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Application of the DNDC model for predicting
soil GHG emissions under shallow water table

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ABSTRACT

In the context of the new Common Agricultural Policy the territorial administration institutions (e.g. regional government) are called to provide evidence of the actions taken and the results obtained to achieve the objectives set by agricultural and environmental policies. DNDC (DeNitrificationDeComposition) is a process-based model of C and N biogeochemical cycles which can model the outcomes from different agricultural practices by simulating greenhouse gases (GHGs) emission, crop yield and leaching from the agroecosystems. Therefore, it can be used to help valuating contrasting agricultural managements. The recent upgrade of the model (DNDCv.CAN) allows to simulate fluctuating and active water table (WT) conditions thanks to new features among which the tile drain option (TD). This is of interest considering the low-lying conditions of the Italian region Veneto's plain. In this work it was attempted to calibrate and validate DNDCv.CAN for a set of lysimeters located at an experimental site of the University of Padova in Legnaro (PD), and to compare the use of TD or not (noTD) in terms of GHGs emissions simulations for carbon dioxide (CO₂), nitrous oxide (N₂O) and methane (CH₄). Observed data used in the comparison with modelling outcomes were soil moisture, water percolation and nitrate leaching, as well as the GHGs emission from soils, which were retrieved between 2011 and 2014 in the lysimeters cultivated with maize (*Zea mays* L.). For the 12 lysimeters considered, two fertilization levels were applied of organic and inorganic N (250 kg ha⁻¹ yr⁻¹ and 368 kg ha⁻¹ yr⁻¹) and three WT setting were employed, that are a WT at the depth of 60 cm (WT60), at 120 cm (WT120), and free drainage conditions (FD). All these field conditions were implemented as input in the model with the addition of meteorological data. The calibration performed was a manual parametrization of specific coefficients and parameters related to the decomposition rate, nitrate and water leaching, N₂O soil emission and crop parameters specific for Veneto. Simulated TD, noTD and observed data were compared, and statistic metrics like the root mean square error (RMSE) the percent bias (PBIAS) and the coefficient of correlation (R²) were evaluated. Daily soil moisture (mm) and nitrate leaching (kg N-NO₃⁻ ha⁻¹ yr⁻¹) were simulated better with TD than noTD. For example, considering lysimeter 7 PBIAS for

the soil moisture was equal to 1.87 with TD and to 52.2 with noTD, while for nitrate leaching values, at WT120 lysimeters RMSE was 4.41 kg N-NO₃⁻ ha⁻¹ yr⁻¹ for TD and 46 kg N-NO₃⁻ ha⁻¹ yr⁻¹ for noTD. Whereas for the simulation of water percolation (mm yr⁻¹), grain production (kg C ha⁻¹ yr⁻¹), CO₂ soil emission (kg C-CO₂ ha⁻¹ yr⁻¹), N₂O soil emission (kg N-N₂O ha⁻¹ yr⁻¹) and CH₄ soil emission (kg C-CH₄ ha⁻¹ yr⁻¹) no significant differences between the two options were detected. For instance, RMSE was equal to 1.50 kg N-N₂O ha⁻¹ yr⁻¹ for TD simulations at WT60, and to 1.58 kg N-N₂O ha⁻¹ yr⁻¹ for noTD records. It is necessary further research to evaluate and calibrate the model in different regions and in a more efficient manner for GHGs emissions. The algorithms at the foundation of biogeochemical fluxes and soil hydrology simulations could be upgraded to improve GHGs emissions output. Nonetheless, for all the parameters mentioned expect CH₄ soil emissions, a good agreement between observed and simulated data was observed considering annual average values, with R² = 0.601 for TD and R² = 0.644 for noTD considering CO₂ emission values and R² = 0.516 for TD and R² = 0.821 for noTD in grain production simulations. This confirmed the positive effect of the parametrization performed, beyond TD or noTD options.

RIASSUNTO

Nel contesto della nuova Politica Agricola Comunitaria, le amministrazioni e le istituzioni territoriali, come per esempio le regioni, sono chiamate a mostrare l'evidenza delle azioni intraprese e dei risultati ottenuti al fine di raggiungere gli obiettivi prefissati da politiche agricole e ambientali. DNDC (DeNitrificationDeComposition) è un modello basato sui processi biogeochimici del ciclo del carbonio e dell'azoto, di cui può predire gli andamenti considerando diverse pratiche agricole, simulando l'emissione di gas serra, percolazione di nitrati e produttività di agroecosistemi. Il recente aggiornamento del modello (DNDCv.CAN) permette di simulare condizioni di tavola d'acqua variabile, grazie a nuove funzionalità, tra cui l'opzione "tile drain" (TD). Ciò è di interesse considerando le condizioni di bassa pianura della regione Veneto in Italia. In questo lavoro, è stato provato a calibrare e validare DNDCv.CAN per un insieme di lisimetri situati in un sito sperimentale dell'Università di Padova a Legnaro (PD), e di confrontare l'utilizzo di TD o meno in termini di simulazione dell'emissione di gas serra, per quanto riguarda il biossido di carbonio (CO₂), il biossido di azoto (N₂O) e il metano (CH₄). I dati osservati utilizzati per la calibrazione erano il contenuto idrico del suolo, la percolazione di acqua, la percolazione di nitrati, così come le emissioni dei sopraccitati gas serra dal suolo. Questi, sono stati misurati tra il 2011 e il 2014 nei lisimetri coltivati a mais (*Zea mays* L.). Per i 12 lisimetri considerati, sono stati applicati due livelli di fertilizzazione organica ed inorganica di azoto (250 kg ha⁻¹ yr⁻¹ e 238 kg ha⁻¹ yr⁻¹), e sono state valutate tre modalità di gestione della tavola d'acqua (falda a 60cm, 120cm e condizioni di drenaggio libero). Tutte queste condizioni sperimentali sono state implementate come input per il modello, oltre ai dati meteo. È stata effettuata una calibrazione manuale, parametrizzando dei coefficienti specifici legati al tasso di decomposizione, alla percolazione di acqua e nitrati, alle emissioni di N₂O dal suolo e parametri colturali specifici per la regione Veneto. In particolare, sono stati confrontati i dati simulati con TD, senza TD e i dati osservati in campo considerando coefficienti statistici come la Radice dell'errore quadratico medio (RMSE), il bias percentuale (PBIAS) e il coefficiente di correlazione (R²). I dati di contenuto idrico del suolo giornalieri (mm) di percolazione

di nitrati ($\text{kg N-NO}_3^- \text{ ha}^{-1} \text{ yr}^{-1}$) sono stati simulati meglio con TD che senza. Per esempio, considerando il lisimetro 7 il PBIAS per il contenuto idrico del suolo era 1.87 con TD e 52.2 senza, mentre per i valori di percolazione di nitrati nei lisimetri WT120 RMSE era $4.41 \text{ kg N-NO}_3^- \text{ ha}^{-1} \text{ yr}^{-1}$ con TD e $46 \text{ kg N-NO}_3^- \text{ ha}^{-1} \text{ yr}^{-1}$ senza. Mentre per quanto riguarda la simulazione della percolazione di acqua (mm yr^{-1}), della produzione di granella ($\text{kg C ha}^{-1} \text{ yr}^{-1}$), dell'emissione di CO_2 dal suolo ($\text{kg C-CO}_2 \text{ ha}^{-1} \text{ yr}^{-1}$), dell'emissione di N_2O dal suolo ($\text{kg N-N}_2\text{O ha}^{-1} \text{ yr}^{-1}$) e dell'emissione di CH_4 dal suolo ($\text{kg C-CH}_4 \text{ ha}^{-1} \text{ yr}^{-1}$) non è stata registrata nessuna differenza significativa tra le due opzioni. Per esempio, RMSE era pari a $1.50 \text{ kg N-N}_2\text{O ha}^{-1} \text{ yr}^{-1}$ nelle simulazioni con TD a WT60 e pari a $1.58 \text{ kg N-N}_2\text{O ha}^{-1} \text{ yr}^{-1}$ per quelle senza TD. Risulta necessaria ulteriore ricerca a riguardo, per valutare e calibrare questa nuova versione del modello in diverse regioni e più precisamente per l'emissione di gas serra in agricoltura, per esempio, implementando gli algoritmi che determinano la simulazione dei flussi biogeochimici. Ciononostante, per tutti i parametri menzionati escluso il metano, è stata osservata una buona concordanza tra i dati simulati e i dati osservati considerando i valori medi annuali con un $R^2=0.601$ con TD e $R^2=0.644$ senza (simulazione di CO_2) e un $R^2=0.516$ con TD e $R^2=0.821$ senza (produzione di granella). Ciò conferma l'effetto positivo della parametrizzazione effettuata, oltre l'opzione TD.

1 Introduction

In recent years climate change is seen as one of the main challenges facing humanity. Political agendas of individual countries and international initiatives proclaim greenhouse gas (GHG) neutrality, e.g., by the year 2050 (European Commission 2019, UNFCCC 2015). Climate change is a challenge in its regulation, monitoring and tackling because it is a complex problem and it is diffused in time and space; so it needs to be addressed with a multidisciplinary approach. Worldwide, greenhouse gas emissions from agriculture, including crop and livestock production, forestry and associated land use changes, are responsible for a significant fraction of anthropogenic emissions, up to 18.4% (figure 1). The crucial issue is the emission of carbon dioxide (CO₂), methane (CH₄) and nitrous oxide (N₂O) from soil due to microbial respiration (Oertel et al., 2016) and crop-related activity like deforestation, land use change and crop burning.

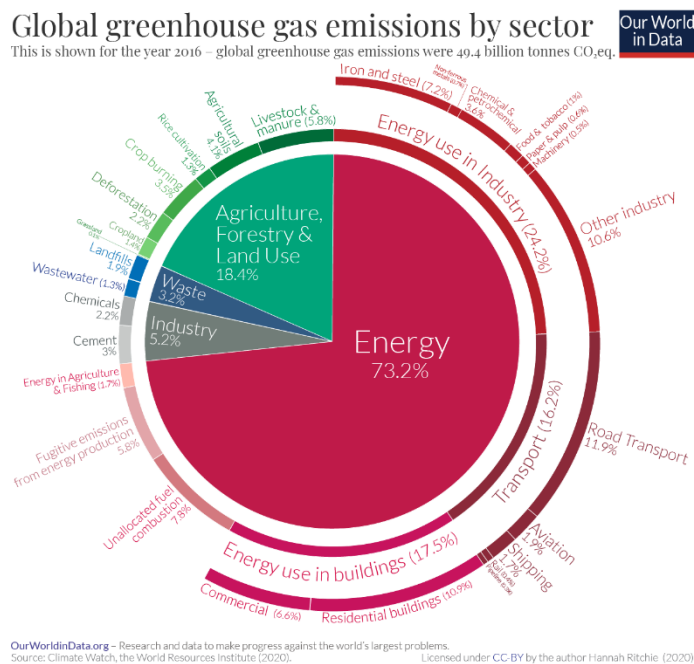


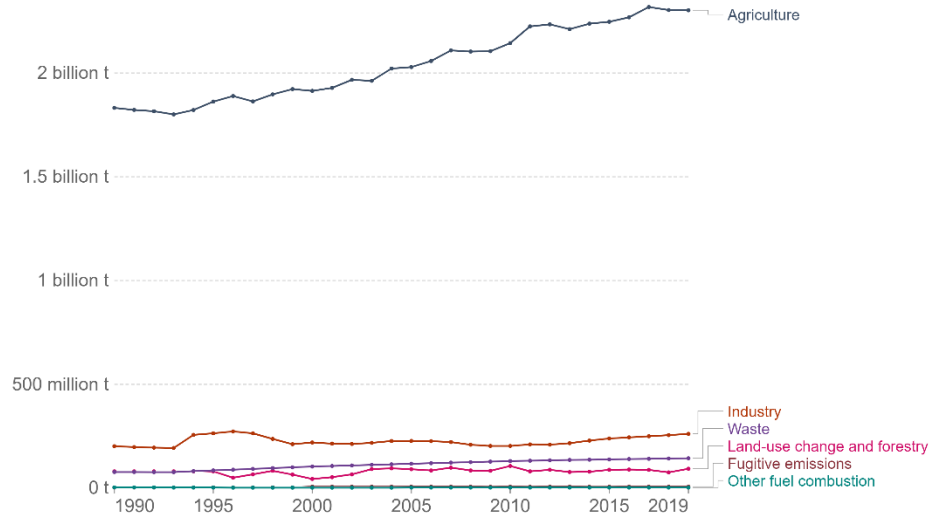
Figure 1: World GHG emissions by sector (OurWorldinData.org)

Carbon dioxide emission from agricultural soils is generated by the organic matter decomposition (heterotrophic respiration), from root respiration, (autotrophic respiration), from microbial decomposition of dead plant remains and from microbial decomposition of rhizodeposits from living roots (rhizomicrobial respiration)

(Kuzyakov, 2006). These fluxes are influenced by the chemical and physical properties of the soil, by meteorological conditions and agricultural management practices. Furthermore, CH₄ emission from soil derives as the result of the balance between the production activity of methanogens bacteria and the degradation activity of methanotrophic bacteria. Agronomic practices that may influence the activity of bacterial strains are tillage, organic fertilization, crop types, irrigation, etc. It follows that irrigated or rainfed croplands and grasslands might be either valuable CH₄ sinks or sources that usually do not exceed a few $\pm \text{kg ha}^{-1} \text{ yr}^{-1}$, e.g. when slurry is used as an organic amendment (Bayer et al., 2012; Hütsch, 2001). Anyway, it must be noted that most of the CH₄ emissions from agricultural management practices are due to paddy rice soils, reaching tens or hundreds of $\text{kg ha}^{-1} \text{ yr}^{-1}$ (Sanchis et al., 2012). Finally, nearly all emissions of N₂O, produced by microbes in nearly all soils, come from agriculture (figure 2), which is also characterized by the highest Global Warming Potential (GWP) among CO₂ (GWP = 1), CH₄ (GWP \approx 30 over 100 years), N₂O (GWP \approx 273 over 100 years). The application of nitrogen fertilizers makes much more nitrogen readily available for microbes – this is because not all of the applied nutrients are taken up by crops. As the application of both inorganic synthetic nitrogen fertilizers and organic fertilizers such as animal manure has rapidly increased over the past 50 years, N₂O emissions have also increased. Raw calculation of N₂O emission directly from cropping systems is based on an emission factor of about $1.25 \pm 1\%$ of total N applied as fertilizer according to the IPCC guidelines (De Klein et al., 2006). However, these guidelines for estimating N₂O emission from agricultural soils have some limitations. They do not consider the pedoclimatic variability of the agroecosystems, which are assumed to be the same throughout the world. Moreover, they do not take into account different crops, tillage operations, and irrigation or fertilization management, all of which are known to affect the nitrification–denitrification equilibrium and therefore the N₂O production and emission (Del Grosso et al., 2005).

Nitrous oxide emissions by sector, World

Nitrous oxide (N₂O) emissions are measured in tonnes of carbon dioxide equivalents (CO₂e) based on a 100-year global warming potential value.



Source: CAIT Climate Data Explorer via Climate Watch OurWorldInData.org/co2-and-other-greenhouse-gas-emissions/ • CC BY

Figure 2: World N₂O emission per sector

1.1 Water table depth in agricultural soils

Wide agricultural areas around the world are cultivated under shallow water table (WT) conditions (e.g., < 3 m), which might modify the biogeochemical fluxes of C N P towards the atmosphere and/or the groundwater. This is the case for the low-lying plain of the Veneto region (figure 3), located in north-eastern Italy.

