Process-oriented simulation and observations of N_2O emission from intensively managed agricultural cropping system

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Abstract — We report experimental observation and model simulations of N_2O emissions in a cropland, located in Southern Italy, candidate ICOS (Integrated Carbon Observation system) level 1 site. Eddy Covariance (EC) and chamber measurements were conducted on sorghum wheat and corn crops over several years. The Agricultural Productions Systems sIMulator (APSIM) model was used to simulate the N_2O emission. Our preliminary results indicate that APSIM was able to catch the seasonal dynamics of the N_2O fluxes, when compared to the EC observations. A considerably lower agreement was found with static chamber measurements. Amount and timing of nitrogen fertilization drive the N_2O emission. Overall, we found APSIM simulations underestimated the cumulative values, compared to both eddy covariance and chambers observations.

Keywords—*GHGs fluxes, nitrogen cycle, agriculture management*

I. Introduction

Nitrous oxide (N_2O) is a major greenhouse gas (GHG) with a global warming potential ~300-fold compared to CO_2 over a 100-y period (**1**). N_2O is the major stratospheric ozone-depleting substance and is projected to remain so for the future (**2**). Soil N_2O emissions are produced predominantly by the microbial processes of nitrification (oxidation of ammonium to nitrate) and denitrification (reduction of nitrate via N_2O to N_2) (**3**), contributing globally to ~50% of anthropogenic N_2O emissions (**1**), mainly as a result of the addition of synthetic nitrogen (N) fertilizers and animal manure to soil (**4**). The environmental drivers of the N_2O emission are well known from the literature, i.e NH_4^+ and NO_3^- concentrations in soil, labile organic carbon as substrate for heterotrophic microorganisms, soil temperature and water content, soil oxygen concentration, and soil pH (**5-6**). Nevertheless, the variation in observed N_2O emissions with known environmental drivers is still posing a challenge for explanation, reflecting the limited ability to comprehensively measure or model N cycling processes and their interactions (**5-7**). Biogeochemical processes models allow for the ex-ante and ex-post estimation of GHG emissions (including N_2O), taking into account the different agronomic practices, fertilization rates and environmental conditions. Among the models currently available, the Agricultural Productions Systems sIMulator (APSIM) (**8**) represents a suite of models used to simulate a wide range of complex agricultural systems. It contains interconnected biophysical and management modules to simulate systems comprising soil, crop, trees, pasture and livestock; it has as well the flexibility to integrate non-biological farm resources such as water storage and farm machinery.

As a process-based model, APSIM describes the main processes of N cycle in ecosystems and synthesizes the current understandings from experimental results. In a complex system like soil – plant – atmosphere, differences between model predictions and observations are rather common for N_2O emissions because of the complicated microbiological, chemical, and physical processes interactions between soil and plants (5).

A particular strength of APSIM is the inclusion of responsive rule-based management where management practices can be dynamically determined by crop or soil conditions (8).

In this study, we use APSIM to compare observed N_2O emissions with modelled simulations in the southernmost cropland observation candidate site of the ICOS (Integrated Carbon Observation System) European infrastructure.

The specific objectives are as follows:

1. To test the performance of APSIM for simulating N_2O emissions;
2. To quantify differences between modelled and measured N_2O emissions, and identify periods of coherence and periods of discrepancies;
3. To assess the cumulative N_2O emission over the period investigated with the approach proposed.

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II. Materials and methods

The data collection occurred during the period 2007-2010 using the static chambers method, and during 2017-2018 using the eddy covariance (EC) technique on a farm located in Southern Italy (Borgo Cioffi, Eboli, 40º31’ 25.5” N, 14º57’26.8” E), the European southernmost cropland observation candidate site of the ICOS (Integrated Carbon Observation System) European infrastructure. The area is characterized by typical Mediterranean climate: over the last 30 years the average annual precipitation was 908 mm with an overall mean air temperature of 15.5 ^{0}C. Most of the precipitation occurs in October-November while the driest month is July. Soil is classified as Calcic Kastanozem Skeletic, with a predominant clay texture (clay: 52%; silt: 28%; sand: 20%). The soil pH and bulk density were 7.5 and 1.2 gcm^{-3}, respectively. The organic matter content was 2.5±0.3%. Parent soil material is calcium carbonate, and most of the soil particles have an alluvial origin, deriving from the nearby Sele River.

