | X | X | X | X | X |
| Soil moisture | X | X | X | X | X | X | X | X |
| Phenology | X | X | X | | | | | X |
| Leaf area index (LAI) | X | X | X | | | X | | |
| Photosynthesis | X | X | X | | | X | | X |
| Respiration | X | X | X | | | X | | X |
| Rooting process | X | X | X | | | X | | |
| N absorption | X | X | X | | X | X | X | X |
| Effect of water on the crop | X | X | X | | X | X | X | X |
| Effect of N on the crop | X | X | X | | X | X | X | X |
| Effect of $CO_2$ on the crop | X | | X | | | X | | |
| Decomposition | X | X | | X | X | X | X | X |
| $CH_4$ emission | X | | | | | X | X | |
| Mineralization | X | X | X | | X | X | X | X |
| Nitrification | X | | X | | X | | X | X |
| Denitrification | X | | X | | X | | X | X |
| N trace gas emission | X | | | | X | | X | |
| **Output Variables** | | | | | | | | |
| Soil temperature | X | X | X | | X | X | X | X |
| Soil moisture | X | X | X | | X | X | X | X |
| Phenological stages | X | X | X | | | | | |
| Leaf area index (LAI) | X | X | X | | | X | | |
| C pool in the plant | X | X | X | | X | X | X | X |
| N pool in the plant | X | X | X | | X | X | X | X |
| C pool in the soil | X | | | X | X | X | X | X |
| N pool in the soil | X | X | X | | X | X | X | X |
| $CH_4$ emission | X | | | | | X | X | |

|  |  |  |  |  |  |  |  |  |
|---|---|---|---|---|---|---|---|---|
| N trace gas emission | X |  |  |  |  |  | X |  |

## DeNitrification-DeComposition (DNDC)

The DeNitrification-DeComposition (DNDC) simulator (UNIVERSITY OF NEW HAMPSHIRE, 2003) is a process-oriented tool developed by Li *et al.* (1992), initially to simulate C and N dynamics in soil and, thereby, estimate C sequestration as well as emission of NO, $N_2O$, $CH_4$ and $NH_3$ for non-flooded agricultural lands.

It was designed to help understand the effects of anthropic activities on increasing greenhouse gas emission rates, seen as a major factor influencing the balance of atmospheric trace gases. In light of this goal, primary processes controlling interactions between ecological variables, soil environment factors and biogeochemical reactions were incorporated. Subsequently, crop growth aspects were incorporated through use of growth curves (Li *et al.*, 1994), while still not considering the effect of climate changes on crop growth, or the resulting interactions with biogeochemical cycles.

Currently, the simulator allows for estimating greenhouse gas fluxes generated by the world's major agricultural ecosystems through integrating detailed aspects on the production system – such as existence of crop rotations, soil management, use of fertilizer and natural manure, irrigation water management, weed control, among others – with biogeochemical processes of nitrification, denitrification, crop growth, water infiltration into the soil and litter production (BABU *et al.*, 2005; LI, 2000).

The simulator considers ecological variables governing environmental factors relevant in the focus of their development, such as: a) local abiotic factors (maximum and minimum temperature, rainfall and solar radiation); b) physical-chemical aspects associated at various depths the with soil type where the crop develops (soil density, field capacity, wilting point, saturation, pH, etc.); c) specific characteristics of cultivated varieties; d) anthropic activities (crop, soil, water, and fertilizer management). These variables impact the environmental factors resulting from the processes contemplated by the tool, which, in turn, impact the soil climate, the effect of temperature and moisture on decomposition, and decomposition itself.

DNDC can be represented by two major components, as established by Li (2000) (Figure 2). The first component includes the soil climate, plant growth and decomposition submodels, which, in turn, allow for evaluation of trends in the effect of variables related to climate, soil properties, existing vegetation and anthropic activities on soil temperature, moisture, pH, redox potential (Eh) and substrate concentration. Generally, the three submodels interact to present information on the variables in a daily time-step. The soil climate submodel calculates temperatures, moisture, and Eh in the soil profile, based on information on air temperature, rainfall, the soil's thermal and hydraulic properties and oxygen availability. This information is considered along with information on crop characteristics, climate and soil properties and management practices, enabling the evaluation of crop growth aspects and their effects on soil temperatures, moisture, pH, Eh, dissolved organic C and available N concentrations, through the crop growth submodel. The same information is also considered by the decomposition submodel to allow simulating substrate concentrations (dissolved organic carbon, $NH_4^+$ and $NO_3^-$). The mathematical equations used to represent the mathematical models of these components are detailed in Li *et al.* (1992, 1994).

CHAP 9 - FIGURE 2

| Variáveis ecológicas | Ecological variables |
|---|---|
| Climáticas | Climatic |
| Solo | Soil |
| Cultura | Crop |
| Manejos | Management practices |
| T média anual | Mean annual T |
| ET potencial diária | Potencial daily ET |
| IAF regulado albedo | Albedo regulated LAI |
| Evaporação | Evaporation |
| Transpiração | Transpiration |
| Fluxo de água entre camadas | Water flow between layers |
| T solo no perfil | Soil T in the profile |
| Umidade do solo no perfil | Soil moisture in the profile |
| Difusão oxigénio | Oxigen diffusion |
| Eh solo no perfil | Soil Eh in the profile |
| Clima do solo | Soil climate |
| Demanda diária de água | Daily water demand |
| Acúmulo diário de biomassa (IAF) | Daily biomass accumulation (LAI) |
| Absorção de água pela raiz | Water absorption through roots |
| Demanda de N | N demand |
| Grãos | Grains |
| Ramos | Branches |
| Raiz | Roots |
| Estresse de água | Water stress |
| Absorção diária de N pela raiz | Daily absorption of N through roots |
| Respiração da raiz | Root respiration |
| Efeito da temperatura e umidade na decomposição | Effects of temperature and moisture on decomposition |
| Muito solúvel | Very solluble |
| Solúvel | Solluble |
| Resistente | Resistant |
| Microbiano lábil | Labile microbial |
| Microbiano resistente | Resistant microbial |

| | |
|---|---|
| Hematos solúveis | Solluble hemato |
| Hematos resistentes | Resistant hemato |
| Humus passivo | Passive humus |
| Decomposição | Decomposition |
| Variáveis ambientais do solo | Soil environmental variables |
| Temperatura | Temperature |
| Umidade | Moisture |
| Substrato ($NH^{4+}$, $NO^{3-}$ e Carbono Orgânico Dissolvido) | Substrate ($NH^{4+}$, $NO^{3-}$ and Dissolved Organic Carbon) |
| Denitrificação | Denitrification |
| Denitrificador nitrato | Nitrate denitrifier |
| Denitrificador nitrito | Nitrite denitrifier |
| Carbono orgânico dissolvido | Dissolved organic carbon |
| Nitrificação | Nitrification |
| Nitrificadores | Nitrifiers |
| Argila | Clay |
| Fermentação | Fermentation |
| Eh do solo | Soil Eh |
| Aerênquima | Aerenchyma |
| Produção | Production |
| Oxidação | Oxidation |
| Transporte | Transport |

**Figure 2.** DNDC simulator and its components. The first component consists of the soil, climate, plant growth and decomposition submodels; the second consists of the nitrification, denitrification and fermentation submodels.