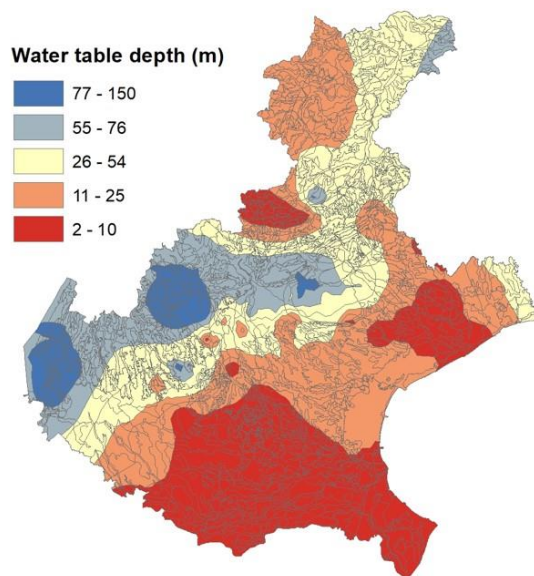


Figure 3: interpolated WT level in the Veneto region (arpav.it)

Water table depth influences environmental impacts in agriculture, for instance, a shallow WT showed to increase the N leaching vulnerability. On the other hand high soil moisture can also lower water N concentrations through denitrification processes (Morari et al., 2012). Moreover, WT level plays a major role in influencing the net flux of GHG emissions from soil, such as N₂O (Cocco et al., 2018), (Jurado et al., 2017), (Shcherbak et al., 2019) and especially CH₄ (Zona et al., 2009), (Topp et al., 1997), (Hütsch, 2001). Nitrification and denitrification are known to be the main pathways of N₂O production and are controlled by soil microbes and their metabolisms. The two factors that most affect N₂O emission are the genetic capability of denitrifiers and nitrifier microorganisms to perform these pathways and the environmental conditions required to sustain and allow these processes (Saggar et al., 2013), (Li et al., 2021). The latter factor includes NO₃⁻ and NH₄⁺ supply, C availability (electron donors), temperature, soil redox conditions linked to waterfilled pore space (WFPS%), consequent aeration status, and pH (Cocco et al., 2018). All these parameters are directly or indirectly influenced by the WT level, which needs to be considered as driving factor in N₂O emissions from soil. In particular, shallow WT level and a consequent O₂ low level (anaerobic condition) is recognised as a potential factor in limiting the emission of such potent GHG (von Arnold et al., 2005), (Li et al., 2021). Recent experiments conducted in the Veneto region revealed that a shallow groundwater can reduce N₂O emissions (Cocco et al., 2018).

1.2 Common Agricultural Policy

Since the 2000s many efforts have been made at European level to enhance the environmental quality of agroecosystems of EU Member State by reducing the GHGs emissions as well as by preserving the ecosystem services that they provide. The main tool provided by EU is the Common Agricultural Policy (CAP), which has been modernised after the CAP reform of 2018. The policy focuses on ten specific objectives, linked to common EU goals for social, environmental, and economic sustainability in agriculture and rural areas. The budget involved in this strategy is remarkable: for the period 2021-27 €387 billion in funding has been allocated. This will come from two different funds: the European agricultural guarantee fund (“first pillar” of the CAP),

which has been set at €291.1 billion; and the European agricultural fund for rural development (“second pillar”), which will amount to €95.5 billion. The first pillar is allocated for income schemes support and for supporting agricultural markets. The budget of the second pillar is destined for financing rural development programs (RDPS). Overall, 40% of total CAP expenditure will be dedicated to climate action (European Parliament, 2020). Farmers are financially supported through the RDPS, specifically, they receive contributes if they implement specific agroclimatic-environmental measures (AEMs). These measures include among the others crop rotations, reduced fertilizer and pesticide application rates, organic farming, undersowing, cover crops, buffered strips and water used reduction. The biggest change of the CAP 2021-2027 against the previous policy (2014-2020) is that money allocation will seek to place more emphasis on a “result-based” approach rather than the traditional “action-based”. Farmers will be no longer be paid for the adoption of specific land management practices only, but part of the funds should be provided according to the production of outcomes with the aim of accompanying any agri-environmental measure with a scientifically based evaluation (Dal Ferro et al., 2016).

1.3 Agroecosystem modelling

Different approaches are still the object of study and debate to quantify the effectiveness of the financially supported measures to reduce GHG emission from agriculture, and consequently to maximize the cost-effectiveness. In fact, favouring certain agro-environmental measures (AEM), can be either effective or not, depending on many different pedo-climatic characteristics.

Process-based biogeochemical models are complex tools that have the potential to describe environmental and agronomic benefits and drawbacks of agro-climate-environment measures implemented by farmers’ over large scale. These cost-effective tools integrate different biogeochemical cycles providing site specific assessment at the regional, national or even global scale. It must be noted that within the renewed interest towards the carbon farming approach –a strategy that encompasses the management of carbon pools, flows, and GHG fluxes at the farm level– agroecosystem models are among the suggested tools for an effective monitoring, reporting, and

verification (MRV) scheme that will provide incentives to farmers and landowners based on the results achieved (COWI, 2021). However, models can provide accurate outcomes under well-known conditions, but they are less consistent when applied to unusual soils or climate. In fact, they must be calibrated under controlled conditions to provide reliable data. The most frequently used calibration procedure is through the optimization of model performances, which is carried out by comparing observed and simulated data. Searching for the best parameter values can be carried by following a trial-and-error procedure, which can be done manually or automatically with algorithms that allow to include several parameters in very short times. The process to estimate in advance which parameters should be used for the calibration is called sensitive analysis. After a model has been calibrated, it needs to be validated to assess the forecasting performance that can offer to the users. Different statistical metrics can be considered to report the results of a validation analysis, such as the root mean square error (RMSE), the relative root mean square error, the model efficiency (EM), the mean difference, and the coefficient of determination (R^2).

Biogeochemical models still have recognized knowledge gaps and thus require new targeted measurements for the development of improved mechanisms to ensure that the iterative process for model development continues. For instance, model structure is often limited by the oversimplified representation of soil and hydrological processes. In a review of nine GHG models, Brilli et al., (2017) found that 46% of the deficiencies in models were due to issues with the simulation of pedo-climatic conditions including soil-water simulation. The DNDC model is the most prominent process-based model used for simulating GHG emissions worldwide, however, it has known issues in simulating soil hydrology (Smith et al., 2019; He et al., 2019; Brill et al., 2017; Congreves et al., 2016; Abdalla et al., 2011).

Veneto, is affected by high anthropogenic pressures due to population increase and highly intensive and productive agriculture, leading to increased GHG emissions. Therefore, in the context of the Rural Development Programs Veneto financed AEMs to obtain good environmental quality targets, especially mitigating climate change.

Aims of the study

The work presented here is part of a wide project in collaboration with the Veneto Region and the DAFNAE department, University of Padova, aiming to assess the effect of alternative practices on soil, water, and air quality.

In particular, with the aim to calibrate and validate a new version of the biogeochemical model DNDC (DeNitrification DeComposition), whose code has been recently upgraded with functions that should be able to describe shallow and fluctuating groundwater conditions and related GHGs emissions at high temporal resolution. This is of high interest considering the conditions of the low-lying Venetian plain, that has peculiar shallow water table fluctuations that can strongly modify the biogeochemical cycles and consequently the GHG emissions. This can help policymakers and consultants, to evaluate the effectiveness of agro-climate-environment measures that are supported by the CAP in the Veneto region to provide ecosystem services.

2 Materials and Methods

2.1. Experimental data description

The data used to test and validate the DNDC model were collected from three experiments conducted between June 2011 and September 2014 at the experimental farm L. Toniolo, Legnaro (PD) of the University of Padova in north-eastern Italy (45°19'N, 11°31'E, 8 m asl) (figure 4, left).

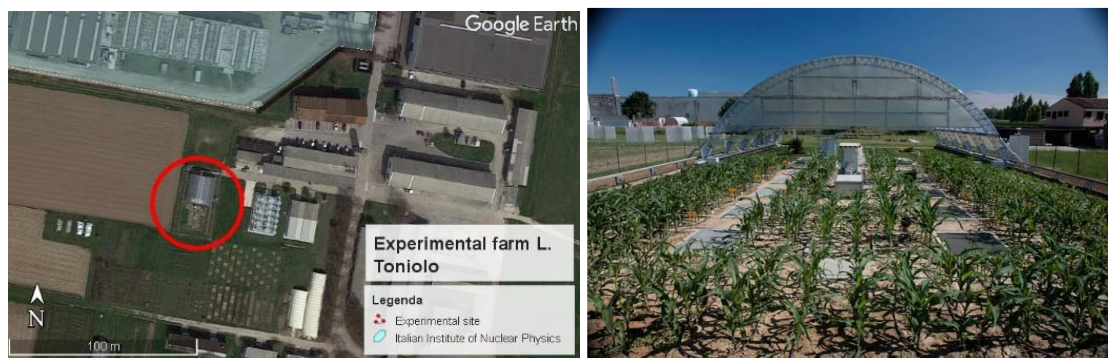


Figure 4: Experimental site location (left) and an on overview of the lysimeters cultivated with maize (right)

The study site consists of 20 drainable lysimeters of size equal to 1-m×1-m×1.5-m (length × width × depth) (figure 4, right), made of reinforced concrete and buried into the soil (Giardini et al.,1988). To prevent border effects, crops are usually grown outside lysimeters, creating a buffer. The principle of communicating vessels was used to control WT conditions. The bottom of each lysimeter is funnel-shaped and connected to an equally high external column (150-cm height) fitted with a valve to regulate both the water table level and leached discharge (figure 5).

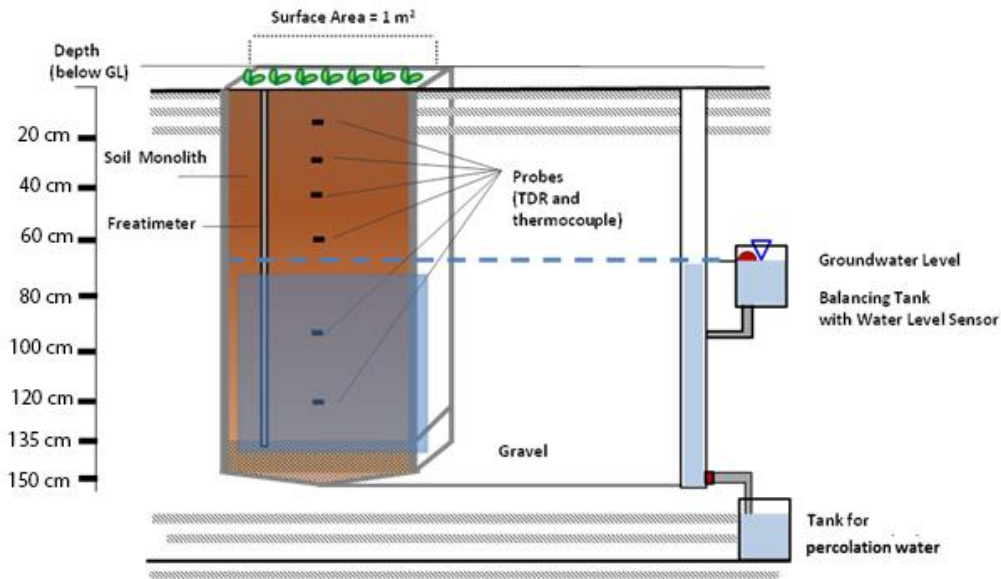


Figure 5: Lysimeter section

Each lysimeter column was equipped with a water level sensor, to avoid the water level deviating more than ± 10 cm from the set reference level. Accordingly, well water was manually added by mean of the external columns to compensate upward flux when water level was at least 10 cm lower than the reference level. On the contrary, percolation water was collected through the bottom valve when, following rainfall or irrigation, the water level raised >10 cm compared with the reference level. Each lysimeter was filled in 1984 with soil excavated from the adjacent experimental farm using a method that preserved the original soil horizons. To facilitate water drainage and prevent soil washout, a 15-cm layer gravel was used to cover the bottom of each lysimeter. The lysimeter soil is a Fluvi-Calcaric Cambisol (CMcf; WRB, 2015) and is representative of $\sim 50\%$ of the low-lying Venetian plain, whose main properties are reported in figure 6. Soil particle size distribution was determined using a particle size analyzer (Mastersizer 2000, Malvern Panalytical; Bittelli et al., 2019); pH and electrical conductivity were measured by an electrode in soil suspensions with a soil/water ratio of 1:2.5 (Kabała et al., 2016) and 1:2 (w/v) (ISO 11265; ISO 1994) respectively; total N was analyzed with the Kjeldahl method (ISO 11261; ISO 1995); soil organic C content was measured with an elemental analyzer (VARIO MACRO, Elementar Analysensysteme); total and active carbonates were measured with the Dietrich-Fruehling calcimeter (ISO 10693; ISO 1995) and ammonium oxalate titration method (Jeffery &

Hutchinson,1981), respectively; available P was measured with the Olsen method (ISO 11263; ISO 1994); and exchangeable K was measured by the extraction with ammonium acetate (Schollenberger & Simon,1945). Field capacity (-33 kPa) and permanent wilting point (WP, -1500 kPa) were derived from the soil water retention curve, which was estimated through the wind's evaporation method and dewpoint potentiometer. In addition, soil texture, bulk density and soil organic C were available for each lysimeter in the following layers: 0–30, 30–55, 55–75, 75–95, and 95–135 cm.

| Soil properties | Soil depth | |
|--|------------|-----------|
| | 0–60 cm | 60–130 cm |
| Sand (%) | 36 | 33 |
| Silt (%) | 49 | 47 |
| Clay (%) | 15 | 20 |
| pH | 8.2 | 8.1 |
| Total Nitrogen (%) | 0.9 | 1.1 |
| Organic Matter (g 100 g ⁻¹) | 1.1 | 1.3 |
| Total Carbonates (%) | 33 | 19 |
| Active Carbonates (%) | 4.1 | 3.2 |
| EC (mS cm ⁻¹)* | 0.28 | 0.35 |
| Available P (mg kg ⁻¹)** | 16 | 50 |
| Exchangeable K (mg kg ⁻¹ ***) | 49 | 132 |