Soil NO_3^--N and NH_4^+-N content were determined on samples collected at a depth of 0–0.30 m. Samples were air dried and sieved up to a particle size of 2 mm prior to analysis. Nitrate and ammonia content were determined in a KCl soil extract. The soil samples were collected in correspondence of the chambers GHGs measurements (i.e. every 15 days during the period May – October of each years). Soil nitrogen content was determined calorimetrically during 2007 – 2008 and 2010 whereas during 2009 this was done by ionic chromatography.

The main features concerning the agronomic management and crop cultivated are reported in Table 1.

	Crop	Sowing	Harv.	N fertilizer	Water supply	
					Rain	Irrig
		Date	Date	N kg ha^{-1}	mm	mm
2007	Corn	05/09	08/24	62.5* 187.0**	111	396
2008	Corn	05/01	08/22	55.1* 120.0**	193	n.a
2009	Corn	06/11	09/08	60.0* 130.0**	24.9	291
2010	Corn	05/01	09/12	60.0* 160.5**	*n.a*	*n.a*
2017	Ryegrass	10/01/ 2017	05/16/ 2018	300.0	n.a	n.a
2018	Sorghum wheat	06/17/ 2018	09/20/ 2018	300.0	75.6	289

Table 1 Summary of sowing and harvesting dates along with management activities on the corn crop during the period investigated

* N fertilization at sowing

** top-dress N fertilisation

n.a not available

Eddy covariance N_2O fluxes The N_2O exchange was measured by the eddy covariance technique, coupling a Gill R3 Ultrasonic anemometer (Gill Instruments Ltd., Lymington, Hampshire, UK) with a CW-QCLTILDAS (Aerodyne Research Inc., Billerica, MA, USA). The 10Hz data was logged to a CR3000 Datalogger (Campbell Scientific Inc., Logan, UT, USA) used for the fast, simultaneous measurement of N_2O, CH_4 and H_2O mixing ratios.

The height of the EC tower varied from 2.15m to 2.60 m according to vegetation growth stages. GHGs were sampled drawing ambient air with a turbulent flow rate greater than 18 l/min through a heated and insulated PTFE buried sampling line of 32.6 m length from the ultra-sonic anemometer to the QCL located in an air-conditioned sea container placed on the field. The EC station is setup approximately in the center of the field, which has a rectangular shape, 300m × 600 m. The fetch in the prevailing wind direction, SW-NE (sea breeze regime), is about 200 m. The flux footprint along the prevalent wind direction (NE-SW) has been already characterized in the past (**19-20**): here it has been investigated for the period used in the modelling exercise, following the model by Kormann and Meixner (**21**), and it is shown in Fig 1.

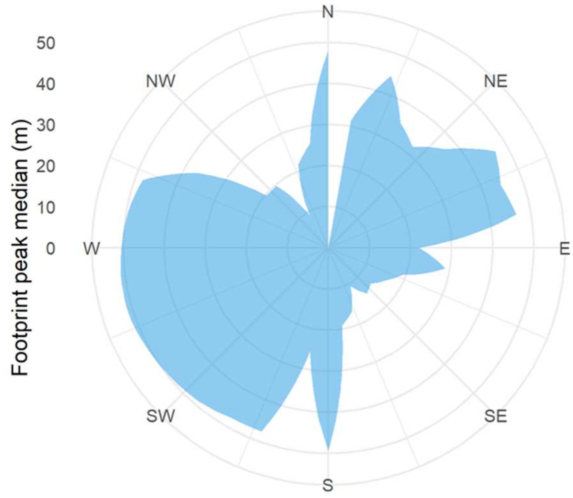

Fig.1 The blue area represents the surface delimited by the median value for each 10° sector of the “footprint peak”, i.e. the distance from the EC station in the direction from which the largest relative individual contribution to the N_2O flux originates.