Source: Li (2000).

The second component of the DNDC conceptual model proposed by Li (2000) is represented by the nitrification, denitrification and fermentation submodels, which allow for estimating fluxes of NO, $N_2O$, $CH_4$ and $NH_3$ generated during simulation of impacts on soil environmental conditions that are relevant to biogeochemical reactions. The factors controlling nitrification in DNDC are: soil temperature, moisture, pH and $NH_4^+$ concentration. The nitrification submodel estimates nitrification rates by following nitrifying activities and $NH_4^+$ concentration. $NH_4^+$ oxidizer growth and mortality rates are calculated based on concentration of dissolved organic C, temperature and moisture. DNDC calculates nitrification induced by production of NO and $N_2O$ as a function of the expected nitrification rate, and based on temperatures (LI, 2000).

The denitrification submodel considers sequential reduction of nitrate into dinitrogen ($N_2$) driven by the presence of denitrifying bacteria under anaerobic conditions (LI, 2000). Thus, in the

DNDC, denitrification rates are controlled by soil moisture and Eh, by temperature and by substrate concentrations (dissolved organic carbon, $NO_3^-$, $NO_2^-$, NO and $N_2O$). The model contemplated by the simulator considers the soil matrix divided into two parts: aerobic and anaerobic, and only the substrate allocated to the anaerobic part is considered for the denitrification effect. The relative growth rate of denitrifiers is described as a multinutrient-dependent growth function. The mortality rate of denitrifiers is a constant fraction of the total denitrifier biomass. The models entered into the simulator also assume that relative growth rates for denitrifiers with various substrates are independent and that bacteria competition occurs via the common substrate of dissolved organic carbon. Substrate consumption rates are calculated using the Pirt equation (LI, 2000). DNDC also allows calculating NO and $N_2O$ diffusion rates in the soil matrix by means of a function which takes into account soil porosity, moisture, temperature and clay content.

In the case of methane ($CH_4$) emission, Li (2000) reports that DNDC takes into account important variables to describe methanogenesis and methanotrophy processes. Methanogenesis occurs by means of the reduction of available C in the soil to $CH_4$ through anaerobic microbial activity, which will necessarily occur when the soil's redox potential (Eh) is at low levels (−150 mV to −200 mV). Additionally, methane production is also strongly influenced by an increase in temperature (with optimal production registered in the 30 °C to 40 °C range). So, to estimate methane ($CH_4$) emission rates, DNDC considers the following variables: carbon content available in soil (i.e., dissolved organic carbon), soil Eh and soil temperature. DNDC also calculates the methane oxidation rate as a function of $CH_4$ concentration in the soil and Eh, as well as diffusion of this gas throughout the soil's layers, as a function of its concentration gradients, and soil porosity and temperature. In addition, the simulator also incorporates estimates on the flux of $CH_4$ carried by plants, as a function of gas concentration and presence of aerenchyma, throughout the cultivation period. In the absence of vegetated soil or of plants with well-developed aerenchyma, DNDC considers the ebullition factor as a source of methane emission, considering that it occurs only on the soil surface layer. Thus, the ebullition rate is evaluated by DNDC as a function of the soil's $CH_4$ concentration, temperature, porosity and the presence of aerenchyma in the plant.

When considering $NH_3$emission, it is known that the concentration of this gas in the soil is governed by chemical reactions in the soil's liquid phase. DNDC calculates liquid $NH_3$ concentration based on $OH^-$ concentrations (depending on soil pH and temperature) and $NH_4^+$ concentrations (provided by the decomposition submodel). Subsequently, $NH_3$ concentration in the soil's gas phase is calculated in proportion to the $NH_3$ concentration found for the liquid phase and the soil temperature. In addition, the simulator assumes that the $NH_3$ fraction emitted daily is related to the soil's air-filled porosity and clay content, due to their effects on the diffusion of $NH_3$. The simulator also incorporates aspects related to the potential for absorption and metabolization of $NH_3$ by plants, since it has been demonstrated that there is a linear relationship between the dry $NH_3$ deposition rate and the $NH_3$ concentration in the air (LI, 2000).

Thus, the concept of N deposition rate can be represented by the ratio of the N absorption rate ($\mu g\ m^{-2}\ s^{-1}$) to the concentration of $NH_3$ in the air ($\mu g\ m^{-3}$), and it ranges from 0.003 $m\ s^{-1}$ to 0.034 $m\ s^{-1}$ for various crops. For this reason, DNDC adopts 0.034 $m\ s^{-1}$ as a default value to calculate the rate of $NH_3$ absorption by crops, although it also considers other factors, such as availability of N in the plant and moisture on the leaf surface (LI, 2000). Further details are available in Li (2000), which notes that DNDC makes it possible to evaluate total N content in the crop for the entire growing season. Upon detecting a decrease in total N content, DNDC reports the reduced part as $NH_3$ flux released from plants.

The fermentation submodel contains equations related to methane and calculates production, oxidation and transport of this gas under submerged conditions. The denitrification submodel calculates production, consumption and diffusion of $N_2O$ and NO during flooding, irrigation or rainfall events; meanwhile, the nitrification submodel also includes functions to estimate $NH_3$ production and volatilization.

DNDC data entry for simulation in local mode requires the following variables:

- Daily temperatures (maximum and minimum).
- Daily rainfall.
- Soil density.
- Soil texture.
- Organic carbon content.
- Soil pH.
- Management practices: crop type, rotation, no-tillage or conventional tillage, fertilization, incorporation of organic manure, irrigation, flooding, pasture and weeds.

Based on the input data, DNDC first calculates soil temperature, moisture, Eh, pH and substrate concentration, on a daily basis, and then uses environmental variables in the nitrification, denitrification, $CH_4$ production/oxidation submodels and in other relevant biogeochemical reactions to present daily estimates of NO, $N_2O$, $CH_4$ and $NH_3$. The soil climate and denitrification submodels run on an hourly time step, unlike the others, which run on a daily time step.

To use the simulator in regional mode, Li (2000) mentions that there is also a need for information previously scanned into databases (data planes) made available in a georeferenced information system (GIS), to allow for spatio-temporal assessment of gas emissions at a regional scale (LI *et al.*, 1996).