Figure 6: Soil characteristics

2.1.1 Treatments and managements techniques

Given the considerable portion of the Veneto Region occupied by shallow water table (ARPAV, 2014), two groundwater (GW) conditions were tested and remained fixed variables throughout all the trials in a comparison with free drainage (FD) conditions. The shallow water table was set at 120-cm depth (WT120) and at 60-cm depth (WT60). Beyond groundwater conditions, the experiment included throughout the years different fertilization levels and mineral/organic N types to determine a factorial combination (170_{organic} + 80_{mineral} kg N ha⁻¹ yr⁻¹ vs. 250_{organic} + 118_{mineral} kg N ha⁻¹ yr⁻¹). Mineral nitrogen was applied as urea and it was distributed for the 40% during the sowing, and the remaining portion on the surface with one dose in 2011 and two doses in 2012-2014. Organic nitrogen was applied as cattle manure in 2011-2012 guaranteeing precise input of organic carbon and fertilizer mineral elements, with the following characteristics: 84% dry matter, 55% OM of the dry matter, 2.8% N, 1.3% P, 1.7% K, and with a C/N =13. In the years 2013-2014, the manure was replaced with

slurry with the following characteristics: in 2013 8% dry matter, 0.28% N, 0.05% P; in 2014 8% dry matter, 0.25% N, 0.035% P. The organic fertilizer was applied during the sowing and incorporated in the first 25 cm of the soil profile digging manually. For the 2011–2014 years, three GW conditions against two N input levels (in total 250 vs. 368 kg N ha⁻¹ yr⁻¹) have been tested. The main crop was maize (*Zea mays* L.), which was grown as monoculture according to conventional tillage operations. Soil was left bared during winter. At the end of each growing season, crop grain and residues were collected and weighted. Crop grain and residue samples were dried at 65 °C in a forced draft oven for 72h for dry weight determination. In all cases, the trials followed a randomized block design with two replicates, such that 12 lysimeters were used (three bottom boundary conditions × two treatment levels × two replicates) (table 1).

| Lysimeters | Organic N <i>kg N ha⁻¹ y⁻¹</i> | Ureic N <i>kg N ha⁻¹ y⁻¹</i> | Total N <i>kg N ha⁻¹ y⁻¹</i> | Drainage | Replicates | Treatments |
|------------|---|---|---|-----------------------|------------|---------------|
| 8 & 20 | 170 | 80 | 250 | free drainage | 2 | 170+80 FD |
| 7 & 13 | 170 | 80 | 250 | water table at 120 cm | 2 | 170+80 WT120 |
| 2 & 11 | 170 | 80 | 250 | water table at 60 cm | 2 | 170+80 WT60 |
| 10 & 12 | 250 | 118 | 368 | free drainage | 2 | 250+118 FD |
| 3 & 6 | 250 | 118 | 368 | water table at 120 cm | 2 | 250+118 WT120 |
| 16 & 19 | 250 | 118 | 368 | water table at 60 cm | 2 | 250+118 WT60 |

Table 1: treatments and WT levels for the 12 lysimeters tested

Surface water input was regulated throughout the period by a mobile plastic roof that automatically closed to cover the lysimeters during rain events, when required. This prevented natural uncontrolled rainfall and protection from extreme weather such as hailstorms. During this period, water inputs were provided by a series of simulated rainfall events applying amounts of water through irrigation, which were previously precisely weighted. Summer simulated-rainfall events were applied according to the average crop water needs measured in FD treatments; in the other seasons, water input was randomly distributed over the typical rainy months. In both cases, manual water application was kept uniform among lysimeters. During each week from 2011 to 2013, an active time domain reflectometry (TDR) sensor (Moisture Point MP-917, ESI Environmental Sensors) connected to previously installed vertical waveguides measured the soil water content (SWC) across three different soil layers (0–15, 15–30,

and 60–90 cm). Starting in 2013, every lysimeter was equipped with an automated monitoring system that allowed the continuous measurement of SWC, soil temperature and soil matrix potential. The system was composed of CS635 TDR probes (Campbell Scientific), electronic tensiometers (T4e probes, UMS GmbH, Munich - Germany) installed at 15, 30, and 60 cm depths. Soil temperature was monitored in continuous utilizing 2 thermocouples per lysimeter at the depth of 15 cm and 30 cm (figure 7).

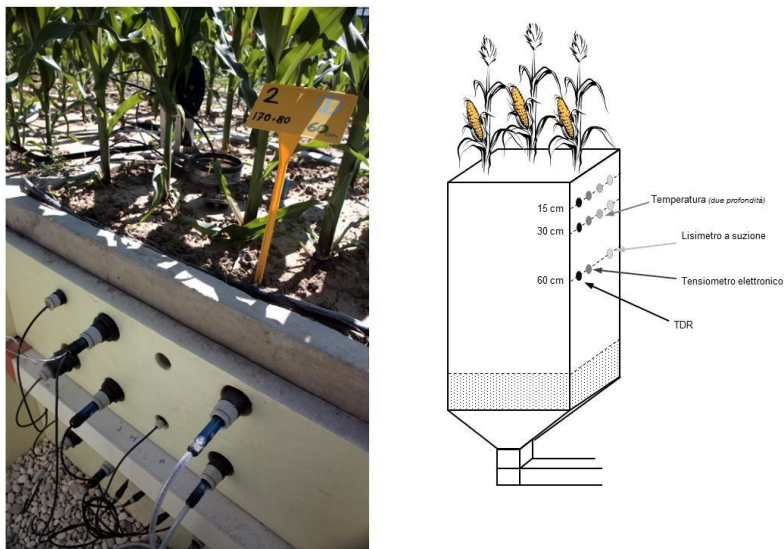


Figure 7: Probes inserted in the lysimeter

The TDR, the tensiometers and the thermocouples probes were connected to a CR-10X datalogger (Campbell Scientific Inc. Lincoln Nebraska - USA) through a series of multiplexers. Measurements were taken every 30 min (figure 8).

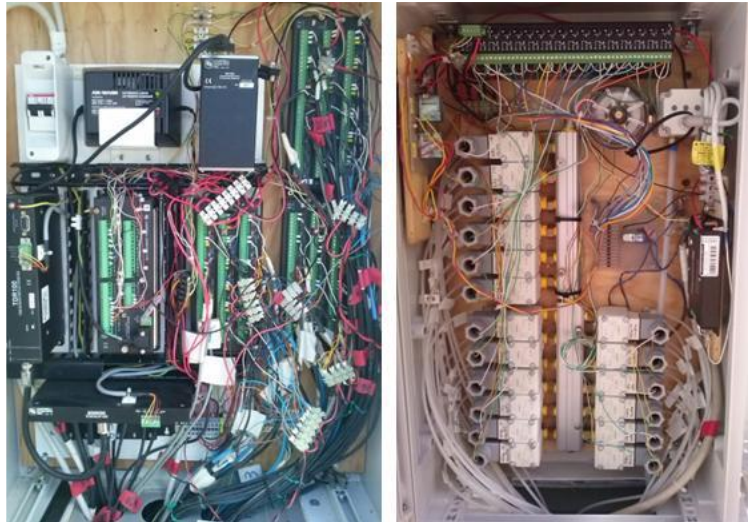


Figure 8: Datalogger and Multiplexers, connected with the measurement probes

2.2 Measurement of greenhouse gases emissions from soil

Besides chemical-physical soil and water soil parameters, it was detected the emission of nitrous oxide (N_2O), methane (CH_4) and carbon dioxide (CO_2) from soil. In order to monitor the fluxes of these GHGs it was installed an automated closed dynamic chamber system (Delle Vedove et al., 2007), accordingly to the definition of Livingston and Hutchinson (1995). The chambers were located in the “250 + 118” and “170 + 80” lysimeters, considering all the water table levels and the replicates (12 chambers in total). The closed chamber is a top-closed and base-open box placed on the soil surface. The chamber method relies on the measurement of increasing, or decreasing, concentration of trace gases of interest inside the chamber’s headspace atmosphere. Each chamber consists of a steel collar (16 cm of diameter and 15 cm height) and a motor closing steel lid is placed on a steel collar inserted into the soil. Tightness of the lid closure is ensured by a neoprene cover on the inner surface of the lid and a rubber ring covering the top perimeter of the collar (figure 9). The CO_2 and N_2O move from where they are produced (soil porosity) to the atmosphere mostly through diffusion even if in certain situations the movement can be due to pressure difference between the chamber and the atmosphere. To avoid air pressure difference between inside and outside the chamber, a pressure vent was built according to the indication of Xu et al. (2006) and placed on the top of the chamber (Hutchinson and Livingston, 2001). The adopted vent design allows static pressure changes inside the chamber to follow

whatever static pressure changes occur in the surrounding air outside the chamber both in calm and windy conditions while remaining insensitive to wind direction. Carbon dioxide analysis was conducted through an infrared beams analyzer (IRGA, infrared gas analyzer). The air circulation in the pipes system was guaranteed thanks to two pumps and 26 electro-valves. A datalogger (CR-1000 Campbell Sci. Inc. Lincoln Nebraska – USA) commands all the operation of the gas emission monitoring through 32 relays, managing the closing of the chambers, the activation of the IRGA analyzer and the pumps. An automated sampling system was employed to monitor N₂O and CH₄. Inside the sampling machine there is a plate with 20 glass vials closed with a specific porous sept that allows the sample gas inlet through needles. The sampling machine has two needles on a mobile component that align with the vials and insert the sample gas. The needles are connected to the chamber through high density PVC tubing and managed form two valves. The gases in the vials have been analyzed with a gas chromatograph (Agilent 7890A, mod. G3440A) equipped with a flame ionization detector (FID) for methane and with an electron capture detector (ECD) for nitrous oxide.

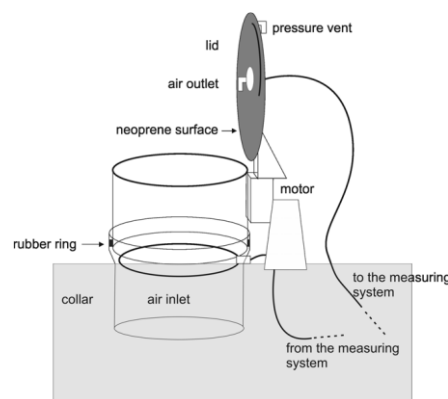


Figure 9: Schematic of chamber's parts with collar inserted into the soil

2.3 The DNDC model

The Denitrification-Decomposition (DNDC) model (Li et al., 1992a, 1992b, 1994, 1996; Li, 2000) is a process-based model of carbon (C) and nitrogen (N) biogeochemistry in agricultural ecosystems. The core of DNDC trace-gas emission predictions consists of microbe-mediated biogeochemical processes commonly occurring in terrestrial soils.

The model DNDC simulates rates of the processes by tracking activities of different groups of microbes which are activated under different environmental conditions including temperature, moisture, pH, redox potential (Eh) and substrate concentration gradient in soils. The DNDC model has been intensively and independently tested by a wide range of researchers worldwide with encouraging results (e.g., Gilhespy et al., 2014; Giltrap et al., 2010) and it has also been widely utilized for inventory and mitigation of GHGs emissions in North America, Europe, Asia and Oceania. The model consists of two components, the first one includes soil climate, crop growth, decomposition sub-models and it predicts soil temperature, soil moisture, pH, Eh, and substrate concentration profiles (e.g. ammonium, nitrate, DOC) based on ecological drivers (e.g., climate, soil, vegetation and anthropogenic activity). The second component, consisting of the nitrification, denitrification and fermentation sub-models, predicts C and N gases fluxes, such as nitric oxide (NO), N₂O, CH₄ and NH₃ fluxes, based on the soil environmental variables.

The DNDC model is the most prominent process-based model used for simulating GHG emissions worldwide, however, it has known issues in simulating soil hydrology as also observed in other biogeochemical models such as Century or EPIC (Smith et al., 2020). Several iterations of the DNDC model have been developed for different region, in order to include additional processes and management options and to overcome problems related to specific pedo-climatic conditions. Specifically, the Canadian version (DNDCv.CAN) has been recently updated with new features of interest that improve soil hydrology simulations (figure 10). In particular Smith et al., (2020) reported that after development, simulation of soil water storage, daily drainage, N loss to runoff and N loss to tile drains were improved. This new version of the model gave good results because of an improved water flow down the profile, thanks to new root density functions, to the setting option for a fluctuating water table and a new mechanistic tile drainage option (TD). Moreover, the new version can include an heterogenous soil profile, extend soil depth to 2 m, accommodate better the effective root penetration, and was implemented with additional crop parameters.

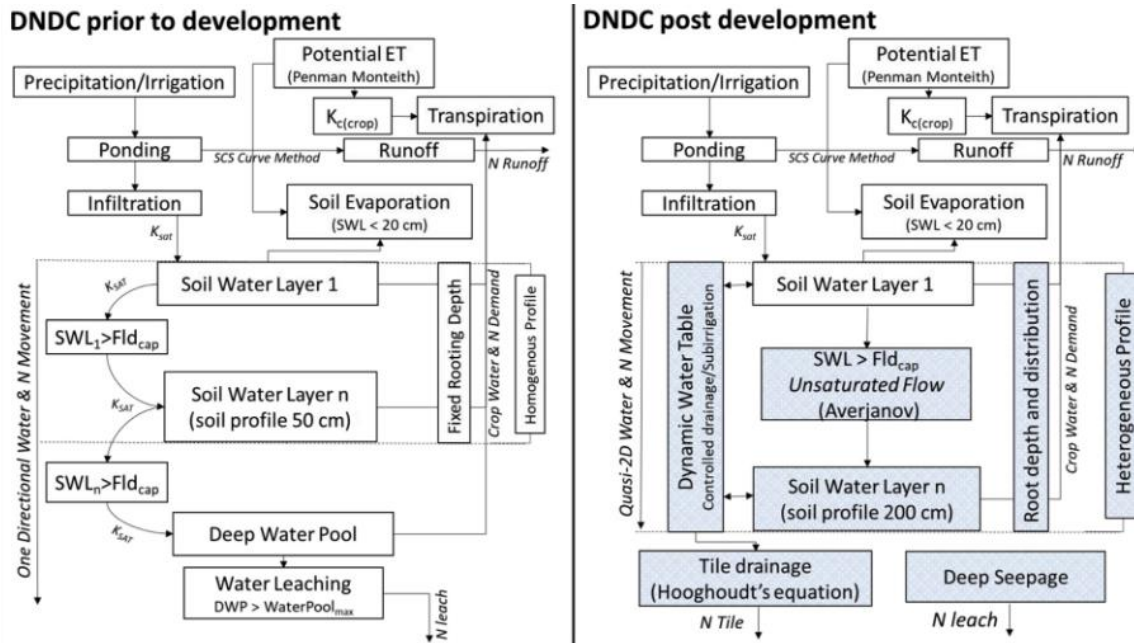


Figure 10: Schematic of Canada DNDC before and after development of improved hydrological processes.

Shaded areas show which algorithms were modified. Revised model version available at

<https://github.com/BrianBGrant/DNDCv.CAN>.

2.4 Description of the simulation experiment

In this thesis work, simulations with DNDCv.CAN have been carried out, the revised version of the DNDC model available at <https://github.com/BrianBGrant/DNDCv.CAN>. The DNDC model runs were performed by comparing soil water, C and N fluxes from simulating WT dynamics with mechanistic tile drainage (TD) versus the absence of a water table control (noTD) (figure 11) according to the traditional model without a water table module. In particular, it is of interest to understand how this new option influences the simulation of the soil moisture and the consequent influence in the GHGs fluxes. The observed data retrieved in the experimental site described above (section 2.1) have been compared with simulated data. More precisely, the latter were the results of simulation recreating the real-field conditions of the 12 lysimeters (table 1) both with active water table and not (TD and noTD). In the following sections are presented the parameters used to create the .dnd files readable from the model, to run the simulations. The 12 lysimeters simulated in this analysis are referred as “2_60_250”, “3_120_368”, “6_120_368”, “7_120_250”, “8_FD_250”, “10_FD_368”, “11_60_250”, “12_FD_368”, “13_120_250”, “16_60_368”, “19_60_368”, “8_FD_250”.