Data processing of the raw data was computed using the software eddypro (www.licor.com/EddyPro.). Data were collected continuously from October 2017 to August 2018. After the QA/QC the % of data coverage was 45% for the entire period of investigation. Due to the absence of a commonly accepted methodology for the gap-filling the missing data were linearly interpolated using the Matlab function Interp1.

Static chamber N_2O fluxes

Eight sampling locations—spaced approximately 30 m from each other—were selected along a NE-SW transect. On each sampling position one collar (0.20 m diameter, 0.15 m height, 4.7 L volume) was inserted into the ground at a depth of 2–3 cm and left in place during the entire measurement season, except when the study area was disturbed by agricultural practices, when each collar was removed. During each measurement campaign, gas samples were always collected at the same time of day, spanning solar noon (i.e. between 1100 and 1300 h). Fluxes from the soil surface were determined by measuring changes in concentration over a 30 min time interval, in the head space of each static chamber. Air samples were collected by means of a PP (Polypropylene) syringe and stored in airtight glass vials (Labco Exetainer, 11 ml, UK) sealed by silicon. Initially, ambient air samples were collected when chambers were still open (t=0); later chambers were closed and air samples collected every 10 min, by washing the vial volume three times with a double needle inlet connected to the chamber headspace. N_2O concentration was determined using a gas chromatograph Fisons Series 800 (9). Cumulative emissions were obtained by linear interpolation between the observed date using the Matlab function Interp1.

APSIM Nutrient module

APSIM (APSIM Next Generation), was employed to simulate the N_2O and NO_3^- dynamics at daily time step. APSIM is a process-oriented simulation model able to reproduce the most relevant ecological and physiological process through a theoretical understanding grounded in state-of the art knowledge. APSIM reproduce specific agro-ecological dynamics under prescribed conditions of climate, soil and management, APSIM simulate functional processes at the basis of SOM (Soil Organic Matter) turnover, gas exchange at the soil-plant-atmosphere interface.

The dynamics of N_2O were modelled using the soil nutrient module SoilN (**8**).

The module operates on a daily time-step, simulating the major processes in soil C and N cycles, including decomposition, mineralisation, immobilisation, nitrification and denitrification (**13 - 14**).

Nitrification follows Michaelis–Menten kinetics and is controlled by soil moisture, temperature and pH (**10**)

$$R_{nitr} = \left[V_{max}\ X\ C_{NH4/(km+C_{NH4})}\ x\ \min\left(f_{sw},\quad f_{pH},\ f_{st}\right)\right] \\ x\ [BD\ x\ D/100] \qquad (1)$$

$$N2O_{nytr} = k1\ x\ R_{nitr} \qquad (2)$$

$$R_{denit} = 0.0006\ x\ NO3\ x\ C_{active}\ x\ f_{sw}\ x\ f_{st} \qquad (3)$$

where, R_{nitr} is the nitrification rate (kg N ha^{-1} day^{-1}) at a given NH_4^+ concentration (C_{NH4}; mg N g^{-1} soil);; V_{max} (mg N g^{-1} soil day^{-1}) is the maximum nitrification rate at the optimum NH_4^+ concentration; Km is the NH_4^+ concentration (mg N g^{-1} soil) that produces a rate of 1/2 Vmax; f_{SW}, f_{pH} and f_{ST} are the nitrification rate modifiers for the effects of soil moisture, pH and temperature conditions respectively; BD is bulk density (g cm^{-3}) of soil layer; D is thickness of soil layer (mm); N_2Onytr is N_2O emissions during nitrification (kg N ha^{-1} d^{-1}), k1 is the proportion of N_2O evolved during nitrification (= 0.002); R_{Denit} is the denitrification rate (kg N ha^{-1} day^{-1}); $NO_3^{\ -}$ is the soil nitrate concentration (mg N g soil^{-1}); and f_{SW} and f_{ST} are the water and temperature modifiers in the range of 0.0–1.0 respectively, affecting denitrification of NO_3 – in each soil layer. C_{active} (mg C g^{-1} soil d^{-1}) is calculated by Eqn 4:

$$C_{active} = 0.0031\ x\ SOC + 24.5 \qquad (4)$$

where, SOC is in mg C g^{-1} soil d^{-1}, which in APSIM-SoilN is calculated as the C concentration (mg C g^{-1} soil d^{-1}) soil C pools (**15**).