What differentiates the DNDC simulator is the ability to create management scenarios, both current and future, which allow for estimating greenhouse gas emissions from agricultural sources resulting from the practices reported. Therefore, provided that it is supported by previous stages of validating the simulator for the Brazilian environment, at the end of the simulated period it provides information that allows for a view of the direct effect of adopted practices on current emissions, as well as proposing management practices combining mitigation with productivity.

## CQESTR

CQESTR is a simulator that has been calibrated and validated for temperate regions and that allows evaluating effects of management practices on carbon stocks (RICKMAN *et al.*, 2001) (Figure 3). The model included in the tool estimates additions of C originating from crop residues, and losses of C resulting from microbial oxidation. In nature, residues added to the soil are decomposed and slowly incorporated into soil organic matter (SOM). In the CQESTR simulator, the period associated with this transformation is approximately four years, obtained from calibrations of the simulator with long-term soil C data.

| CHAP 9 - FIGURE 3 | |
|---|---|
| Resíduos da planta | Plant residues |

| | |
|---|---|
| Decomposição | Decomposition |
| Fase | Stage |
| Resíduo superfície | Surface residues |
| Preparo do solo | Soil preparation |
| Resíduo incorporado (Camadas 1,…n) | Incorporated residue (layers 1,…n) |
| Resíduo na raiz (Camadas 1,…n) | Residue on roots (layers 1,…n) |
| Transição | Transition |
| Matéria orgânica do solo (Camadas 1,…n) | Soil organic matter (layers 1,…n) |

**Figure 3.** CQESTR simulator and its components.

Source: Rickman *et al.* (2001).

To estimate total C stocks (*CT*), CQESTR considers, for a daily time step and for multiple layers, the unit of weight of crop residues per unit of area within each layer: $CT = (COM - DOM) + (CR - DR) + (CA - DA)$. *COM* is the amount of organic matter present in the soil at a given initial point, to which organic matter in the form of crop residues (*CR*) or organic amendments (*CA*) are added. Soil carbon is lost through daily decomposition of the organic matter (*DOM*), decomposition of crop residues (*DR*) and decomposition of organic amendments (*DA*). The net gain or loss of *COM* is determined by the cumulative daily loss (*DOM*) and the periodical contributions (in the simulator) due to $CR - DR$ and $CA - DA$. *CT* is a dynamic value, varying with monthly additions of residues and daily losses through decomposition. The organic matter in the soil, *COM*, is a relatively static variable. The daily amounts to be decomposed (*DR* and *DA*) are small, but ever-present, and both $CR - DR$ and $CA - DA$ are small after the four year composting period used in the simulator.

In CQESTR, the decomposition equation contains a decomposition rate k, the quantity of heat accumulated (in cumulative degree days, CDD), and four terms related to residues or environment, which modify the decomposition rate. These terms include a factor of nitrogen content in the residue (*fN*), a water factor (*fW*), a soil texture factor (*fX*) and a biomass factor (*fB*). The term fN provides different decomposition rates for residues rich and poor in nitrogen. The value for fW is determined by the location of the residue, incorporated or on the surface of the soil and by the presence or absence of crops in growth stage. The texture factor is not yet functional in the current version of the simulator. Its value varies between 0 and 1, depending on the impact of clay and sand contents, as advocated by Parton *et al.* (1987). The biomass factor differentiates fresh residues, roots, decomposed material and native soil organic matter. Values for *fB* were determined by calibration with long-term observations of SOM, obtained at the USDA Research Center, Oregon. The remaining residue stock (in units of weight of residue per unit of area) is computed through the addition to each layer from the initial amount of residue (Ri) and amount of heat accumulated at the time of the addition of the residue to the soil:

$$Rr = Ri * exp\,(k * fN * fW * fX * fB * CDD)$$

where *exp* is an exponential function.

CQESTR is considered a simple simulator, primarily due to the lesser number of input variables required for its use. The main input variables are initial SOM content, bulk density, textural class, N content in crop residues and mean monthly temperatures and rainfall.

### Century – DayCent

Century incorporates a mechanistic model to simulate, in the long term (10,000 years), the dynamics of soil organic matter (SOM) and nutrients in the soil-plant system. Thus, it makes it possible to evaluate the impact of various management practices on C and N dynamics, as well as P and S dynamics. The Century simulator is composed of several submodels: the submodel for soil organic matter dynamics, the water submodel and the plant production submodel. The water and plant production submodels include most of the variables (soil temperature and moisture, nutrient uptake by plants and quantity and quality of plant residues) required for the SOM dynamics submodel. The simulator runs on a square-meter scale and simulates the 0 cm to 20 cm surface layer, using a monthly time step. The main input variables are: mean, minimum and maximum monthly air temperature, monthly rainfall, soil texture (sand, silt and clay content), nitrogen content, plant material lignin content, N intake from the atmosphere and soil and initial contents of C and N in various pools of the soil.

Century includes three SOM pools (active, slow and passive), with different decomposition rates, plant residue pools above and below the soil and a surface microbial pool (Figure 4). Plant residues are divided into: surface – comprising shoot residues; and soil – comprising root system residues. These fractions are partitioned into two pools: structural, which presents a recycling time of 1 to 5 years; and metabolic, immediately decomposed by microbial action, with a recycling time from 0.1 to 1 year. The partitioning into these pools is done in accordance with the tissues' lignin-to-nitrogen ratio (L/N). As the ratio increases, most of the residue is allocated to the structural pool. The SOM is divided into three pools: active – consisting of soil microbial biomass and its products, easy decomposable and with short recycling time (1-5 years) depending on environment and sand content; slow – derived from resistant plant material (lignin) and from chemically and physically protected OM, with an intermediate recycling time (20 to 40 years); and passive – material very resistant to decomposition, being chemically recalcitrant and physically protected, with long recycling time (200 to 500 years).

| CHAP 9 - FIGURE 4 | |
|---|---|
| Parte aérea | Above-ground part |
| Estrutural Lignina \| Celulose | Structural Lignin \| Cellulose |
| Metabólico | Metabolic |
| Microbiano da superfície | Surface microbial |
| Parte raiz | Root |
| Ativo | Active |
| Lento | Slow |
| Lixiviado | Leachate |
| Passivo | Passive |

| | |
|---|---|
| L/N = Lignina / Nitrogénio | L/N = Lignin / Nitrogen |
| A= Fator de decomposição abiótico | A= Abiotic decomposition factor |
| T= Teor silte + argila | T= Sand + clay content |
| $T_s$= Teor de areia | $T_s$= Sand content |
| $T_c$= Teor de argila | $T_c$= Clay content |
| $L_s$= Fração do carbono estrutural que é lignin | $L_s$= Fraction of structural carbon that is lignin |
| Água lixiviada na camada abaixo de 30 cm | Leachate water in layer below 30 cm |
| Taxa de decomposição maxima (ano$^{-1}$) | Maximum decomposition rate (year$^{-1}$) |
| Fração do resíduo metabólico | Metabolic residue fraction |
| Taxa de decomposição do carbono (ano$^{-1}$) | Carbon decomposition rate (year$^{-1}$) |

**Figure 4.** Century simulator pools and fluxes.

Source: Parton *et al.* (1987).