From now on in order to describe the main parameters that the model requires as input, it will be taken into account the lysimeter “2_60_250” as example.

| | | | |
|---|--------------------------------|--------------------------------|--------------------------------|
| WaterTable Depth (m) | <input type="text" value="2"/> | Water Table (0=Yes 1=No) | <input type="text" value="0"/> |
| 2m=WaterTable Active: >2m= NoWaterTable | | 0=TileDrainActive, 1=FreeDrain | |

Figure 11: Water Table setting: "0" to set an active WT (TD), "1" to set free drainage conditons (noTD)

2.4.1 Climate Tab

First model information are related to site name, latitude and longitude, number of years simulated and the climate conditions (figure 12). In this work the simulations were conducted for a 5-year time span that was related to the experimental one. Despite the observed data that were used for the comparison have been retrieved between 2011 and 2014, on year more is run. The run of 2010 was used as a spin-up period to let the model set up and arrange itself, but output data will not be considered. Moreover, the observed data for 2011 were not complete, so the comparison was performed for 2012,2013 and 2014. Daily meteorological data files have been prepared in advance with 365 days for a year; each year has an individual file in a plain text format. In this set of simulations, minimum/maximum temperature (° C) and precipitation (cm) were included in the meteorological files. Between 2011 and 2013 meteorological data were retrieved from a database collected by ARPAV, while in 2014 it was implemented an *in situ* meteorological station. Meteorological data are important because they are implemented by the model to calculate the potential evapotranspiration (PET) of the site.

Input Information

Climate | Soil | Cropping | TileDrain and Model Params | Save |

Site: 2_60_250
 Latitude: 45.34
 Simulated years: 5
 Record daily results:

Obtain meteorological data from your database
 Select Climate Files: [Down] [Up] Use 1 year climate file for all years:

C:\DND\meteo\legnaro.2010\NowindNoRad.bt
 C:\DND\meteo\legnaro.2011\NowindNoRad.bt
 C:\DND\meteo\legnaro.2012\NowindNoRad.bt
 C:\DND\meteo\legnaro.2013\NowindNoRad.bt

N concentration in rainfall (mg Nl or ppm) = 0
 Atmospheric background NH3 concentration (ug N/m³) (0.06) = 0.06
 Atmospheric background CO2 concentration (ppm) (350) = 380
 Annual increase rate of atmospheric CO2 concentration (ppm/yr) = 0
 Or read annual CO2 concentrations from a file:
 CO2 File Name:

Select a format matching your climate file(s)
 Jday, MeanT, Prec
 Jday, MaxT, MinT, Prec
 Jday, MaxT, MinT, Prec, Radiation
 Jday, MaxT, MinT, Prec, WindSpeed
 Jday, MaxT, MinT, Prec, WindSpeed, Radi, Humi
 Jday, MaxT, MinT, Prec, WindSpeed, Humidity
 Jday, MaxT, MinT, Prec, Humidity
 Prec (cm), Radiation (MJ/m2/day), WindSpeed (m/s), Humidity (%)

Accept

OK Cancel Apply Help

Figure 12: Climate tab input

2.4.2 Soil tab

In this section, soil physical-chemical characteristics of each lysimeter were implemented (figure 13). Firstly, the land-use was selected. Parameters like texture (“loam” in our case) and pH were the same for every lysimeter, while bulk density (g/cm³), water-filled porosity at field capacity and at wilting point (0-1), porosity (0-1), saturated water conductivity (m/hr), and clay fraction (0-1) were specific for each lysimeter. These parameters were included according to the soil layer of sampling and analysis (figure 14). Free drainage conditions or active WT were selected in this tab.

Input Information

Climate | Soil | Cropping | TileDrain and Model Params | Save |

Land-use: (1) Upland crop field
 Top soil properties
 Texture: (S) Loam 0.19
 Depth of Soil Profile (m): 2
 Define soil texture profile by specifying
 top soil (0-10cm) texture: Bulk density: 1.531 Field capacity (wfps): 0.25 Clay fraction (0-1): 0.17
 Heterogeneous profile: Soil pH: 8.1 Wilting point (wfps): 0.124 Porosity (0-1): 0.422
 Soil structure
 Bypass flow rate (0-1): 0.422 Water Table Depth (m): 2 Water Table (0=Yes 1=No): 0
 2m=WaterTable Active, >2m=NoWaterTable 0=TileDrainActive, 1=FreeDrain

Initial soil organic C (SOC) content, partitioning and profile
 SOC at surface soil (0-10cm) (kg C/kg soil): 0.0085
 SOC partitioning
 Re-define: Bulk C/N: 10.0908
 V.L litter Labile litter Resistant litter Humads Humus Biochar
 Fraction: 0 0 0.01 0.0177 0.9723 0
 C/N: 5 25 100 10 10 500

Modify decomposition rates by multiplying a factor for SOC pools
 Litter Humads Humus

Initial N concentration at surface soil (mg N/kg): nitrate: 0.5 ammonium: 0.05
 Microbial activity index (0-1): 1
 Slope (0-90 degree): 0.05
 Soil salinity index (0-100): 1
 Rain water collection index: 1
 Use SCS and MUSLE functions:
 Define hydro-parameters:

Accept / Save Changes

OK Cancel Apply Help

Figure 13: Soil tab

Define heterogeneous soil profile ×

Thickness of soil profile (m) Number of texture layers

| | Thickness (m) | Density (g/cm ³) | SOC (kgC/kg) | pH | Texture | Clay (fraction) | Fldcap (wfps) | Wiltpt (wfps) | Porosity (v/v) | Hydro-Cond. (m/hr) |
|-----------|------------------------------------|------------------------------------|------------------------------------|----------------------------------|---|-----------------------------------|------------------------------------|------------------------------------|------------------------------------|------------------------------------|
| Layer 1: | <input type="text" value="0.05"/> | <input type="text" value="1.531"/> | <input type="text" value="0.008"/> | <input type="text" value="8.1"/> | <input type="text" value="(S) Loam 0.1"/> | <input type="text" value="0.17"/> | <input type="text" value="0.25"/> | <input type="text" value="0.124"/> | <input type="text" value="0.422"/> | <input type="text" value="0.008"/> |
| Layer 2: | <input type="text" value="0.075"/> | <input type="text" value="1.463"/> | <input type="text" value="0.008"/> | <input type="text" value="8.1"/> | <input type="text" value="(S) Loam 0.1"/> | <input type="text" value="0.17"/> | <input type="text" value="0.27"/> | <input type="text" value="0.107"/> | <input type="text" value="0.448"/> | <input type="text" value="0.012"/> |
| Layer 3: | <input type="text" value="0.05"/> | <input type="text" value="1.463"/> | <input type="text" value="0.007"/> | <input type="text" value="8.1"/> | <input type="text" value="(S) Loam 0.1"/> | <input type="text" value="0.17"/> | <input type="text" value="0.2"/> | <input type="text" value="0.183"/> | <input type="text" value="0.448"/> | <input type="text" value="0.010"/> |
| Layer 4: | <input type="text" value="0.1"/> | <input type="text" value="1.463"/> | <input type="text" value="0.007"/> | <input type="text" value="8.1"/> | <input type="text" value="(S) Loam 0.1"/> | <input type="text" value="0.17"/> | <input type="text" value="0.28"/> | <input type="text" value="0.146"/> | <input type="text" value="0.448"/> | <input type="text" value="0.010"/> |
| Layer 5: | <input type="text" value="0.05"/> | <input type="text" value="1.521"/> | <input type="text" value="0.007"/> | <input type="text" value="8.1"/> | <input type="text" value="(S) Loam 0.1"/> | <input type="text" value="0.17"/> | <input type="text" value="0.384"/> | <input type="text" value="0.105"/> | <input type="text" value="0.426"/> | <input type="text" value="0.011"/> |
| Layer 6: | <input type="text" value="0.25"/> | <input type="text" value="1.576"/> | <input type="text" value="0.006"/> | <input type="text" value="8.1"/> | <input type="text" value="(S) Loam 0.1"/> | <input type="text" value="0.17"/> | <input type="text" value="0.311"/> | <input type="text" value="0.118"/> | <input type="text" value="0.405"/> | <input type="text" value="0.022"/> |
| Layer 7: | <input type="text" value="0.05"/> | <input type="text" value="1.545"/> | <input type="text" value="0.006"/> | <input type="text" value="8.1"/> | <input type="text" value="(S) Loam 0.1"/> | <input type="text" value="0.17"/> | <input type="text" value="0.331"/> | <input type="text" value="0.102"/> | <input type="text" value="0.416"/> | <input type="text" value="0.011"/> |
| Layer 8: | <input type="text" value="0.125"/> | <input type="text" value="1.545"/> | <input type="text" value="0.007"/> | <input type="text" value="8.1"/> | <input type="text" value="(S) Loam 0.1"/> | <input type="text" value="0.17"/> | <input type="text" value="0.299"/> | <input type="text" value="0.166"/> | <input type="text" value="0.416"/> | <input type="text" value="0.029"/> |
| Layer 9: | <input type="text" value="0.2"/> | <input type="text" value="1.57"/> | <input type="text" value="0.008"/> | <input type="text" value="8.1"/> | <input type="text" value="(S) Loam 0.1"/> | <input type="text" value="0.17"/> | <input type="text" value="0.253"/> | <input type="text" value="0.152"/> | <input type="text" value="0.407"/> | <input type="text" value="0.020"/> |
| Layer 10: | <input type="text" value="1.05"/> | <input type="text" value="1.57"/> | <input type="text" value="0.008"/> | <input type="text" value="8.1"/> | <input type="text" value="(S) Loam 0.1"/> | <input type="text" value="0.17"/> | <input type="text" value="0.365"/> | <input type="text" value="0.112"/> | <input type="text" value="0.407"/> | <input type="text" value="0.016"/> |

Figure 14: Heterogeneous soil profile

2.4.3 Cropping tab

All information related to the crop system is reported in the “Cropping tab”, including farm management practices for every single year of the simulation such as date of sowing and harvest, crop growth parameters, etc. The first section (“Crop”) was the same for all lysimeters, including the number of crops per year, the crop type, the planting and harvest day and the crop variety (figure 15). These parameters have been implemented considering a specific database available for the study area of interest, the adjusted values can be observed in the following figure.

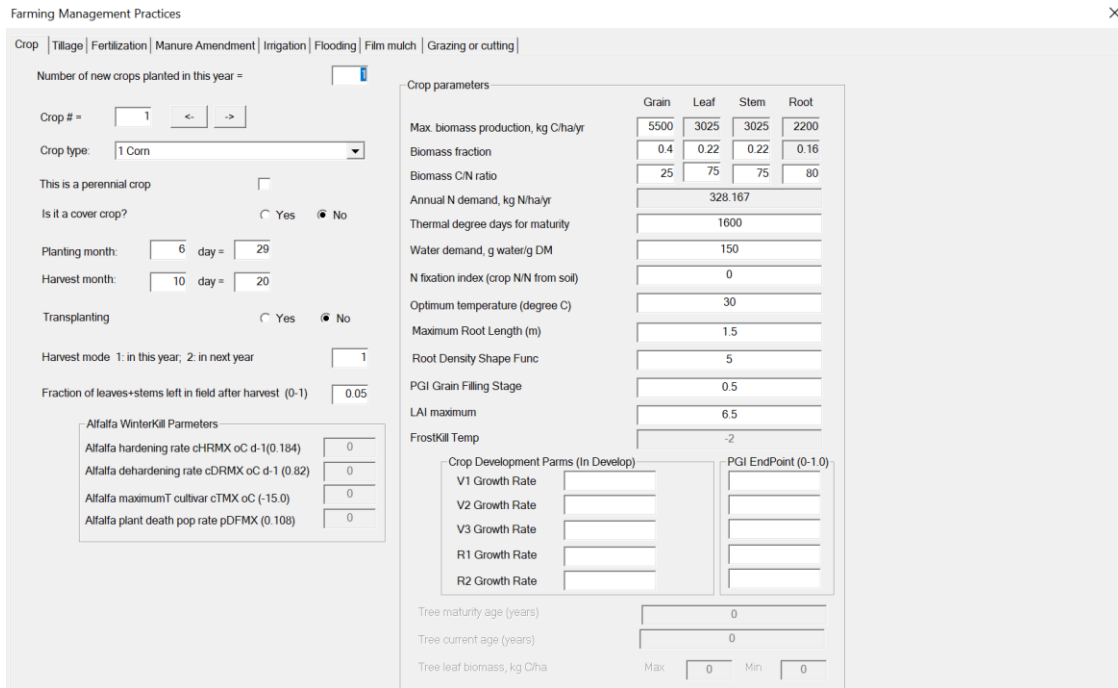


Figure 15: Crop section

Besides, in the cropping tab it can be set up the tillage activity and the fertilization and manure amendment characteristics. For all the 12 lysimeters the tillage activity selected was “ploughing with moldboard, 20cm”, performed at the day of the planting. Beyond the soil characteristics, what differentiates the .dnd files representing the lysimeters is the amount of inorganic N fertilization and of manure amendment applied (see section 2.1.1). The last sections of this tab (irrigation, flooding, film much, grazing) have not been considered in this analysis. The irrigation was not applied through this tab because since the model reads both precipitation and irrigation as input sources of water. In this work, all input water that entered each lysimeter was provided through the climate file. Finally, conditions such as film much, flooding conditions and grazing were not applied being not representative of the study site.

2.4.4 Tile Drain and Model parms tab

The “Tile drain” tab (figure 16) has been added with the upgraded version of the DNDC model and it presents some sub-sections. The tile drain module was designed by Smith et al. (2020) in DNDC model to better emulate what is observed in Eastern Canada (high water table in the spring, then drops during the summer and returns during the

late fall-winter). It is meant to define the general tile drain setup for the simulation and allows for a greater control over internal parameters that affect major outputs. Specifically, it is possible to set the drain depth (m), the drain spacing (m) and its radius (m), the depth to bedrock (m) and a factor (keDrain) that controls the rate of horizontal effective saturated conductivity to the tiles. Other parameters specific for NO₃ percolation, urea hydrolysis, N runoff, trace gas fluxes, soil temperature and water balance can be calibrated. More information that describe all these new parameters are available at <https://github.com/BrianBGrant/DNDCv.CAN/blob/master/DNDCvCAN%20User%20Guide.pdf>.

Figure 16: Tile drain parameters

2.5 Calibration and evaluation of model performance

In this work, one of the parameters used for calibration was the drain depth, in order to match the experimental soil moisture with the modelled one. It follows that best performances were found by setting the tile drain at 100 cm depth for WT60, and at 130 cm for WT60. The drain depth values arise after an empirical manual calibration performed considering the daily soil moisture (mm) in the two year-period 2013-2014, when the daily observed data have been retrieved on field with the new TDR system.