The N_2O emission from denitrification ($N_2ODenit$, kg N ha^{-1} d^{-1}) is calculated by combining predictions of denitrification with the ratio of N_2 to N_2O emitted during denitrification (**16**);

$$\frac{N2}{N2Odenit} = \Big[(0.16\ x\ k2), \\ (k2\ xe^{\left(-0.8\ x\frac{NO3}{CO2}\right)})\Big]\ x\ \max(0.1{,}1.5\ x\ WFPS - 0.32) \qquad (5)$$

where, k_2 is the constant related to gas diffusivity in soil at field capacity, CO_2 is the heterotrophic soil respiration (mg C g soil^{-1} d^{-1}) and WFPS is the soil water-filled pore space. Site-specific measurements of bulk density, organic C, pH, clay content, water and N content, as well as crop residue before cultivations, were used to parametrize the model.

III. Results

The comparison between simulated and measured N_2O emissions, obtained with the EC technique, are shown in Fig1: the APSIM model was able to catch the seasonal dynamics of the emissions that abruptly occurred after the first N fertilization.

The simultaneous presence of an elevated level of N in the soil, and an adequate level of soil water content (data not shown) determined the optimal conditions for the soil microbial communities to produce N_2O, that was observed by both approaches adopted in this study (EC observation and APSIM simulation). Before N fertilization, N_2O emissions were practically constant, at very low levels with values < 0.01 Kg ha^{-1} day^{-1}. About 80 % of the overall annual emission occurred in the 2 months (May and June) after the first fertilization event, as indicated by the down arrows in Fig 2. Our results are in line with several previous studies (i.e **11-12**) indicating that soil N_2O emissions are characterized by 'hotspots' or 'hot-moments, with peak of emissions, resulting in considerable temporal variability. The ability of the measurement techniques or model simulation adopted to capture such episodes, represents a key factor for reliable annual budgets of N_2O emissions.

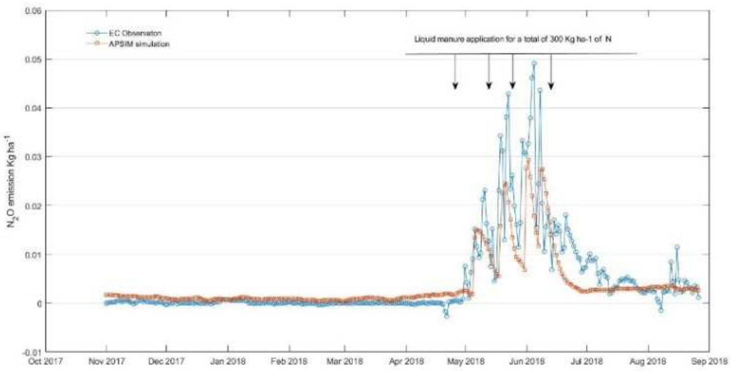

Fig 2. Temporal dynamics of N_2O emissions: each point represent the daily cumulative emission observed with the EC technique and simulated by APSIM model during the period November 2017-August 2018. Down arrows represent the fertilization events

The scatter plot (Fig 3) between observed and predicted values showed an Adj r^2 of 0.72 and a RMSE of 0.0029. Differences between observed and simulated data were more remarkable at high level of emission (e.g. during the emission peak) with an overall underestimation of APSIM simulation compared to the observations (Fig 2 and Fig 3).