DayCent is the daily version of the Century simulator and it estimates C and N fluxes between the atmosphere, vegetation and soils. The Century simulator operates on a monthly time step because this degree of resolution is suitable for simulating medium- and long-term changes (10–100 years) in SOM, plant production and other ecosystem variables, in response to changes in climate, land use and concentration of atmospheric $CO_2$. Simulations of gas fluxes, however, require a shorter time scale, as the majority of total gas flux resulting from short-term rainfall or irrigation and the processes resulting in emission of these gases are constantly responding to changes in soil water content in a non-linear way.

Submodels for plant production, residue decomposition and soil organic matter, in addition to soil water, temperature dynamics and trace gas fluxes, are included in the DayCent simulator (Figure 5). Plant growth is controlled by nutrient availability, water and temperature. Carbon and nutrients are allocated to leaves, stem and root biomass, depending on the type of vegetation. Transfer of C and nutrients from dead material to SOM pools and transfer of available nutrients is controlled by material's lignin content and C/N ratio, decomposition factors related to water and temperature, and soil texture. Maximum and minimum temperatures and daily rainfall, description of management practices and soil texture data are required as input variables. Recent modifications made to DayCent have included effects of solar radiation on plant growth (DEL GROSSO *et al.*, 2002). Comparisons of the simulator's results with measured data have shown that the model adequately simulates crop production, SOM stocks and trace gas fluxes for various native and managed systems (DEL GROSSO *et al.*, 2002, 2005).

| **CHAP 9 - FIGURE 5** | |
|---|---|
| Absorção N | N absorption |
| Componentes da Planta | Plant components |

| | |
|---|---|
| Folhas | Leaves |
| Raízes finas | Fine roots |
| Galhos | Twigs |
| Tronco | Trunk |
| Raízes grossas | Thick roots |
| N entrada | N intake |
| morte | death |
| Material da planta morto | Dead plant material |
| Estrutural | Structural |
| Metabólico | Metabolic |
| MOS | SOM |
| Ativo | Active |
| Lento | Slow |
| Passivo | Passive |

**Figure 5.** DayCent simulator and its components.

Source: Del Grosso *et al.* (2001).

In DayCent, the submodel for gaseous N simulates emissions of $N_2O$, NOx and $N_2$ originating from the soil and resulting from nitrification and denitrification processes (Figure 6). The simulator assumes that release of gaseous N from the soil due to nitrification is proportional to nitrification rates and that these rates are controlled by $NH_4^+$ concentration, water content, temperature, pH and texture. Nitrification is limited by water stress on microbial activity when the amount of pore space occupied by water (PSOW) is low, and by $O_2$ availability when this amount is high. Nitrification peaks occur when soil water content is approximately 50% of PSOW. Nitrification is not limited when pH is greater than 7, but it decreases exponentially as pH drops below 7, due to acidity. The denitrification submodel first calculates the total flux of gaseous N from denitrification ($N_2 + N_2O$) and then uses a $N_2 / N_2O$ ratio to estimate $N_2O$ and $N_2$ emissions of. Denitrification is controlled by availability of labile C (electron donor), concentration of $NO_3^-$ in the soil (electron acceptor) and $O_2$ availability.

| CHAP 9 - FIGURE 6 | |
|---|---|
| Nitrificação | Nitrification |
| solo | soil |
| Textura | Texture |
| Desnitrificação | Denitrification |

**Figure 6.** Nitrogen gas flux in the DayCent submodel.

Source: Del Grosso *et al.* (2001).

# Application of DNDC, Century and CQESTR simulators to estimate greenhouse gas emissions

## Using DNDC to estimate methane emissions from flood-irrigated rice cultivation in a Gleysol in Pindamonhangaba, São Paulo (SP)

Rice cultivation in a flood-irrigated planting system is a source of methane emissions ($CH_4$). Anaerobic decomposition of organic matter in rice fields under this cultivation system produces methane that escapes into the atmosphere, initially by diffusion-controlled transport, through aerenchyma of rice plants during the growing season.

These emissions also depend on climate factors, plant varieties used and types of soil where they are grown (where soil physical-chemical factors and management factors are also important), as well as on organic matter added, fertilizers applied and especially water management (ALBRITTON; MEIRA FILHO, 2001; BABU *et al.*, 2005; EGGLESTON *et al.*, 2007; LI; FENG, 2002; LI *et al.*, 2004; LIMA *et al.*, 2001; YAN *et al.*, 2005). Therefore, local practices and climate aspects of the crop environment must be considered concurrently when evaluating factors that contribute to methane emissions during crop development under flooding conditions (LIMA *et al.*, 1999, 2003, 2006).

Embrapa Environment, under the Agrogases and Carboagro projects, conducted studies aimed at generating scenarios in the DeNitrification-DeComposition (DNDC) simulator to represent the irrigated rice crop management system in a cultivation area located in Pindamonhangaba, São Paulo (SP). This work was done in order to allow  using simulation to evaluate trends in effects of management practices adopted in a continuous rice flooding regime on seasonal methane emissions, as well as variations in daily rates of seasonal methane emissions over various crop cycles. Version 8.9 of DNDC (of June 2006) was used with simulator input data including information gathered in the field combined with other data from laboratory tests on these experiments, conducted by Embrapa Environment in an area of the São Paulo State Agribusiness Technology Agency (APTA) [*Agência Paulista de Tecnologia dos Agronegócios*] / Paraíba Valley Regional Agribusiness Technology Development Hub (PRDTA Vale do Paraíba) [*Pólo Regional de Desenvolvimento Tecnológico do Vale do Paraíba*], in the 2003–2004, 2004–2005 and 2005–2006 harvests in Pindamonhangaba, São Paulo (SP).

The most important data on these crops used for the purpose of the simulations conducted is presented in summary form in Table 2. Additional information used included local environmental factors measured daily (maximum and minimum temperature, rainfall, solar radiation), as well as crop management and irrigation water and physical-chemical characteristics of the soil (classified as a Gleysol with clayey to loamy-clayey texture). Daily climate data was provided by the APTA / PRDTA Vale do Paraíba Experimental Station and the organizing of information, as well as treatments and conversions of resulting values were performed using Microsoft Excel and SAS.