More precisely, the target of this calibration was to choose the drain depth setting that allowed to have the trend and the average of soil moisture daily values the more similar as possible to the observed data. Slight variations in SOM mineralization coefficients, N leaching, and crop growth parameters were also made across lysimeters (not lysimeter-specific calibration was performed) to close experimental and modelled yearly averaged data. In addition to the drain depth, the parameters were changed as reported in the following table (2), in order to better simulates the fluxes of GHG emissions and water and nitrate percolation.

| Parameter | Original value | Changed value |
|---------------------------|----------------|---------------|
| Bypass flow rate | 0.422 | 0 |
| Adjusted_litter_factor | 0.0179 | 3 |
| Adjusted_humads_factor | 0.9721 | 3 |
| Adjusted_humus_factor | 1 | 3 |
| MaxNF overall N movement | 0.5 | 0.05 |
| N not pref leach when sat | 0.75 | 0.95 |
| N2:N2O factor | 2 | 100 |

Table 2: DNDC parameters before and after calibration

In order to evaluate the performance of the model three statistic metrics have been considered, that are the root mean square error (RMSE), the percent bias (PBIAS) and the coefficient of determination (R^2). They have been calculated considering observed data measured directly in the study area and corresponding simulated data, obtained running the model both with the WT option active (TD) and not (noTD). Particularly, for the following parameters: grain production ($\text{kg C ha}^{-1} \text{ yr}^{-1}$), N_2O soil emission ($\text{kg N ha}^{-1} \text{ yr}^{-1}$), CO_2 soil emission/consumption ($\text{kg C ha}^{-1} \text{ yr}^{-1}$), CH_4 soil emission/consumption ($\text{kg C ha}^{-1} \text{ yr}^{-1}$), NO_3^- percolation ($\text{kg N ha}^{-1} \text{ yr}^{-1}$) and water percolation (mm). While for soil moisture, a graphical analysis of time series of simulated and observed data was carried out.

RMSE is very common in modelling evaluation (Moriasi et al., 2007), and it is considered an excellent general purpose error metric for numerical predictions. It is defined as in equation (1):

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^n (\text{Obs}_i - \text{Sim}_i)^2}{n}}, \quad (1)$$

where Obs_i are the real observed values, Sim_i the predicted values, and n the number of observations available for analysis. RMSE is a good measure of accuracy, but only to compare forecasting errors of different models or model configurations for a particular variable and not between variables, as it is scale dependent. RMSE values of 0 indicate a perfect fit.

PBIAS measures the average tendency of the simulated data to be larger or smaller than their observed counterparts (Gupta et al., 1999). It is calculated with equation (2)

$$PBIAS = \frac{\sum_{i=1}^n (Obs_i - Sim_i) * 100}{\sum_{i=1}^n Obs_i}. \quad (2)$$

The optimal value of PBIAS is 0, with low-magnitude values indicating accurate model simulation. Positive values indicate model underestimation bias, and negative values indicate model overestimation bias (Gupta et al., 1999).

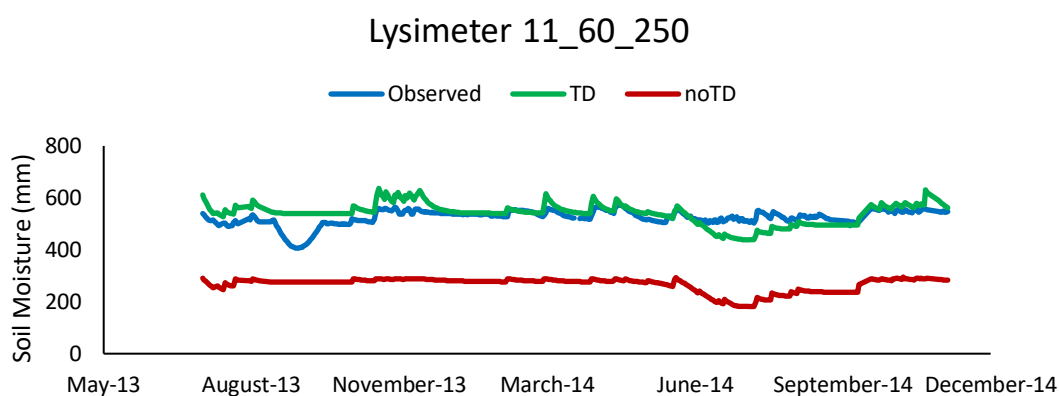
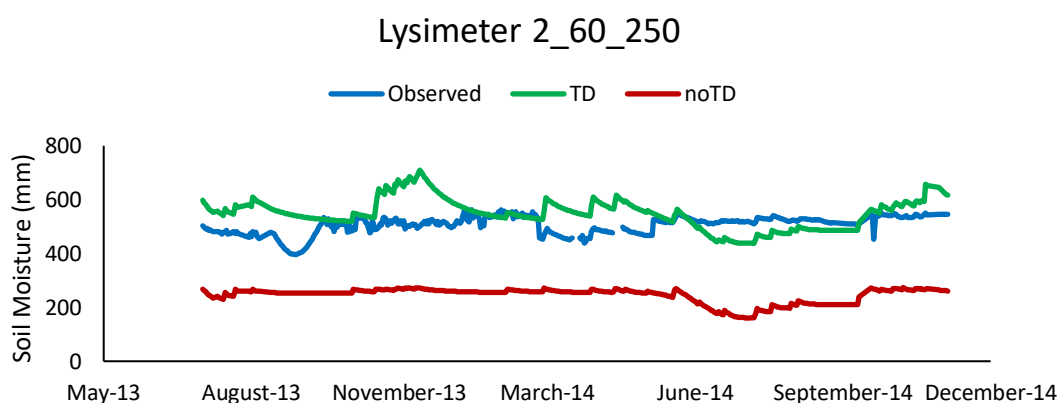
The coefficient of determination (R^2) describes the degree of collinearity between simulated and measured data. The correlation coefficient, which ranges from -1 to 1 , is an index of the degree of linear relationship between observed and simulated data. If $r = 0$, no linear relationship exists. If $r = 1$ or -1 , a perfect positive or negative linear relationship exists.

These analyses were done using Microsoft Excel software.

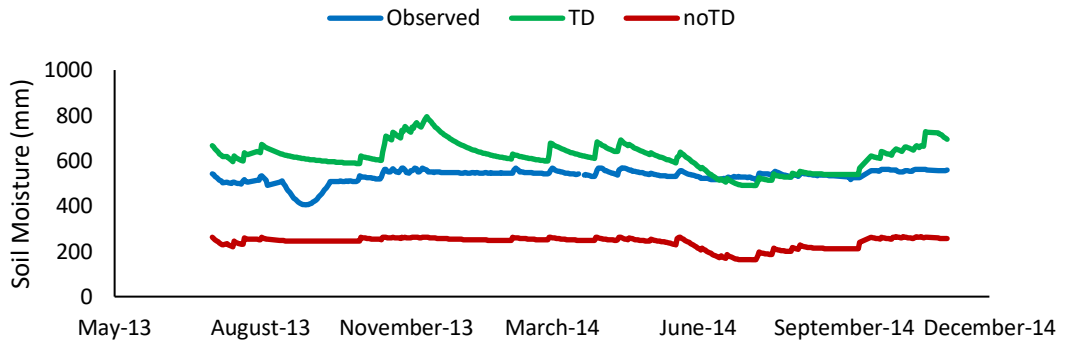
3 Results and Discussion

3.1 Soil moisture calibration and model performance

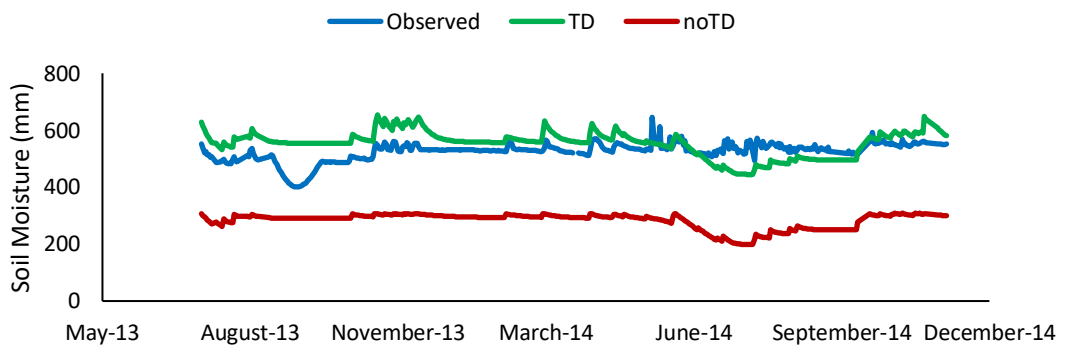
Smith et al., (2020) asserted that the enhancements to DNDC hydrological framework should enable the development of improved biogeochemical processes. With the purpose of investigating this development, the starting point was to reproduce a similar dynamic of water in the soil profile, between observed daily data and simulated data with TD. The parameterization (i.e., drain depth and bypass flow rate setting) was satisfying and a good conformity was observed. In the following graphs the simulated and observed trends of daily soil water were reported for all the WT60 and WT120 lysimeters, during the two-year period 2013-2014 (figure 17).



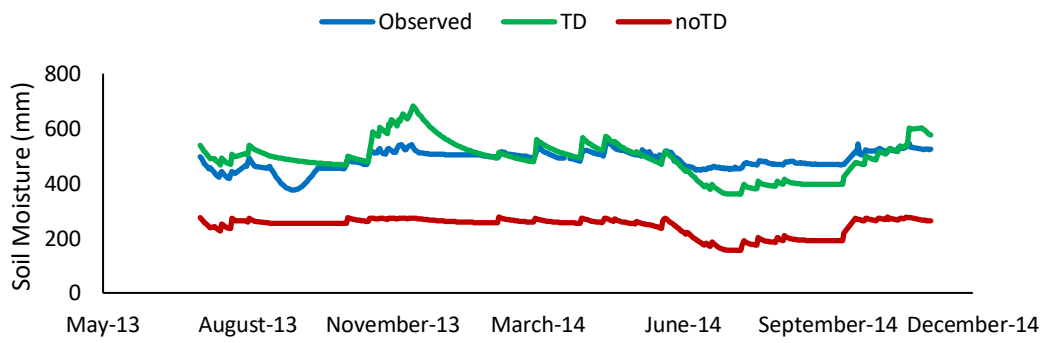
Lysimeter 16_60_368



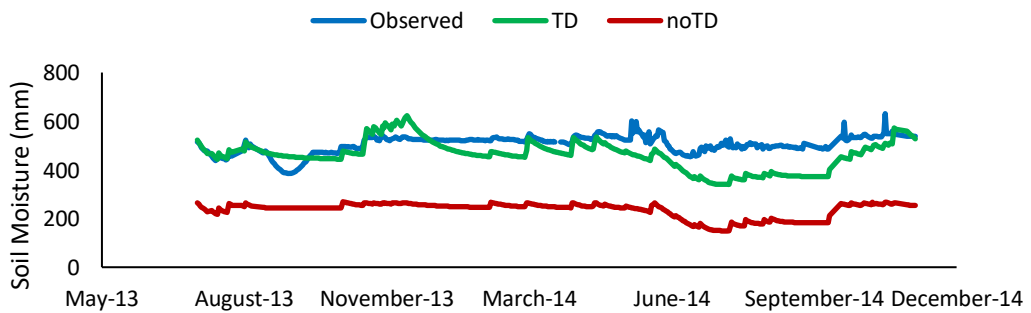
Lysimeter 19_60_368



Lysimeter 3_120_368



Lysimeter 6_120_368



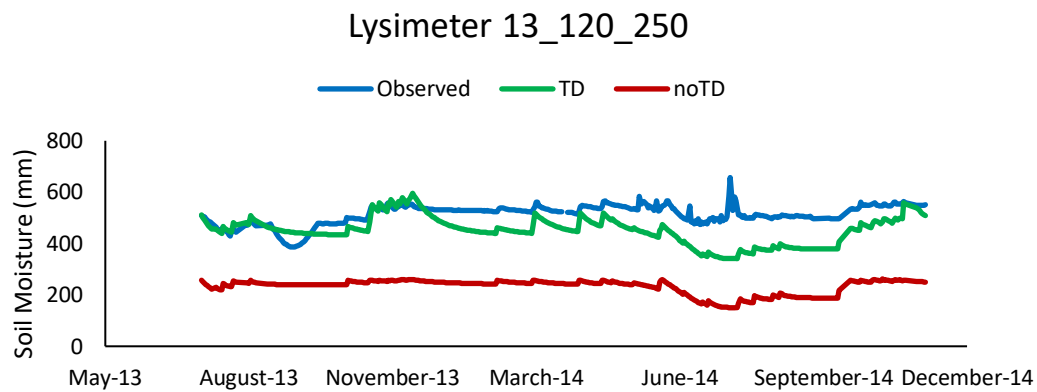
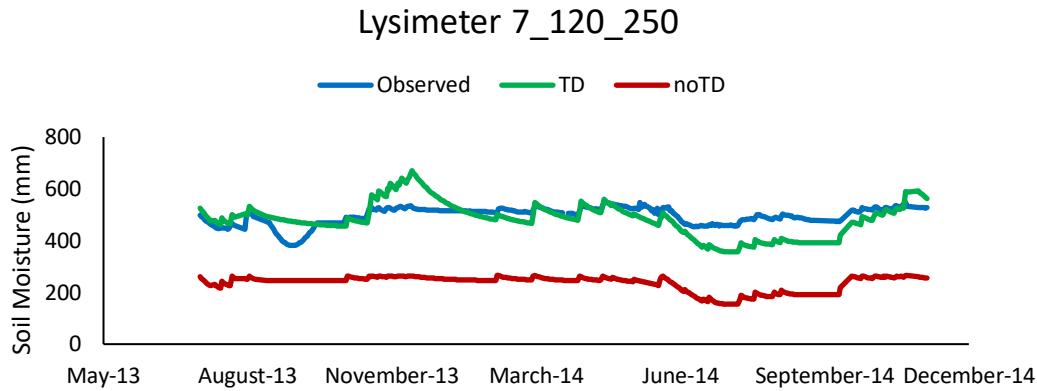


Figure17: Observed and simulated (TD and noTD) soil moisture (mm) daily data in 2013-2014, for the 8 lysimeters with WT60 and WT120

The above results suggested that the calibrated TD option improved the effectiveness of soil hydrology simulations in respect with noTD conditions (Smith et al., 2020). As reported in table 3, the average values of soil moisture (mm) were more similar to the observed ones when simulated with TD option than noTD, leading to a high underestimation using the latter. Furthermore, RMSE and PBIAS coefficients were closer to 0 for every lysimeter. In our case, soil water was overestimated in a few events, namely in September and November 2013, causing an overall overprediction of the average values. In the former event, experimental WT dropped causing a fall in soil moisture, which could not be reproduced by the model. In the latter event, the model did not catch the high amount of water loss through percolation. To be mentioned, DNDC simulates soil hydrology through the empirical cascade (tipping bucket) flow algorithm, which may lead to an overestimation of soil moisture in free drained soils, as observed by (Macharia et al., 2021), (Li et al., 2017), (Uzoma et al., 2015), Smith et al. (2019). Likewise, Zhang & Niu, (2016) contended that this is also

possible because DNDC does not include unsaturated flow and underestimates the rainfall loss caused by surface runoff and leaf interception. Nevertheless, with the presence of a WT an underestimation of soil water content may occur because the model does not take into account capillary rise in its simulations. In fact, the amount of water deriving from WT up-flux is not considered. Finally, we can confirm also for the peculiar Veneto pedoclimatic conditions the better performance of DNDCv.CAN, run with the TD option, in simulating soil hydrology, as already observed by Smith et al., (2020).