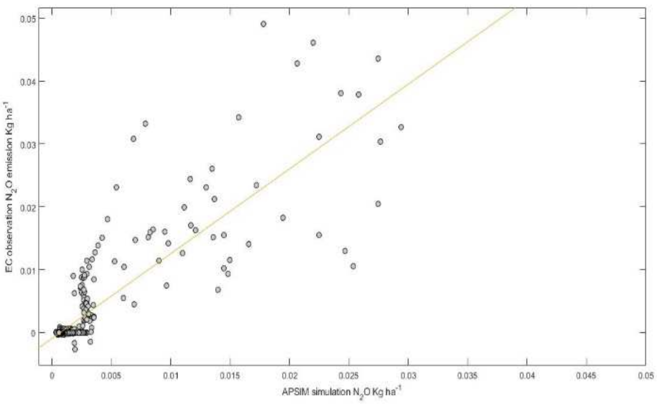

Fig 3. Scatter plot between the observed and simulated daily cumulative N_2O emission

In order to produce a guess of the annual N_2O emission (Fig 4) the data obtained using EC observations and APSIM simulations were cumulated at daily time step: APSIM data showed an underestimation of 0.27 Kg ha^{-1} over the period November 2017-August 2018. Cumulative N_2O emission were 1.35 and 1.08 kg ha^{-1} with the EC and APSIM simulation respectively.

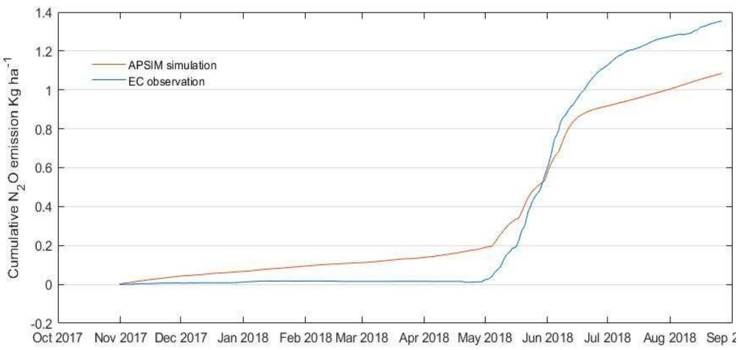

Fig 4 Comparison between the cumulative N_2O emission simulated and observed over the period November 2017-August 2018

The temporal dynamics of N_2O emissions over the years 2007 - 2010, simulated with APSIM and measured using the static chambers, are shown in Fig 5.
Emissions measured in 2007 were largely higher than those measured for the two following years with maize crops (2008-2010). The lowest N_2O fluxes were detected for maize crop in 2009, corresponding to low soil water content values and soil N content (data not shown). It should be noted that in 2007 the maize crop followed a fennel crop: a highly fertilized winter-time vegetable, which for the great part was not harvested and was instead incorporated in to the soil by ploughing-thus providing a substantial organic N and C source for the summer crop (9).

Chamber observations were in general characterized by an elevated variability, reflecting the high spatial heterogeneity of the field in terms of N_2O emissions; however, the APSIM simulated values fall within the standard deviation of the observed data. The scatter plot between observed and simulated data was overall not satisfactory (r^2 0.013, data not shown) highlighting the considerable difference between the two approaches proposed: on one hand, an integrated homogeneous approach simulated by the model, on the other the spot observations of a heterogeneous source.

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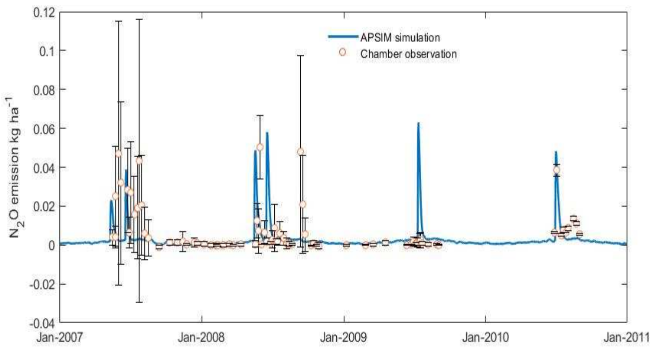

Fig 5 Annual temporal dynamics of the N_2O emission observed with the static chambers (error bars represent the standard deviation of the daily observations) and simulated using the APSIM model over the year 2007

Such differences are of course reflected in the cumulative values of the N_2O emission over the 4 years investigated (Fig 6): APSIM simulation underestimate the observed data by a factor of 1.69kg ha^{-1}. Cumulative emission observed with the chambers was 5.69 kg ha^{-1} while the APSIM-simulated was 3.99 Kg ha^{-1}.