Specific aspects of rice variety IAC-103, available in a publication on the cultivar by Agronomical Institute of Campinas / São Paulo Agency of Agribusiness Technology (IAC/APTA) [*Instituto Agronômico de Campinas / Agência Paulista de Tecnologia dos Agronegócios*], were incorporated into the simulator database. This variety was chosen because it was one of the most widely used in the region during the period studied. For each harvest evaluated, a specific scenario was created in DNDC, considering the information presented in Table 2. At the end of the simulated period, the estimated seasonal methane emission was compared to that observed in the field.

**Table 2.** Management and climate factors for harvests of flooded rice evaluated at Pindamonhangaba, São Paulo (SP).

| Harvest | Sowing and harvest dates | Fertilizer application (urea) | Flooding period considered |
|---|---|---|---|
| 2004 | Dec. 5 and Apr. 14 | Feb. 3 (30 kg)<br>Mar. 1 (30 kg)<br>Mar. 14 (30 kg) | Jan. 1 to Apr. 10 |
| 2005 | Dec. 6 and May 9 | Jan. 10 (33 kg)<br>Feb. 14 (33 kg) | Dec. 22 to Apr. 20 |
| 2006 | Dec. 17 and May 5 | Jan. 27 (40 kg)<br>Feb. 14 (40 kg)<br>Mar. 8 (40 kg) | Jan. 2 to Apr. 11 |

As a reference standard for generated emissions, both for quantified local information and information estimated by DNDC, the default emission factor provided by the Intergovernmental Panel on Climate Change (IPCC) was used for flooded rice systems under a continuous water regime and without addition of organic fertilizer, obtained by Yan *et al.* (2005) for the IPCC in 2006, of 1.3 kg $CH_4$ $ha^{-1}$ $day^{-1}$ (0.80 – 2.20 error limit).

The first considerations focusing on studying the DNDC software and its requirements in order to applied in this environment were presented by Plec *et al.* (2007) and later evolved to include more reliable field data, carefully entered into the simulator, This made it possible to present considerations focusing on using the DNDC simulator in flooded rice production systems in local mode (Pindamonhangaba, São Paulo (SP)), and on aspects related to validating it for the Brazilian environment. Analysis of results provided by DNDC also made it possible to identify aspects management practices which contributed to increase methane emission rates throughout the harvests analyzed.

For the 2003–2004 harvest, DNDC estimated seasonal methane emissions of 20,560.87 mg $CH_4$ $m^{-2}$, whereas the measured value of gas collections made in the field for that same period was 8,923.02 mg $CH_4$ $m^{-2}$ ± 1,048.52 mg $CH_4$ $m^{-2}$. Considering the 101-day flooding period, it was found that the simulated value was about 2.04 kg $CH_4$ $ha^{-1}$ $day^{-1}$, whereas the observed value was 0.88 kg $CH_4$ $ha^{-1}$ $day^{-1}$ and, therefore, both are within the limit error range reported by Yan *et al.* (2005). It was found that, in this harvest, the simulator overestimated seasonal emissions by 130.42% compared to the quantified value. For the 2004–2005 harvest, the DNDC estimate was 18,765.22 mg $CH_4$ $m^{-2}$ whereas the measured value of gas collections made in the field for that same period was 18,906.13 mg $CH_4$ $m^{-2}$ ± 2,384.47 mg $CH_4$ $m^{-2}$. It was observed that the simulated value was about 1.56 kg $CH_4$ $ha^{-1}$ $day^{-1}$ whereas the observed value was 1.58 kg $CH_4$ $ha^{-1}$ $day^{-1}$ for that harvest, considering the flooding period of 120 days, both within the limits reported by Yan *et al.* (2005). In this harvest, DNDC underestimated the seasonal emission potential by 0.77%.

Meanwhile, for the 2005–2006 season the seasonal gas emission estimate simulated by DNDC was 11,578.26 mg $CH_4$ $m^{-2}$, whereas the value of quantified samples collected in the field for the same period was 16,631.45 mg $CH_4$ $m^{-2}$ ± 2,328.51 mg $CH_4$ $m^{-2}$. Thus, considering the 100-day flood period of this harvest, it was observed that the simulated value was 1.16 kg $CH_4$ $ha^{-1}$ $day^{-1}$, whereas the observed value was 1.66 kg $CH_4$ $ha^{-1}$ $day^{-1}$ for this harvest, and therefore, also both within the limits reported by Yan *et al.* (2005). In the case of this harvest (2005–2006), DNDC underestimated the seasonal emission potential by 30.38%. Generally, it was found that DNDC reflects seasonal emissions within expected international reference limits for irrigated rice cultivation, as it also presented them in the DNDC-to-quantified ratios of 2.30, 0.99 and 0.70, respectively for the harvests of 2003–2004 (year 2004), 2004–2005 (year 2005) and 2005–2006 (year 2006) (Figure 7). The DNDC-to-quantified ratio observed for 2004 can be justified as a result of necessary adjustments to the collection and transport method used for quantifying field gases, as the value of quantified emissions for that year was well below the values observed in measurements recorded for the following harvests.

| CHAP 9 - FIGURE 7 | |
|---|---|
| Emissão de metano | Methane emission |
| Ano | Year |
| Quantificdo | Quantified |

**Figure 7.** Comparison between estimates of seasonal methane emissions quantified (observed in the field) and estimated by DNDC for flooded rice harvests in Pindamonhangaba, São Paulo (SP).

Source: Pessoa *et al.* (2010).

It was also found that the simulator constitutes a potential tool for identifying management strategies having fewer impacts in terms of seasonal methane emissions. There is also an intention to carry out sensitivity tests on DNDC, since there are variations in climate and in aspects related to carbon content, bulk density and soil nitrogen that should be further investigated in order to explain the variations observed. Thus, new quantification studies, being conducted under the Carboagro project, address a more detailed tracking of parameters potentially related to methane fluxes emitted during the crop growing season. They also contemplate activities aiming to assess the behavior of the DNDC simulator in other major areas of flooded rice production in Brazil, such as those found in Santa Catarina (SC), which will be critical to present increasingly reliable results. These results will also contribute to preparing estimates of greenhouse gas emission factors as part of reference reports for nationwide greenhouse gas emission inventories.

