horticulturae

Supplementary materials: overview of the other N_2O modeling approaches

The IPCC (Integrated Pollution Prevention and Control), established in 1988 by the United Nations, serves as the global authority for evaluating climate change science. Its primary task is to produce comprehensive reports that assess our understanding of climate change [41]. These reports consider assessment reports, special reports, and methodology reports that offer guidance for constructing greenhouse gas inventories. The methodology utilized to estimate nitrous oxide (N_2O) emissions from agriculture is based on empirical data and mathematical models. The guidelines outline a comprehensive approach using available input data, aiming to include all N_2O emissions related to agriculture, both direct and indirect, while providing default factors for emission estimation. The guidelines classify agricultural N_2O sources into three categories: direct emissions from agricultural land, emissions from animal waste management systems, and indirect emissions linked to nitrogen processes such as volatilization, leaching, removal in biomass, or export from agricultural land [102]. The three fractions of N_2O are derived by multiplying the N input of each one with the relative emission factor [45,103].

$$N_2O = N_2O_{direct} + N_2O_{animal} + N_2O_{indirect}$$

The IPCC categorized methodologies based on complexity and accuracy level. Tier 1 offers basic estimates based on general fertilizer consumption data, resulting in some uncertainty. Tier 2 provides more detailed estimates by incorporating specific agricultural practices, crop types, and local climate data. Tier 3 is the most advanced level, relying on farm-specific data, which demands detailed information on agricultural practices, soil conditions, and climate to provide the most accurate estimates. The choice of tier depends on data availability and the desired level of precision in emissions estimation [104].

A more detailed description of this methodology (https://www.ipcc-nggip.iges.or.jp/public/2019rf/index.html, accessed on 16 November 2023), [105] consists of the following key steps:

- Data collection, which typically involves agricultural surveys, farmer interviews, and national data, involves information on agricultural practices like crop types, fertilizer use, irrigation methods, and organic fertilizer application;
- Estimation of N_2O emissions from soils, primarily result from biological processes like nitrification and denitrification. Here, the methodology considers local factors such as soil type, climate, and agricultural practices;
- Calculation of emission factors to estimate N_2O emissions from specific agricultural activities. These factors account for diverse variables, including fertilizer types, specific farming practices, and local conditions;
- Data collection, emission factors, and estimation are combined at regional or national levels, offering an overall perspective on N_2O emissions from agriculture within specific geographical areas.

While this methodology represents a valuable method of estimating the agricultural contribution to global nitrous oxide emissions, it does have limitations due to the constrained availability of agricultural and monitoring data. Furthermore, the accuracy of this methodology depends heavily on the availability of data in diverse environments at both local and national levels, which has a significant impact on emission rates.

Statistical models, often referred to as empirical models, represent the simplest modeling approach. These models predict environmental performance by examining observed relationships between a process and one or more independent variables. Unlike complex biogeochemical or agronomic process models, these models rely primarily on observed data and statistical methods. The models establish region-specific functional relationships based on data obtained from field experiments or environmental surveys that pertain to specific cropping systems, soil types, or climatic conditions. In the context of agricultural greenhouse gas emissions, statistical models have been used to simplify the intricate measurements and modeling of N_2O emissions from nitrogen (N) gases [106-108]. Various empirical models are employed to estimate nitrous oxide (N_2O) emissions. The IPCC has developed statistical models at both Tier 1 and Tier 2 levels to estimate N_2O emissions from agriculture. Tier 1 relies on national or global data to derive estimates, employing category data and average emission factors. In contrast, Tier 2 is more detailed, relying on region-specific data and mathematical models. Bayesian statistical methods have been applied to develop Bayesian models that can incorporate observed data and expert knowledge to enhance estimation accuracy. Multiple regression models employ regression analysis to explore relationships between input variables (such as agricultural practices and soil conditions) and N_2O emissions, identifying the most influential factors. Time series models consider seasonal variations and trends in N_2O emissions over time, facilitating the assessment of the long-term impacts of agricultural practices.

Machine learning models, including algorithms such as linear regression, logistic regression, neural networks, and decision trees, can be employed to create sophisticated models based on input data for estimating N_2O emissions. As reported earlier, statistical models offer simplicity, which reduces the risk of spurious predictions compared to process models. However, because statistical models rely solely on the observations used to derive relationships, regionally specific (Tier 2), they generally have a narrower geographic range of application compared to process models [109].