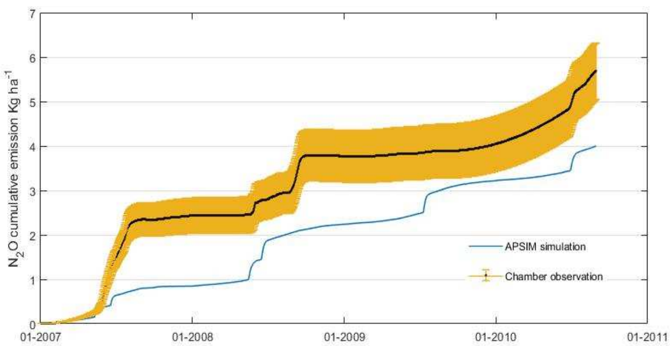

Fig 6 Cumulative emission of the N2O observed and modeled using ASPIM over the years 2007-2010

IV Discussion and conclusions

We have simulated the temporal dynamics of N_2O emissions from an intensively managed agricultural site, and compared the results with experimental observations of N_2O obtained with the EC technique and the static chambers method. The background N_2O fluxes for the greater part of the monitored period were very low. Seasonal emissions came largely from the main crops (maize and sorghum), in response to mineral nitrogen supplies.

This study confirms that measured N_2O fluxes are highly variable in time and space and controlled by the N availability (assuming an adequate level of soil water content and temperature) in the soil. The irrigation regime was key determinant in N_2O emission.

In a recent ensemble model simulation to determine N_2O emissions, Ehrhardt et al (**17**) report that for uncalibrated individual models, results were within 1 standard deviation of the observed N_2O emissions, while after the partial model calibration the prediction error was reduced to a variable extent for N_2O emissions across the sites investigated.

In a comparison study to simulate N_2O emissions with different models, (DAYCENT, DNDC, and YLRM) Yue et all (**18**) highlight how all models underestimate the N_2O emission with a r^2 between simulated and observed seasonal cumulative N_2O emissions ranging from 0.17 to 0.31

Our results, after the model calibration with site specific parameters, indicate that the APSIM model was able to catch the annual dynamics of the N_2O emissions, especially when compared to the EC observations. A lower agreement was found with the static chamber measurements: the larger footprint (compared to the static chambers), that characterizes EC observations, better represents the emission at field level simulated by the model. Chamber measurements are field “spot” observations that do not capture the whole EC (or model) footprint. Moreover, during the “peak” of emission that characterizes the post-fertilization phase, N_2O fluxes measured by EC showed a well-defined, regular temporal behavior with the peak of emission around noon. This indicates that, at elevated emissions, N_2O EC fluxes follow the daily development of turbulence in the mixed surface layer (while at lower level of emission no daily structure is observed), and the highest recorded fluxes were around midday.

Chamber observations were always conducted between 11:00 AM and 13:00 PM, therefore the linear interpolation was possibly conducted considering the peak conditions for emission and not the daily mean value. This might be a factor in explaining the considerable higher estimation of the chamber observation compared to the APSIM simulation, although further comparison measurements need to be conducted simultaneously over this environment between the two different techniques, in combination with a model simulation. In addition to the sensitivity to soil parameters and climate conditions, this study underlines the importance of the timing of fertilization events: this might have significant impacts on the model output and cumulative N_2O emission. In general, models have the ability to increase our understanding of N_2O emissions from soils compared with what would be possible from experimental observations. There's still a lack of knowledge related to a suitable methodology for gap filling the measured data, that might be overcome by model applications; this however will require well detailed management information especially for amount and timing of N fertilizations.

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