## Use of Century and CQESTR to estimate carbon emissions in Latosols [US: Oxisols] under conventional tillage and no-tillage with soybean and maize cultivations in Viçosa, Minas Gerais (MG), and Baixa Grande do Ribeiro, Piauí (PI)

In Brazil, excessive soil tillage has favored emergence of erosion and compaction processes, and medium- and long-term physical, chemical and biological degradation of the soil. It has also increased biological oxidation of organic carbon into $CO_2$, through increased microbial activity due to increased soil aeration, and increased contact between soil and plant residue. This has resulted in more favorable conditions for decomposition and increased exposure of carbon protected in soil aggregates to microbial attack, causing decreased organic matter stocks and, consequently, increased $CO_2$ concentration in the atmosphere. These factors, in isolation or in combination, have contributed to decrease crop productivity and create an unbalanced environment. Therefore, in recent years, adoption of no-tillage has been encouraged, as it is premised on sustainability of the production process, maintaining or restoring organic matter stocks by avoiding soil movements and incorporating residues, which ensures a lower decomposition rate (LEITE *et al.*, 2003; ROSCOE, 2006). Despite these benefits, studies using simulators have shown that no-tillage, when not associated with other practices, such as inclusion of cover crops with significant biomass yield, may, in the long run, fail to increase C stocks.

In an Red-Yellow Argisol [Argisol = US: Ultisol], in Viçosa, Minas Gerais (MG), the Century simulator estimated the dynamics of total organic carbon (TOC) and its pools, since the cutting of the Atlantic Forest in 1930, and subsequent adoption of conventional agriculture, up until the experiment period (1984–2000), with application of treatments (no-tillage, disc plow, heavy harrow + disc plow and heavy harrow), and extending to the year 2050 (LEITE *et al.*, 2004). In all systems, including no-tillage, cultivated with a maize – beans succession, there was a decrease in simulated C stocks, which indicated the need for changes in management strategies, such as inclusion of cover crops with high inputs of residues (Figure 8). In the same study, the CQESTR simulator also estimated, for all systems, decreases in TOC stocks (LEITE *et al.*, 2009) (Figure 9A).

| CHAP 9 - FIGURE 8 | |
|---|---|
| COT | TOC |
| C ativo | Active C |
| C Lento | Slow C |
| C passivo | Passive C |
| Ano | Year |
| PD | NT |
| AD | DP |
| GPAD | HH+DP |
| GP | HH |
| Período anterior ao experimento | Period before the experiment |
| Início do experimento | Beginning of experiment |

**Figure 8.** Century simulation of the dynamics of total organic carbon (TOC) and carbon pools (C) in a Red-Yellow Argisol [Argisol = US: Ultisol], in Viçosa, Minas Gerais (MG). NT: no-tillage; DP: disc plow; HH+DP: heavy harrow + disc plow; HH: heavy harrow.

Source: Leite *et al.* (2004).

In Baixa Grande do Ribeiro, in the Cerrado of Piauí (PI), in a Red-Yellow Latosol [Latosol = US: Oxisols; Red-Yellow Latosol = US: Rhodic/Xanthic Haplustox] cultivated with soybean – maize, the CQESTR simulator also evaluated the impact of replacing the native Cerrado forest (1988) with a conventional tillage system (1988–1996) and with reduced tillage and no-tillage systems (1996–2033). CQESTR estimated a decrease in TOC stocks after conversion of native forests into agroecosystems, and this reduction was maintained, even with the subsequent adoption of no-tillage. The amount of residues added via cover crops (second-crop corn, 4 Mg ha$^{-1}$) was not sufficient to produce increases in TOC stocks (LEITE *et al.*, 2009) (Figure 9B).

| CHAP 9 - FIGURE 9 | |
|---|---|
| COT | TOC |
| Ano | Year |
| PD | NT |
| PC | CT |
| PR | RT |
| PR1 | RT1 |
| PR2 | RT2 |
| Início do experimento | Beginning of experiment |

**Figure 9.** CQESTR simulation of the dynamics of total organic carbon (TOC) in a Red-Yellow Argisol [Argisol = US: Ultisol] (Viçosa, Minas Gerais (MG)) (A); and a Red-Yellow Latosol [Latosol = US: Oxisol; Red-Yellow Latosol = US: Rhodic/Xanthic Haplustox] (Baixa Grande do Ribeiro, Piauí (PI)) (B). NT: no-tillage; RT1: reduced tillage with disc plow; RT2: reduced tillage with heavy harrow; CT: conventional tillage with disc plow and heavy harrow; RT: reduced tillage with heavy harrow.

Source: Leite *et al.* (2009).

**Table 3.** Carbon (C-$CO_2$) emission estimated by the CQESTR simulator and from values measured in a Red-Yellow Argisol [Argisol = US: Ultisol] (AVA) in Viçosa, Minas Gerais (MG) and a Red-Yellow Latosol (LVA) [Latosol = US: Oxisol; Red-Yellow Latosol = US: Rhodic/Xanthic Haplustox] (LVA) in Baixa Grande do Ribeiro, Piauí (PI), under various tillage systems.

| **Tillage system** | **C stock** | | | **Rate**$^{(1)}$ | **Sequestration(+) Emission (-) of C** |
|---|---|---|---|---|---|
| | **Initial** | **Final** | **Variation Δ** | | |
| | **Mg ha$^{-1}$** | | | **Mg ha$^{-1}$ year$^{-1}$** | |
| | **AVA (Viçosa)** | | | | |

|  |  |  |  |  |  |
|---|---|---|---|---|---|
| CQESTR |  |  |  |  |  |
| NT | 43.4 | 34.79 | −8.60 | −0.53 | −0.36 |
| RT1 | 43.4 | 28.45 | −14.94 | −0.93 | −0.96 |
| CT | 43.4 | 27.18 | −16.21 | −1.01 | −1.05 |
| RT2 | 43.4 | 28.80 | −14.59 | −0.91 | −0.94 |
| Measured |  |  |  |  |  |
| NT | 44.0 | 38.54 | −5.46 | −0.34 | −0.17 |
| RT1 | 44.0 | 31.23 | −12.77 | −0.79 | −0.82 |
| CT | 44.0 | 30.90 | −13.10 | −0.82 | −0.86 |
| RT2 | 44.0 | 31.24 | −12.76 | −0.79 | −0.82 |
|  | **LVA (Baixa Grande do Ribeiro)** |  |  |  |  |
| CQESTR |  |  |  |  |  |
| NT | 42.7 | 36.07 | −6.63 | −0.51 | −0.30 |
| CT | 42.7 | 32.53 | −10.17 | −0.78 | −0.82 |
| RT | 42.7 | 33.75 | −8.95 | −0.69 | −0.72 |
| Measured |  |  |  |  |  |
| NT | 45.1 | 40.68 | −4.42 | −0.34 | −0.14 |
| CT | 45.1 | 34.72 | −10.38 | −0.80 | −0.84 |
| RT | 45.1 | 35.76 | −9.34 | −0.72 | −0.75 |

Note: NT: no-tillage; RT1: reduced tillage with plow; CT: conventional tillage; RT2: reduced tillage with harrow; RT: reduced tillage with harrow.