| Lysimeter | Observed | TD | noTD | TD | noTD | TD | noTD |
|-----------|----------|---------|---------|------|------|-------|-------|
| | Average | Average | Average | RMSE | RMSE | PBIAS | PBIAS |
| 2 | 506 | 549 | 245 | 109 | 266 | -10.3 | 50.8 |
| 3 | 486 | 494 | 244 | 70 | 244 | -2.34 | 49.4 |
| 6 | 506 | 462 | 235 | 81 | 273 | 7.98 | 53.1 |
| 7 | 496 | 484 | 236 | 70 | 263 | 1.87 | 52.2 |
| 11 | 525 | 540 | 266 | 62 | 261 | -3.50 | 48.9 |
| 13 | 514 | 451 | 232 | 91 | 285 | 11.6 | 54.5 |
| 16 | 533 | 618 | 239 | 116 | 295 | -16.8 | 54.8 |
| 19 | 525 | 554 | 283 | 75 | 247 | -6.14 | 45.9 |

Table 3: Average soil moisture (mm), RMSE (mm²) and PBIAS, for TD and noTD conditions

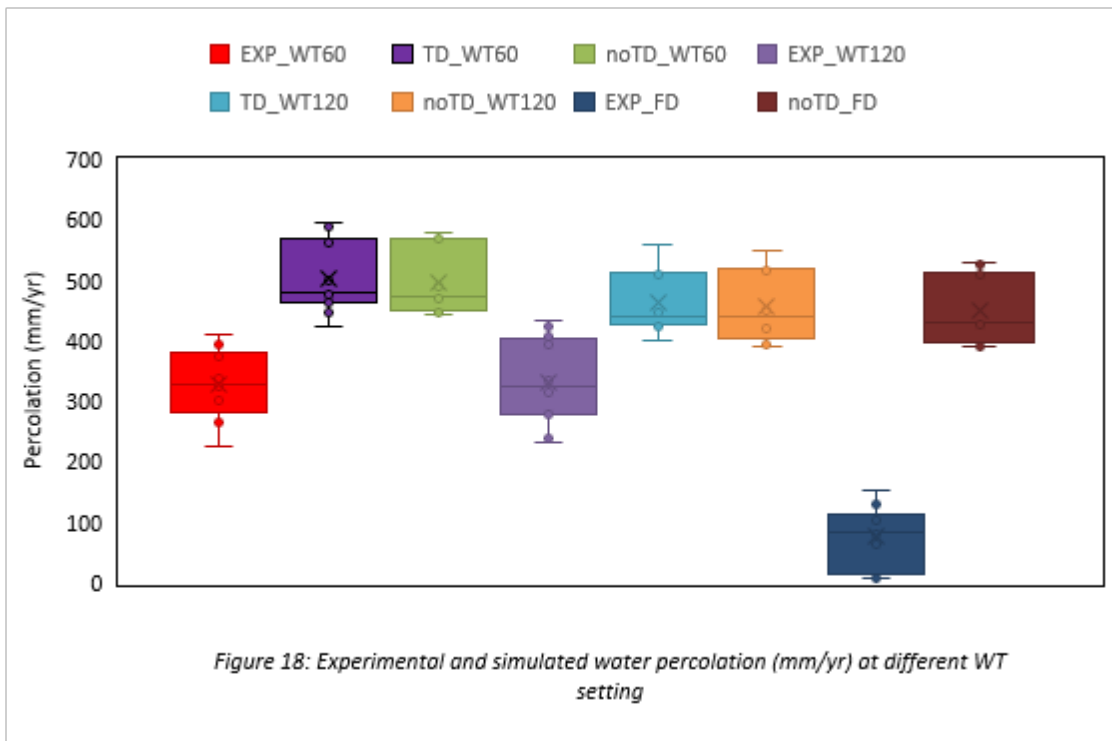
During the calibration stage, it was important to obtain simulated values in agreement with observed ones beyond soil hydrology, and some improvements were observed after the parameterization process. An overall evaluation of the model performances both with TD and noTD can be accomplished considering the RMSE, PBIAS and R² calculated after grouping the lysimeters considering the WT conditions (table 4). The evaluation was developed for grain production (kg C ha⁻¹ yr⁻¹), N₂O soil emission (kg N ha⁻¹ yr⁻¹), CO₂ soil emission/consumption (kg C ha⁻¹ yr⁻¹), CH₄ soil emission/consumption (kg C ha⁻¹ yr⁻¹), NO₃⁻ leaching (kg N ha⁻¹ yr⁻¹) and water percolation (mm). More considerations about each one of these parameters will be discussed specifically in the following sections. In particular TD_WT60 and noTD_WT60 include lysimeters “2_60_250”, “11_60_250”, “16_60_368” and “19_60_368”. TD_WT120 and TD_noTD120 include lysimeters “3_120_368”, “6_120_368”, “7_120_250” and “13_120_250”. While noTD_FD include “8_FD_250”, “10_FD_368”, “12_FD_368” and “8_FD_250”.

| | | TD_WT 60 | noTD_WT 60 | TD_WT1 20 | noTD_WT1 20 | noTD_F D |
|---|------|---------------------|-----------------------|----------------------|------------------------|---------------------|
| Grain production | RMS | | | | | |
| | E | 1275 | 1232 | 1534 | 1533 | 1317 |
| | PBIA | | | | | |
| | S | 4.58 | 5.82 | 16.6 | 18.1 | -24.4 |
| | R2 | 0.443 | 0.615 | 0.516 | 0.821 | 0.030 |
| N₂O soil emission | RMS | | | | | |
| | E | 1.50 | 1.58 | 1.65 | 1.68 | 1.62 |
| | PBIA | | | | | |
| | S | -19.2 | 24.2 | -18.8 | 23.0 | 30.6 |
| | R2 | 0.058 | 0.050 | 0.008 | 0.003 | 0.001 |
| CO₂ soil emission/consumption | RMS | | | | | |
| | E | 1677 | 1391 | 1188 | 1083 | 1820 |
| | PBIA | | | | | |
| | S | 21.7 | 17.3 | 16.0 | 14.4 | 23.0 |
| | R2 | 0.119 | 0.224 | 0.601 | 0.644 | 0.117 |
| CH₄ soil emission/consumption | RMS | | | | | |
| | E | 3.11 | 3.10 | 3.14 | 3.14 | 2.76 |
| | PBIA | | | | | |
| | S | 1326 | 1322 | 1238 | 1236 | 8334 |
| | R2 | 0.356 | 0.352 | 0.366 | 0.370 | 0.368 |
| NO₃⁻ percolation | RMS | | | | | |
| | E | 6.60 | 46.1 | 4.41 | 46.0 | 29.9 |
| | PBIA | | | | | |
| | S | 12.9 | -388 | -23.5 | -484 | 13.4 |
| | R2 | 0.032 | 0.482 | 0.564 | 0.571 | 0.892 |
| water percolation | RMS | | | | | |
| | E | 195 | 188 | 162 | 161 | 387 |
| | PBIA | | | | | |
| | S | -53.2 | -51.3 | -39.9 | -37.8 | -540 |
| | R2 | 0.043 | 0.037 | 0.081 | 0.173 | 0.025 |

Table 4: RMSE, PBIAS and R2 for water percolation, NO₃⁻ percolation, CH₄ soil emission/consumption, CO₂ soil emission/consumption, N₂O soil emissions, and grain production for the simulations of WT60, WT120, FD lysimeters with TD and noTD

3.2 Water percolation

In order to evaluate DNDCv.CAN in its soil hydrology simulation performances, also water percolation was taken into account. Simulated percolation data showed to be higher than the observed ones, both in TD and noTD run. This appears both graphically, considering figure 18, and statistically. In fact, PBIAS is negative for all the combination of WT setting and TD/noTD options, in particular: -53.2 for TD_WT60, -51.3 for noTD_WT60, -39.9 for TD_WT120, -37.8 for noTD_WT120, -540 for noTD_FD. This overestimation of water percolation by DNDC is even larger if FD lysimeters are taken into account. In this case observed data were lower, while simulated (TD and noTD) data did not differ much in respect with WT60 and WT120 lysimeters. This higher overestimation is well depicted by the PBIAS coefficient, which is one order of magnitude lower (-39.9 for TD_WT120 and -540 for noTD_FD). Furthermore, no correlation between observed and simulated data appeared, considering all the combination of WT setting and TD/noTD options, with a maximum R^2 of 0.173 for noTD_WT120.



Moreover, in simulating water percolation TD option did not demonstrate to be better than noTD. Specifically, in 2012 the average values of the replicated lysimeters simulated showed to be comparable among these two options (table 5), in 2013 TD simulated data were closer to the observed ones, while in 2014 the opposite occurred.

| Percolation (mm) | | EXP | TD | noTD | EXP | TD | noTD | EXP | TD | noTD |
|-------------------------|--------------|------|------|------|------|------|------|------|------|------|
| WT | Treat | 2012 | 2012 | 2012 | 2013 | 2013 | 2013 | 2014 | 2014 | 2014 |
| 60 | 250 | 258 | 400 | 465 | 331 | 465 | 547 | 402 | 552 | 422 |
| 120 | 250 | 249 | 437 | 474 | 333 | 479 | 564 | 405 | 577 | 438 |
| FD | 250 | 8.40 | | 435 | 83.1 | | 528 | 133 | | 391 |
| 60 | 368 | 263 | 451 | 429 | 296 | 427 | 518 | 401 | 517 | 393 |
| 120 | 368 | 288 | 448 | 462 | 333 | 471 | 568 | 401 | 567 | 446 |
| FD | 368 | 11.8 | | 429 | 81.5 | | 513 | 108 | | 399 |

Table 5: Average water percolation values (mm) of observed, TD simulated and noTD simulated data

DNDC simulates soil moisture in each layer by calculating both surface and vertical water movements, including surface runoff, transpiration, evaporation, infiltration, water redistribution, and drainage. Primary factors influencing soil moisture include weather conditions (e.g., temperature, humidity, and wind speed), soil properties (e.g., texture, field capacity, wilting point, and hydrological conductivity, and previous soil water availability), crop growth, and FMPs (irrigation, flooding, film mulch etc.). Since all of these factors are similar or identical among the different lysimeters the simulated water balance is similar too. Hence, water percolation, that is a component of this balance, showed to be quite regular in all the records.

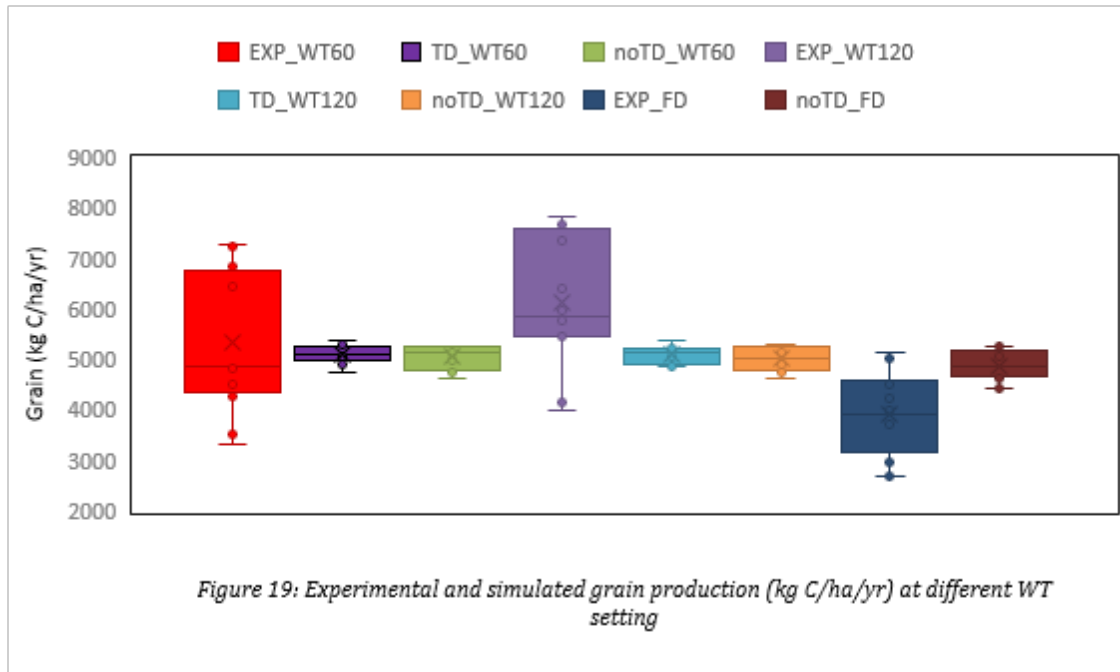
One possible factor that may have played a role is that transpiration was quite low in respect with the observed ones, and consequently the evapotranspiration (no data showed). If there is a certain amount of water in the system and runoff is more or less constant, either this amount of water leaves the system through the plant-soil system or it percolates. If the plant transpires less water, water percolation can increase.

On a broader sense, it is more likely that this overestimation was due to the core of DNDC model water simulation system. That is, like already reported, the employment of empirical tipping bucket system that neglects the role of water potentials in driving water flow in soil. In fact, the conceptual basis of a tipping bucket flow model does not

allow for upward water flows, which control both evaporation at the soil surface as well as capillary rise from groundwater into the root zone to maintain crop transpiration during dry summer periods (McBean et al., 2020; Longo et al., 2021; Jarvis et al., 2022). More specifically, in the cascade approach, water percolates if field capacity in a soil layer is reached. This also explains why with TD option the simulation did not improve, since this setting does not change the empiricism at the base of soil hydrology simulation. This limitation is not specific for the DNDC model, but for many crop models that relies on empirical components to describe soil hydrology. Capacity or tipping bucket models of soil water flow can be classified as phenomenological/empirical as they attempt to mimic the physical process of water flow without directly addressing the physical forces driving the flow, nor the soil hydraulic properties that control it. As Jarvis et al., (2022) stated, when a physics-based approach is just as easy to use as a corresponding (more) empirical approach, then it should be preferred, and that there are not any convincing reasons to still use empirical models of soil water flow. In fact, there are many studies reporting that models based on Richards' equation (physic-based approach) generally perform better (e.g. Diekkrüger et al., 1995; Maraux et al., 1998; Vancloster and Boesten, 2000; Herbst et al., 2005; Wegehenkel et al., 2008; Kröbel et al., 2010; Soldevilla-Martinez et al., 2014; Guest et al., 2017; McBean et al., 2020; Groh et al., 2022).