(1) A contribution of 6 Mg ha$^{-1}$ from cover crop (0.17 Mg ha$^{-1}$ year$^{-1}$ and 0.20 Mg ha$^{-1}$ year$^{-1}$ for AVA and LVA, respectively, considering 45% as C) (SALTON *et al.*, 2005) was assumed for the no-tillage system. C emissions (0.045 Mg ha$^{-1}$ year$^{-1}$ and 0.031 Mg ha$^{-1}$ year$^{-1}$, for conventional tillage and reduced tillage, respectively) were included to represent additional fuel use (DIECKOW *et al.*, 2004).

Source: Leite *et al.* (2009).

For the studies in Viçosa and Baixa Grande do Ribeiro, CQESTR estimated the emission of C (C-$CO_2$) into the atmosphere. In Viçosa, emissions were 0.36 Mg C ha$^{-1}$ year$^{-1}$ and 1.05 Mg C ha$^{-1}$ year$^{-1}$ under no-tillage and conventional tillage, respectively. The estimate using measured values also indicated C emission for all systems, although of smaller magnitude (LEITE *et al.*, 2009) (Table 3). These estimates differ from those reported in most studies where there is C sequestration under no-tillage. The difference can be attributed to the method used to calculate the estimates. In this study, C stocks at the beginning of the experiment, i.e., at time zero, were used as reference in order to verify the real contribution of no-tillage, whereas in other studies the reference values were those observed in conventional tillage. If that had been the case, there would be sequestration of C in the no-tillage system, on the order of 0.47 Mg ha$^{-1}$ year$^{-1}$ (simulated) and 0.48 Mg ha$^{-1}$ year$^{-1}$ (measured), which would be consistent with the values observed by other authors for the same type of soil (0.52 Mg ha$^{-1}$ year$^{-1}$) (LOVATO *et al.*, 2004). In Baixa Grande do Ribeiro, emissions of C were also observed. The values ranged from 0.30 Mg ha$^{-1}$ year$^{-1}$ (no-tillage) to 0.82 Mg ha$^{-1}$ year$^{-1}$ (conventional tillage) estimated by CQESTR, and from 0.14 Mg ha$^{-1}$ year$^{-1}$ (NT) to

0.84 Mg ha$^{-1}$ year$^{-1}$ (CT) calculated using measured values (Table 3). However, taking TOC stocks in conventional tillage as reference, the no-tillage system presented a C sequestration rate of 0.18 Mg ha$^{-1}$ year$^{-1}$ to 0.38 Mg ha$^{-1}$ year$^{-1}$ for measured and simulated values, respectively.

## Comparison of simulation of carbon dynamics by Century in CQESTR in Latosols [US: Oxisols] under conventional tillage and no-tillage

In an analysis of CQESTR and Century simulators, Leite and Doraiswamy (2007) observed, in a Red-Yellow Latosol (LVA) [Latosol = US: Oxisol; Red-Yellow Latosol = US: Rhodic/Xanthic Haplustox] in Baixa Grande do Ribeiro, Piauí (PI), that Century presented a better correlation ($R^2$ = 0.96) between simulated and measured values than CQESTR ($R^2$ = 0.88) (Figure 10), which can be explained by its more robust structure, with several residue pools (surface and soil, subdivided into structural and metabolic) and soil organic matter pools (active, slow and passive) with different residence times. Decomposition rates for these pools are obtained through several multiplicative functions of soil temperature and moisture, lignin-to-nitrogen ratio and clay content, which allows for greater control of processes involved in carbon dynamics. In the CQESTR simulator, there is a lesser number of residue pools (surface and soil) and soil organic matter is unicompartmental, suggesting a greater simplification of the model's equations and assumptions. In addition, the texture factor is limited to a texture class descriptor (clay = −1 and sand = 1). Soils with the same texture class descriptor, however, may have different clay contents, and, as a result, will have different cation exchange capacities, which will influence carbon stabilization differently. Therefore, this is a limitation to the model. Despite the absence of important mechanisms, however, differences in TOC stocks simulated by CQESTR in relation to those simulated by Century and to those measured by analytical techniques were of low magnitude, in all tillage systems. In the no-tillage system, differences between simulated and measured were, on average, 2.9% for CQESTR and −10.5% for Century. In remaining systems, differences were 1.9% and −4.7% (for conventional tillage) and 3.9% and 5.3% for (for reduced tillage) for Century and CQESTR, respectively (Figure 11). CQESTR's greater simplicity and differences between simulated and measured TOC stocks (<10%) make this model suitable for tropical Cerrado soil under various tillage systems.

| CHAP 9 - FIGURE 10 | |
|---|---|
| Simulado | Simulated |
| Medido | Measured |

**Figure 10.** Correlation between measured values and values estimated by Century (A) and CQESTR (B) simulators.

Source: Leite & Doraiswamy (2007).

## Using CQESTR to estimate carbon emissions (C-CO$_2$) in a Latosol [US: Oxisol] under a crop-livestock integration system in Santo Antônio de Goiás, Goiás (GO)

Crop-livestock integration (CLI) has been recommended as an efficient management strategy to improve soil quality in areas of the Brazilian Cerrado. It is a hybrid production system for parallel production of grain and meat in the same area, alternating between farming and grazing. CLI has benefits for both sides. Introducing annual crops in degraded pasture, when the cycle returns to the grazing stage, improves soil conditions for meat or milk production. In addition, introduction of pasture grass species (usually *Brachiaria* sp.) improves the soil's physical conditions (deep rooting) and chemical/biological conditions (increase in organic matter) for grain production. In Santo Antônio de Goiás, Goiás (GO), in a Dystrophic Dark Red Latosol [Dark Red Latosol = US: Rhodic Haplustox], studies were conducted on the effects of CLI on the increase of C stocks, on the long term. The area studied had been covered by native Cerrado forest until the year 1983. From then on, soybean was cultivated under conventional tillage for about 10 years until the establishment of the experiment, in 1993. The systems studied were: crop-livestock integration with rotation (soybean – maize – upland rice – beans/*Brachiaria*) every 4 years (CLI4); crop-livestock integration with rotation (soybean – maize – upland rice – beans/*Brachiaria*) every 2 years (CLI2); no-tillage with soybean – maize – upland rice – beans rotation (NT-SM); crop-livestock integration with rotation (soybean – maize – upland rice – beans/*Brachiaria*) every 3 years (CLI3); and conventional tillage with rice cultivation (CT-R). Systems CLI4 and CLI2 were under no-tillage in the grain cultivation stage. In CLI3, rice was sown under conventional tillage. CQESTR estimated a decrease in TOC stocks after removal of the native forest. This trend continued even after adoption of the management systems. In 2000, TOC stocks ranged from 34 Mg ha$^{-1}$ (NT-SM and CT-R) to 36 Mg ha$^{-1}$ (CLI4 and CLI2), which represented a reduction of 26% to 22%, respectively, compared to the original stock (LEITE *et al.*, 2007) (Figure 12). From 2007 onwards, however, systems with crop-livestock integration under no-tillage began to show an increase in TOC stocks, and the model estimates for were from 57 Mg ha$^{-1}$ (CLI4) to 49 Mg ha$^{-1}$ (CLI2). These results highlight the importance of CLI associated with no-tillage to improve soil quality and contribute to carbon sequestration. In addition, the trend toward TOC stock decreases was maintained for CLI3 (rice in rotation under conventional tillage) and systems with only crop rotation . For 2040, the estimated values were 26 Mg ha$^{-1}$, 22 Mg ha$^{-1}$ and 16 Mg ha$^{-1}$ for CLI3, NT-SM and CT-R, respectively. In these systems, greater oxidation of organic carbon caused by excessive tillage and lower biomass input, assumptions considered in the model, contributed to these declines.

| CHAP 9 - FIGURE 11 | |
|---|---|
| COT | TOC |
| Ano | Year |
| Medido | Measured |

**Figure 11.** Comparison between total organic carbon (TOC) stocks, simulated by Century and CQESTR and measured under no-tillage (A), conventional tillage (B) and reduced tillage (C) systems.

Source: Leite & Doraiswamy (2007).

Crop-livestock integration with rotation every 4 and 2 years sequestered 0.4 Mg ha$^{-1}$ and 0.34 Mg ha$^{-1}$ year$^{-1}$, respectively. There was also sequestering of C in CLI3, although of lesser magnitude (0.12 Mg ha$^{-1}$ year$^{-1}$). All remaining systems, where there was no crop-livestock integration, emitted carbon into the atmosphere (0.09 Mg ha$^{-1}$ and 0.30 Mg ha$^{-1}$ year$^{-1}$) (LEITE *et al.*, 2010) (Table 4). Crop-livestock integration is a suitable system for Brazilian Cerrado and it may indeed become an excellent alternative to improve soil quality and reduce greenhouse gas emissions.

| CHAP 9 - FIGURE 12 | |
|---|---|
| COT | TOC |
| Ano | Year |
| ILP4 | CLI4 |
| ILP2 | CLI2 |
| PD-SM | NT-SM |
| ILP3 | CLI3 |
| PC-A | CT-R |

**Figure 12.** CQESTR simulation of total organic carbon (TOC) dynamics (0 cm – 20 cm) under various management systems: crop-livestock integration with rotation (soybean – maize – upland rice – beans/*Brachiaria*) every 4 years (CLI4); crop-livestock integration with rotation (soybean – maize – upland rice – beans/*Brachiaria*) every 2 years (CLI2); no-tillage with soybean – maize – upland rice – beans rotation (NT-SM); crop-livestock integration with rotation (soybean – maize – upland rice – beans/*Brachiaria*) every 3 years (CLI3); conventional tillage with rice cultivation (CT-R).

Source: Leite *et al.* (2007).

**Table 4.** Carbon (C-$CO_2$) emission or sequestering estimated by the CQESTR simulator and from values measured in a Dark Red Latosol [US: Rhodic Haplustox] (LVE) in Santo Antônio de Goiás, Goiás (GO), under various management systems.

| **Management system** | **C stock** | | | **Rate** (1) | **C sequestering (+) / emission (−)** |
|---|---|---|---|---|---|
| | **Initial** | **Final** | **Variation Δ** | | |
| | **Mg ha$^{-1}$** | | | **Mg ha$^{-1}$ year$^{-1}$** | |
| CQESTR | | | | | |
| CLI 4 years | 36.6 | 39.0 | 2.42 | 0.16 | 0.40 |
| NT-SM | 36.6 | 32.5 | −4.04 | −0.27 | −0.09 |
| CLI 2 years | 36.6 | 38.1 | 1.54 | 0.10 | 0.34 |
| CLI 3 years | 36.6 | 34.8 | −1.79 | −0.12 | 0.12 |
| CT-R | 36.6 | 32.1 | −4.44 | −0.30 | −0.30 |
| Measured(2) | | | | | |
| CLI 4 years | 28.0 | 35.9 | 7.9 | 0.61 | +0.88 |
| CLI 2 years | 28.0 | 35.3 | 7.3 | 0.56 | +0.84 |
| CLI 3 years | 28.0 | 31.8 | 3.8 | 0.29 | +0.57 |
| CT-R | 28.0 | 32.0 | 4.0 | 0.31 | +0.26 |

Note: Crop-livestock integration with rotation (soybean – maize – upland rice – beans/*Brachiaria*) every 4 years (CLI4); crop-livestock integration with rotation (soybean – maize – upland rice – beans/*Brachiaria*) every 2 years (CLI2); no-tillage with soybean – maize – upland rice – beans rotation (NT-SM); crop-livestock integration with rotation (soybean – maize – upland rice – beans/*Brachiaria*) every 3 years (CLI3); conventional tillage with rice cultivation (CT-R).

(1) A contribution of 8 Mg ha$^{-1}$ (CLI4, CLI2 and CLI3) and 6 Mg ha$^{-1}$ (NT-SM) from cover crop (0.24 Mg ha$^{-1}$ year$^{-1}$ and 0.18 Mg ha$^{-1}$ year$^{-1}$ considering 45% as C) (SALTON *et al.*, 2005) was assumed for the no-tillage system. An emission of 0.045 Mg ha$^{-1}$ year$^{-1}$ of C was included for conventional tillage to represent additional use of fuel (DIECKOW *et al.*, 2004).

(2) Values measured in 2005, except for the soybean – maize NT system.

Source: Leite *et al.* (2010).

## Final considerations

The use of computer simulators has been widely required to estimate the dynamics of C and N and greenhouse gas emissions in various agroecosystems. They are extremely useful and essential tools to aid in decision making. However, to optimize the efficiency of these simulators, and, consequently, of the modeling activities, some measures must be considered: 1) proposing databases, especially databases that provide information still scattered throughout Brazil, about low-variation aspects related to specific characteristics of crop varieties and daily climatological information throughout the year, which are essential for simulations on a local scale; 2) identifying, organizing and, most importantly, make electronically available (via the Agrogases network website) information from other sites containing databases and technical studies with relevant information, as well as contacts of entities (researchers, institutions, universities, etc.) working on the topic, thus avoiding redundant work and unnecessary expenses in gathering information already collected by other research institutions or of little use; 3) validate simulators for various Brazilian environments and respective production systems; and 4) develop models and simulators to estimate gas emissions while incorporating specific factors for conditions found in tropical environments.

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