3.3 Grain production

Crop growth and yields are controlled by complex interactions of weather, soil conditions and crop physiological properties. Because crop growth affects soil water content, DOC, soil N pools, and production of plant litter incorporated into SOC pools, it influences almost all the biogeochemical processes in DNDC through influencing soil environmental factors and/or substrates concentrations. Hence, a good agreement between observed crop production and modelled productivity is necessary to satisfactorily simulate N and C biogeochemical cycles and consequent GHG emissions. Despite the model did not fully reproduce the high variability of observed grain yield, independently from the WT level, nevertheless, the average values were comparable (table 6), (figure 19).



| Grain (kg C/ha) | | EXP | TD | noTD | EXP | TD | noTD | EXP | TD | noTD |
|-----------------|-------|------|------|------|------|------|------|------|------|------|
| WT | Treat | 2012 | 2012 | 2012 | 2013 | 2013 | 2013 | 2014 | 2014 | 2014 |
| 60 | 250 | 5299 | 4806 | 4935 | 6233 | 5207 | 5234 | 3826 | 4993 | 4698 |
| 120 | 250 | 5226 | 4866 | 5006 | 5516 | 5155 | 5195 | 3644 | 4942 | 4777 |
| FD | 250 | 3207 | | 4663 | 4372 | | 5074 | 4280 | | 4652 |
| 60 | 368 | 7774 | 5183 | 5229 | 7516 | 5354 | 5278 | 5478 | 5098 | 4795 |
| 120 | 368 | 6636 | 5166 | 5209 | 7240 | 5354 | 5241 | 4393 | 5113 | 4685 |
| FD | 368 | 2802 | | 5156 | 4352 | | 5246 | 4472 | | 4414 |

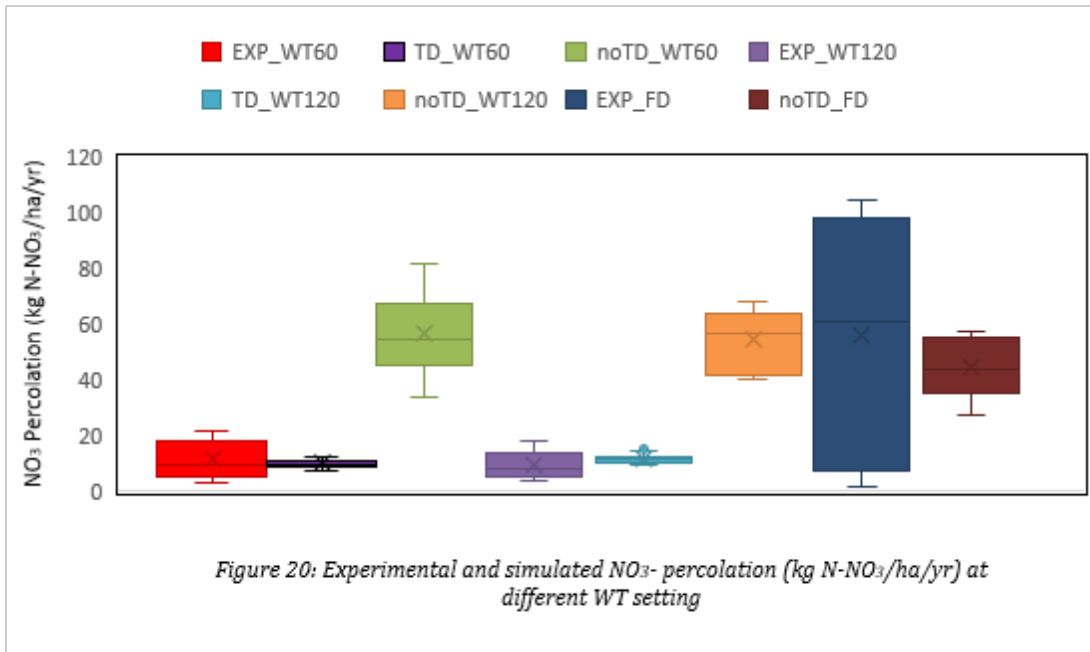
Table 6: Average grain production values (kg C/ha) of observed, TD simulated and noTD simulated data

Besides, a good agreement was observed between simulated and observed data ($R^2 > 0.5$ for noTD_WT60, TD_WT120 and noTD_WT120). Considering that DNDC model was not specifically developed to simulate crop growth and yield, results of the internal plant growth sub-model were adequate. Focusing on the differences between TD and noTD simulations in all WT conditions, no significant discrepancies arose (PBIAS and RMSE were 4.58 and 1275 kg C ha⁻¹ yr⁻¹ for TD_WT60 and 5.82 and 1232 kg C ha⁻¹ yr⁻¹ for noTD_WT60), being the presence of a simulated WT the only different parameter. The fact that TD and noTD determined similar outcomes denotes that the model did not simulate a condition of stress for the plant in the absence of WT simulation. But this is not in agreement considering the observed FD data (in 2012, 2802 kg C/ha in

average in FD_368 records) and FD lysimeters grain production results simulated with noTD (figure 19, EXP_FD).

3.4 Nitrate leaching

Running the DNDC model with the default tile drain and model parms tab parameters resulted in a large overestimation of NO_3^- percolation simulated data in respect with the observed ones. Though, after adjusting of “MaxNF overall N movement” and “N not pref leach when sat” parameters, TD simulations exhibited good agreement with the observed NO_3^- percolation values. In fact, “MaxNF overall N movement” is a factor that controls that maximum threshold value that primary controls the maximum nitrogen movement across soil layers, and it was highly decreased. While “N not pref leach when sat” regulates the fraction of N that is not susceptible to preferential leaching when the water table is above the tiles, so its increase also played a big role. After this manual calibration an important result was observed, that is, with TD the simulation of NO_3^- percolation was much better than with noTD. In fact, for TD_WT60 and TD_WT120 RMSE is $6.60 \text{ kg N ha}^{-1} \text{ yr}^{-1}$ and $4.41 \text{ kg N ha}^{-1} \text{ yr}^{-1}$, while for noTD_WT60, noTD_WT120 and noTD_FD is $46.1 \text{ kg N ha}^{-1} \text{ yr}^{-1}$, $46.0 \text{ kg N ha}^{-1} \text{ yr}^{-1}$ and $29.9 \text{ kg N ha}^{-1} \text{ yr}^{-1}$. In fact, noTD simulations gave as result an overestimation of NO_3^- percolation, with PBIAS coefficient that is equal to -388 and -484 for noTD_WT60 and noTD_WT120. This is clear also considering figure 20, where for WT60 and WT120 records the simulated values were significantly higher than the observed ones.



A possible explanation about these differences is that the calibration performed, despite having a positive influence in both the simulation settings (TD/noTD), was developed for parameters that are specifically referred for the TD option system, like expressed in DNDCv.CAN manual user guide (Grant, 2020). If averaged values are considered for TD and noTD simulations (table 7), this pattern was even clearer, suggesting that different soil N dynamics occurred between TD and noTD.

| N - NO ₃ (kg/ha) | | EXP | TD | noTD | EXP | TD | noTD | EXP | TD | noTD |
|-----------------------------|-------|------|------|------|------|------|------|------|------|------|
| WT | Treat | 2012 | 2012 | 2012 | 2013 | 2013 | 2013 | 2014 | 2014 | 2014 |
| 60 | 250 | 4.95 | 9.41 | 41.9 | 6.95 | 12.1 | 63.6 | 8.53 | 11.4 | 54.8 |
| 120 | 250 | 5.36 | 9.00 | 42.6 | 15.8 | 10.1 | 64.8 | 13.5 | 9.66 | 55.9 |
| FD | 250 | 2.05 | | 29.8 | 60.0 | | 47.3 | 55.1 | | 41.9 |
| 60 | 368 | 4.07 | 10.3 | 41.8 | 13.0 | 12.2 | 67.7 | 15.8 | 14.9 | 63.8 |
| 120 | 368 | 3.74 | 8.93 | 40.6 | 21.2 | 11.2 | 66.7 | 13.0 | 10.8 | 63.3 |
| FD | 368 | 4.65 | | 35.3 | 101 | | 56.6 | 85.1 | | 55.4 |

Table 7: Average soil NO₃-percolation values (kg N-NO₃/ha) for observed, TD simulated and noTD simulated data

Except for 2012, average experimental values for FD lysimeters were higher than WT60 and WT120 lysimeters, which is predictable in the conditions of an absent water table. In fact, there was a high correlation between observed FD NO₃⁻ percolation values and noTD_FD simulations, with R² equal to 0.892. Lastly, considering the simulation of the of TD_WT60, TD_WT120 and noTD_FD and the respective observed values, there is a

high correlation ($R^2 = 0.768$) that again depicts the positive effect of different TD and noTD simulations for different WT conditions (figure 21).

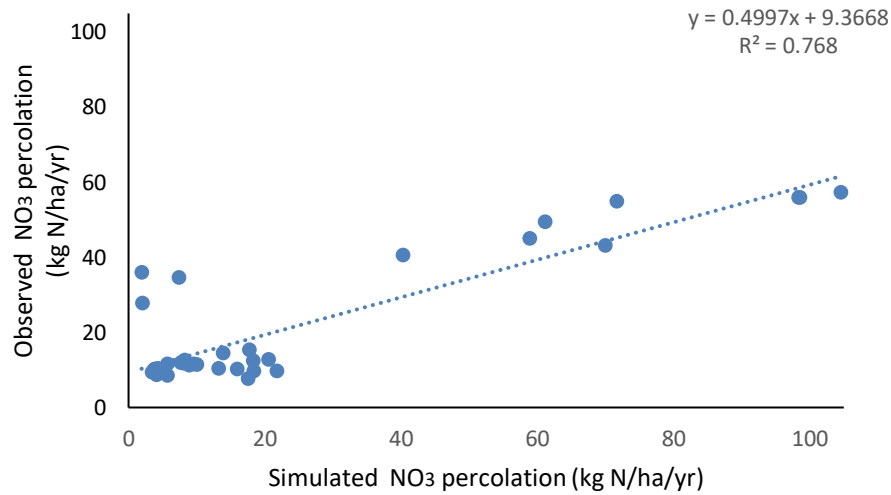


Figure 21: Linear regression between observed and simulated NO₃ percolation values (kg N/ha/yr)

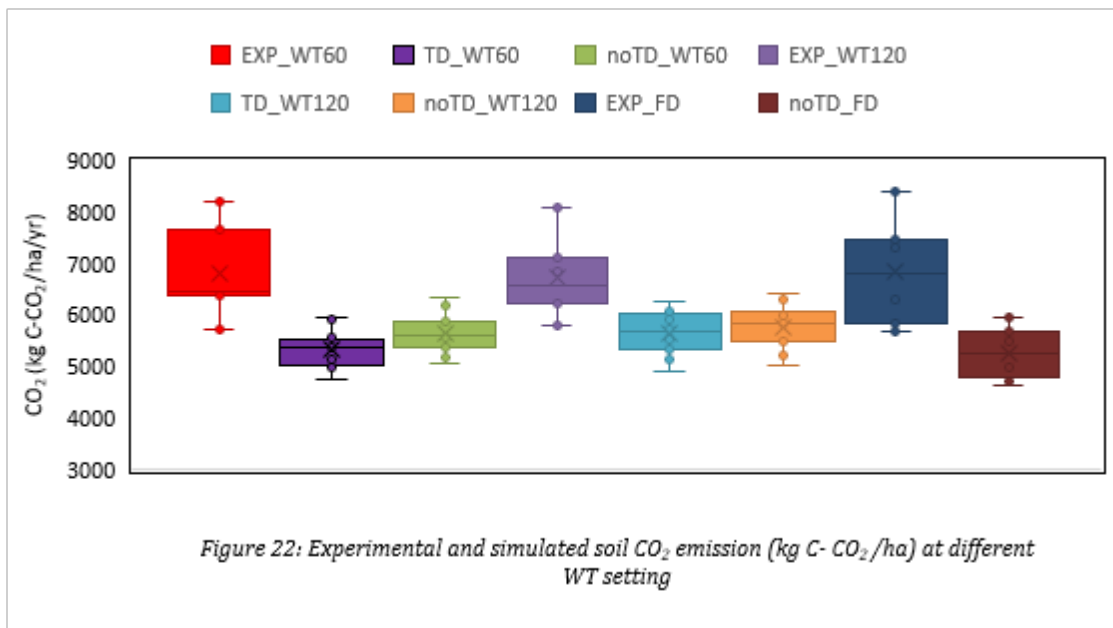
The noTD nitrate movement in DNDC is described simply as a function of the water flux and nitrate concentration per layer. Soil nitrate is considered to be mobilized by a positive water flux (90% mobilized) and transferred to the layer below as a one-dimensional vertical N flux towards the bottom soil profile. Additionally, another fraction (10% of the NO₃⁻ in a layer) was considered to be lost through preferential water flow via macropores directly out of the soil profile. This preferential loss was calculated regardless of whether the soil layer directly below also met the condition of having a positive water flux. For simulations with tile drainage, the movement of nitrate is an iterative step through each of the saturated layers per hour that are drained to tiles. In DNDCv.CAN this preferential N leaching function has been modified to ensure correlation with water movement. In fact, It was previously found that DNDC sometimes simulated N losses when there was no water flux out of the bottom of the soil profile. In DNDCv.CAN the fraction of NO₃⁻ available to be transferred to the layer below at an hourly time step can now be parameterized as described above. Nitrate losses to tile drains are calculated starting from the layer situated at the top of the saturated water table down to the layer at the bottom of the tile drains (Smith et al., 2020).

3.5 CO₂ soil emission

The modification of the decomposition rates by multiplying a factor 3 to each of the three-soil organic carbon (SOC) pools led simulated CO₂ values in line with the observed ones. This was true for WT120 lysimeters ($R^2=0.601$ for TD simulations) but not for WT60 and FD lysimeters ($R^2=0.119$ and $R^2=0.117$ for TD simulations). In fact, decomposition in DNDC is a process mediated by the microbes living in the soil describing degradation of the organic matter; part of the SOC is employed as energy source resulting in CO₂ production, and another part of the SOC is utilized for the microbial construction. During the decomposition, labile C is gradually lost with resistant C become relatively more abundant in the soil. DNDC simulates SOC decomposition by simultaneously calculating the decomposition rate for each of the SOC sub-pools (i.e., litter, microbes, humads and humus). The parameterization that increased the decomposition rate was performed for all the lysimeters combination, resulting in average soil CO₂ emissions similar among the different lysimeters (table 8). Moreover, also crop properties in the DNDC model were adjusted to conform to Veneto standards for all the lysimeters, in particular actual yield, temperature degree-day (TDD), grain:stem:root ratio and the C/N ratio of grain, stem and root. Furthermore, since CO₂ emissions are positively correlated with temperature, water filled pore space and soil temperature (Chen et al., 2013) and since these parameters are similar in the lysimeters, it is possible that this can lead in similar CO₂ emission amounts for all of them. Still, the simulated emissions underestimate the observed ones ($14.4 < \text{PBIAS} > 23.0$ for TD_WT60, noTD_WT60, TD_WT120, noTD_WT120, noTD_FD), (figure 19).

| C - CO ₂ (kg/ha) | | EXP | TD | noTD | EXP | TD | noTD | EXP | TD | noTD |
|-----------------------------|-------|------|------|------|------|------|------|------|------|------|
| WT | Treat | 2012 | 2012 | 2012 | 2013 | 2013 | 2013 | 2014 | 2014 | 2014 |
| 60 | 250 | 7524 | 5380 | 5736 | 5753 | 5055 | 5330 | 6394 | 5342 | 5496 |
| 120 | 250 | 7524 | 5350 | 5678 | 5753 | 4935 | 5199 | 6394 | 5264 | 5441 |
| FD | 250 | 5849 | | 4993 | 5675 | | 4707 | 7476 | | 4748 |
| 60 | 368 | 8088 | 6196 | 6350 | 6220 | 5805 | 5913 | 7120 | 5993 | 6019 |
| 120 | 368 | 7670 | 5660 | 5963 | 6385 | 5210 | 5467 | 6448 | 5762 | 5825 |
| FD | 368 | 6289 | | 5953 | 7293 | | 5501 | 8393 | | 5669 |

Table 8: Average soil CO₂ emission values (kg C- CO₂/ha) for observed, TD simulated and noTD simulated data



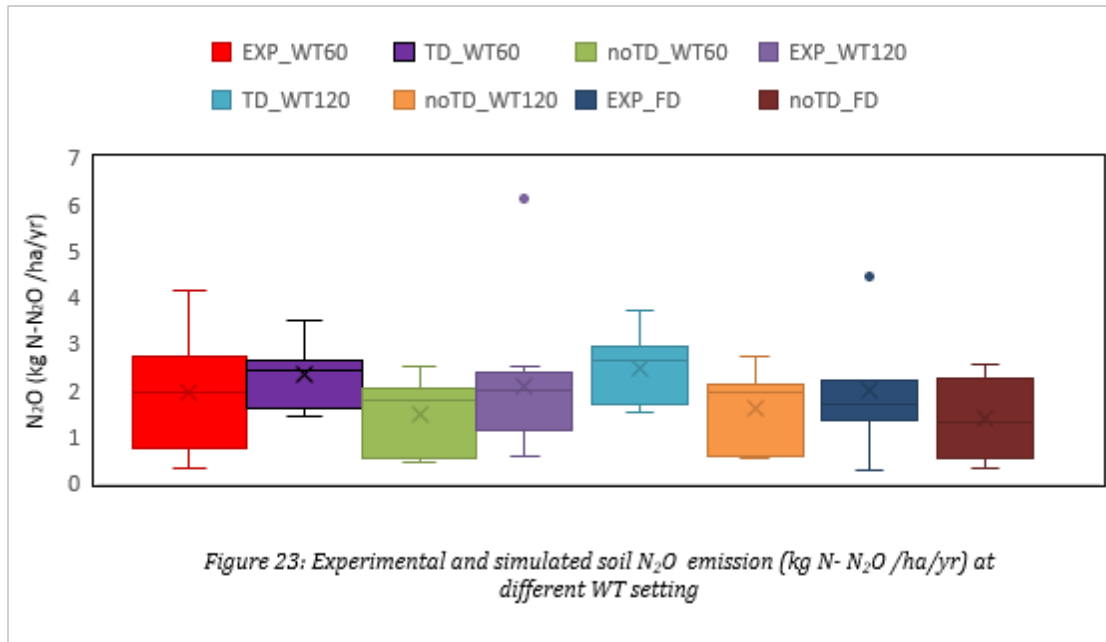
Despite the parameterization described above, that allowed a good agreement between observed and simulated data, further development is still possible. In fact, the manual calibration performed was simply to increase the decomposition rates, but it is also possible to calibrate the SOC pools and their C/N ratio in order to better describe C biogeochemical cycle. Moreover, another possibility to decrease this underestimation is to increment the spin up period run, in order to allow the model to equilibrate itself and auto-calibrate the SOC pools.

Anyway, the improved model was not able to differentiate heterotrophic CO₂ emissions according to different soil moisture conditions, being CO₂ values similar between TD and noTD. This suggest that further improvement is required to better simulate the relationship between SOM mineralization conditions and soil moisture.

3.6 N₂O soil emission

The modification of N₂:N₂O factor allowed to increase the amount of N₂ formed from N₂O, which was shown to be necessary considering the initial high N₂O soil emission values simulated by the DNDC model. Since this parameterization occurred for both TD and noTD simulations, and WT60, WT120, FD settings, in general the model responded well despite the peculiar conditions (RMSE was 1.50 kg N- N₂O ha⁻¹ yr⁻¹ for TD_WT60, 1.58 kg N- N₂O ha⁻¹ yr⁻¹ for noTD_WT60, 1.65 kg N- N₂O ha⁻¹ yr⁻¹ for TD_WT120,

1.68 kg N- N₂O ha⁻¹yr⁻¹ for noTD_WT120, 1.62 kg N- N₂O ha⁻¹yr⁻¹ for noTD_FD). An overall agreement among observed and simulated N₂O values can be inferred by figure 23, in which the distribution of the data is not significantly different, in any records.



Considering the improvement of soil moisture simulations with TD option active, it was expected a possible progress in the simulation of N₂O soil emission in these conditions. In fact, the nitrification/denitrification scheme at the foundation of the model is the concept of an “anaerobic balloon” which swells or shrinks according to redox potential of the soil (Li et al., 2004a). For each layer substrates (such as DOC, NH₄⁺ and NO₃⁻) are allocated to the anaerobic or aerobic compartments based on oxygen availability. In these terms, improved soil hydrology description would imply a more accurate redox potential evaluation. However, TD option in the simulation improves soil hydrology in the whole soil profile (2m), but in DNDC, nitrification and denitrification reactions occur primarily near the soil surface where substrates are high (Smith et al., 2020), and water content here is not necessarily improved in respect with noTD option.

| N-N ₂ O (kg/ha) | | EXP | TD | noTD | EXP | TD | noTD | EXP | TD | noTD |
|----------------------------|-------|------|------|-------|-------|------|------|------|------|------|
| WT | Treat | 2012 | 2012 | 2012 | 2013 | 2013 | 2013 | 2014 | 2014 | 2014 |
| 60 | 250 | 2.29 | 1.64 | 0.555 | 0.57 | 2.70 | 1.93 | 2.16 | 2.45 | 1.78 |
| 120 | 250 | 1.43 | 1.57 | 0.544 | 1.06 | 2.68 | 1.95 | 2.97 | 2.24 | 1.66 |
| FD | 250 | 3.18 | | 0.378 | 0.450 | | 1.45 | 1.51 | | 1.20 |
| 60 | 368 | 1.69 | 1.64 | 0.575 | 1.00 | 3.60 | 2.65 | 4.23 | 2.88 | 2.09 |
| 120 | 368 | 3.22 | 1.54 | 0.504 | 1.23 | 3.07 | 2.28 | 2.45 | 2.89 | 2.05 |
| FD | 368 | 1.90 | | 0.540 | 1.71 | | 2.55 | 3.36 | | 2.28 |

Table 9: Average soil N₂O emission values (kg N- N₂O/ha for observed, TD simulated and noTD simulated data

For TD_WT60 and TD_WT120 PBIAS was -19.2 and -18.8, while for noTD_WT60, noTD_WT120 and noTD_FD is 24.2, 23.0 and 30.6. These values depicted a clear tendency by TD simulations to overestimate N₂O soil emission, and a tendency by noTD simulations to underestimate them. The trend was also confirmed by considering observed TD and noTD averages between the replications (table 7). Especially for 2012, this underestimation was clear. The simulation option with noTD was comparable with the DNDC model version before the recent upgrade, in fact in different studies evaluating N₂O soil emission such as Abdalla et al., (2009), Macharia et al., (2021), Smith et al. (2008) and Gaillard et al., (2018), there were simulated lower values in respect with measured data. It is worth noting that N₂O production often occurs above field capacity, usually at about 80% WFPS (Butterbach-Bahl et al., 2013). It is therefore likely that a significant lower soil water content using noTD than TD (section 3.1) was sometimes reached, leading to a slight underestimation. As a final remark, more work is left to be done in understanding the biogeophysical system that produces soil N₂O and in harmonizing the process-based models that simulate that system (Gaillard et al., 2018).

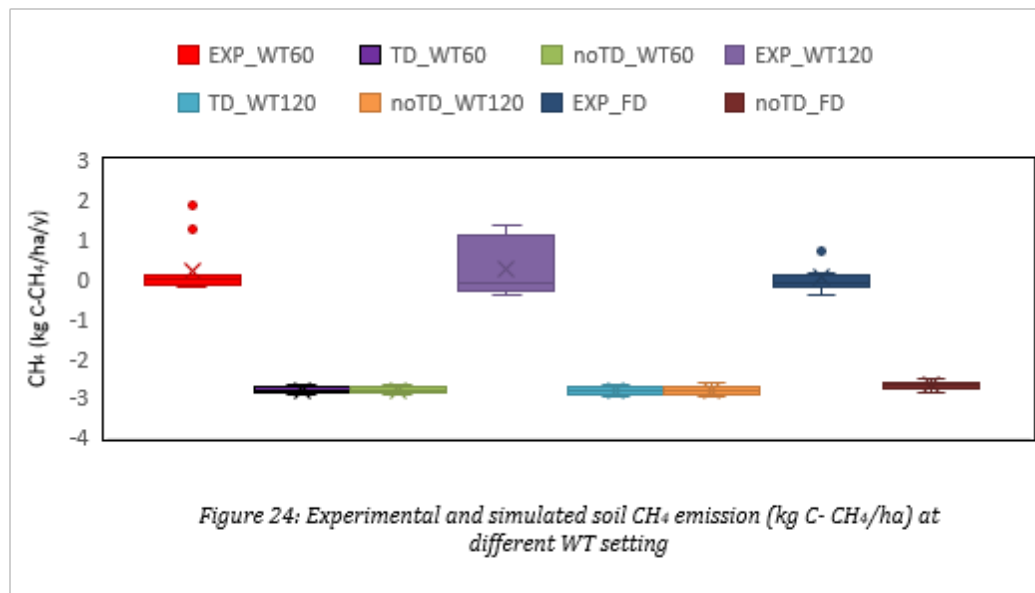
3.7 CH₄ soil emission

Figure 24 depicts CH₄ soil emissions (positive values) and sink (negative values) trends for observed and TD and noTD simulated data, at different WT settings. There were no differences arising between TD and noTD simulated data, like it is also clear observing the average values for every simulated year (table 10). In fact, considering both TD and noTD simulations in 2012-2013-2014 for all the lysimeters replicates, there was a CH₄

consumption (between 2.54 and 2.95 kg C⁻¹ ha⁻¹ yr⁻¹) by the soil, which acted as a sink. While considering observed data, the sink effect was less present with a maximum of 0.379 kg C⁻¹ ha⁻¹ yr⁻¹ consumed in 2013 in the replicates FD_368.

| C - CH ₄ (kg /ha) | | EXP | TD | noTD | EXP | TD | noTD | EXP | TD | noTD |
|------------------------------|-------|--------|-------|-------|--------|-------|-------|--------|-------|-------|
| WT | Treat | 2012 | 2012 | 2012 | 2013 | 2013 | 2013 | 2014 | 2014 | 2014 |
| 60 | 250 | -0.071 | -2.85 | -2.84 | -0.192 | -2.71 | -2.70 | 0.661 | -2.92 | -2.91 |
| 120 | 250 | -0.208 | -2.87 | -2.86 | -0.170 | -2.76 | -2.76 | 1.29 | -2.95 | -2.94 |
| FD | 250 | 0.031 | | -2.63 | -0.066 | | -2.54 | -0.089 | | -2.69 |
| 60 | 368 | 0.009 | -2.78 | -2.78 | -0.268 | -2.69 | -2.68 | 1.30 | -2.86 | -2.86 |
| 120 | 368 | -0.089 | -2.76 | -2.76 | -0.102 | -2.69 | -2.68 | 0.693 | -2.86 | -2.85 |
| FD | 368 | -0.110 | | -2.77 | -0.379 | | -2.66 | 0.808 | | -2.84 |

Table 10: Average soil CH₄ emission values (kg C - CH₄/ha) for observed, TD simulated and noTD simulated data



Probably, the model is not particularly sensitive to varying soil conditions originating from different WT setting. Hence, since the model does not simulate capillary rise, it most likely underestimates soil moisture in the surface layers, where the dynamics of formation of GHGs are more effective. DNDC simulates denitrification, reductions of Mn⁴⁺, Fe³⁺, and SO₄²⁻, and methane production as consecutive reactions with each reaction occurring under certain Eh conditions (Li et al., 2004). DNDC simulates methane production after depletions of NO₃⁻, Mn⁴⁺, Fe³⁺, and SO₄²⁻, when soil Eh is below -150 mV (Li et al., 2004). Methane consumption is simulated as an oxidation reaction involving electron exchange between CH₄ and oxygen. This means that in

respect with the real conditions, in this work DNDC probably detected a major presence of oxygen in the soil pore space. This determines more methane consumption than production because soil Eh does not reach levels low enough to allow methanogenesis bacteria to work. Another important factor that surely influences methane cycle is the substrate, that is SOC. As already stated in CO₂ section DNDC allows to parametrize the distribution of SOC in different pools. It is possible that a calibration of these parameters would increase the agreement between simulated and observed methane emissions/consumption. Furthermore, during the two-year period 2011-2012 it was applied a commercial typology of manure as organic input, with high level of maturity of the organic component and low water content. On the contrary, during 2013-2014 it was applied cattle slurry with significantly higher water content and chemical properties variable during the years. Probably, the slurry applied in 2014 was not completely mature. Because of this, the production of methane may have already happened during the storage period, or in the days immediately after its application. Since in the input section of the model, It is not possible to describe the peculiar and variable characteristics of 2013 and 2014, it is not possible for DNDCv.CAN to depict these higher emissions of CH₄. On the contrary, it simulated a constant sink effect of the soil because of the redox conditions and because of constant manure and slurry compositions.

4 Conclusion

In this study a new version of the DNDC model (DNDCv.CAN) was tested after calibration for a set of lysimeters with shallow WT in an attempt to simulate the Veneto low-lying plain conditions. Among the new features of this upgraded version, the model ability to simulate soil moisture conditions was encouraging, being a fluctuating shallow groundwater condition and maintenance of high soil moisture well described in correspondence with rainfall events. Considering soil moisture, we can therefore assess even for these peculiar pedoclimatic conditions the better performance of DNDCv.CAN, run with the TD option which allows to simulate an active WT. Notwithstanding, simulated percolation data showed to be higher than the observed ones, although this was observed regardless the use of TD or noTD. So, the improvement of soil hydrology is not fully accomplished. In fact, the absence of capillary rise and low evapotranspiration rate has likely determined more water output from the system than under field experimental conditions. This disagreement is probably due to the fact that DNDCv.CAN remains a biogeochemical model, not specifically developed for soil hydrology. In fact, the empiricism applied in the hydrological sub-model may be limiting if compared for example with a physics-based simulation's algorithm. Additionally, it was also observed a good agreement between the simulated and observed data of crop growth and yields, thanks to the utilization in input of crop parameters specific for the Veneto region. This was important since N and C biogeochemical cycles and consequent GHG emissions are indirectly dependent on this parameter. With a new N leaching function correlated with water movement, and with the possibility to parameterize the fraction of nitrate available to be transferred to the layer below, DNDCv.CAN with TD allowed to model in a good way NO_3^- leaching when a WT was present. With regard to GHGs, it was detected a nice overall agreement between observed and simulated data of CO_2 and N_2O soil emission. This was possible thanks to the parametrization of the decomposition rates and of the $\text{N}_2:\text{N}_2\text{O}$ ratio coefficient. Considering CH_4 , the model simulated soil as a sink, whilst this was not observed in every lysimeter and every year under real conditions. In general, for the fluxes of GHGs no significant differences arose between TD and noTD simulated data, suggesting that improvement of average soil moisture conditions

along the soil profile was not a driving factor to affect the C and N biogeochemical fluxes. It is likely that the model inability to simulate the capillary rise had low effects on the surface moisture conditions, in turn limiting changes in C and N forms. Hence, in this study the improvement of soil moisture and nitrate leaching simulation employing the TD option of DNDCv.CAN emerged, but this did not result in a significant improvement of soil GHGs emission simulations. In the end, this work helped in the purpose of advancing the prediction of agroecosystems water, C and N fluxes under shallow groundwater conditions, therefore helping policymakers and practitioners in the valuation of ecosystem services provided by the agricultural sector. Anyway, this was one of the first attempts of calibration and validation of agroecosystem outcomes under shallow conditions typical for the Venetian low-lying plain. This determines an important first step, but more work and research is required to implement soil hydrology dynamics and effects on GHGs emissions.

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