Meta-analysis is a statistical technique used to combine and synthesize the results of primary studies addressing a specific research question. It is not common to directly use meta-analysis models to estimate nitrous oxide (N_2O) emissions since meta-analysis focuses on synthesizing the results of existing studies rather than directly predicting emissions [110]. However, meta-analysis could be used in a later stage to combine the results of studies that address the effects of different agricultural practices or mitigation policies on N_2O emissions. In this case, meta-analysis models can help assess the effectiveness of various mitigation strategies based on the results of different studies [111]. Compared to emission simulation models, meta-analysis models are statistical tools used to synthesize the results of existing studies, while emission models are specifically designed to directly estimate greenhouse gas emissions, including nitrous oxide, based on agricultural data and specific conditions. In agriculture, the use of meta-analysis to estimate nitrous oxide (N_2O) emissions may require the application of various meta-analysis approaches and methods, depending on the research questions and data availability [112].

Whole-farm models are higher-level models that aim to represent the overall functioning of a farm as a whole. These agricultural models can estimate and evaluate the farm system's performance and functionality. These models consider various aspects of agricultural activities, including the agronomic process, crop management, animal breeding, management of natural resources, economic aspects, and environmental impact [113]. They are often used for management, planning, and evaluation purposes at the agricultural system level, and they provide a general overview of farm performance but may not penetrate specific details of biogeochemical or physiological processes occurring within the farm. They often rely on empirical data collected from the farm, including economic data, production data, and other operational data [114]. Some examples of farm models are FSSIM (Farm System Simulator), AgriPoliS, and APSIM (Agricultural Production Systems sIMulator). FSSIM was developed by the United States Department of Agriculture (USDA) and is widely used to simulate the operation of farms, including aspects such as crop production, livestock farming, economic management decisions, and interactions with the environment [115]. Agripolis is a whole-farm model developed in Germany that integrates agricultural, economic, and environmental aspects to assess the impacts of agricultural policies and management decisions on the farm [116]. APSIM, introduced as a process-based model, is also a whole-farm model widely used to simulate agricultural production dynamics, including crop cycles, crop performance, and interactions with soil and water resources [117]. While whole-farm models provide a general overview of farm performance and decisions at the farm level, process-based models focus on the detailed dynamics of specific processes occurring within the farm. Both have different purposes and applications and can be used in combination for a more comprehensive understanding of agriculture and to make informed decisions about farm management and planning.

References

Lapitan, R.; Wanninkhof, R.; Mosier, A. Methods for stable gas flux determination in aquatic and terrestrial systems. *Dev. Atmos. Sci.* **1999**, *24*, 29–66. https://doi.org/10.1016/S0167-5117(98)80023-2.

Nevison, C. Review of the IPCC methodology for estimating nitrous oxide emissions associated with agricultural leaching and runoff. *Chemosphere—Glob. Chang. Sci.* **2000**, *2*, 493–500. https://doi.org/10.1016/S1465-9972(00)00013-1.

Brown, L.; Brown, S.A.; Jarvis, S.C.; Syed, B.; Goulding, K.W.T.; Phillips, V.R.; Sneath, R.W.; Pain, B.F. *An inventory of nitrous oxide emissions from agriculture in the UK using the IPCC methodology: emission estimate, uncertainty and sensitivity analysis*, **2001**. *Atmospheric Environment*, *35*.

Mosier, A.; Kroeze, C.; Nevison, C.; Oenema, O.; Seitzinger, S.; Van Cleemput, O. An overview of the revised 1996 IPCC guidelines for national greenhouse gas inventory methodology for nitrous oxide from agriculture. *Environmental Science & Policy* **1999**, *2*, 325–333.

Lokupitiya, E.; Paustian, K. Agricultural Soil Greenhouse Gas Emissions. *Journal of Environmental Quality* **2006**, *35*, 1413–1427, doi:10.2134/jeq2005.0157.

Amon, B.; Çinar, G.; Anderl, M.; Dragoni, F.; Kleinberger-Pierer, M.; Hörtenhuber, S. Inventory reporting of livestock emissions: The impact of the IPCC 1996 and 2006 Guidelines. *Environ. Res. Lett.* **2021**, *16*, doi:10.1088/1748-9326/ac0848.

Leip, A.; Busto, M.; Winiwarter, W. Developing spatially stratified N2O emission factors for Europe. *Environmental Pollution* **2011**, *159*, 3223–3232, doi:10.1016/j.envpol.2010.11.024.

Millar, N.; Robertson, G.P.; Grace, P.R.; Gehl, R.J.; Hoben, J.P. Nitrogen fertilizer management for nitrous oxide (N 2O) mitigation in intensive corn (Maize) production: An emissions reduction protocol for US Midwest agriculture. *Insectes Sociaux* **2010**, *57*, 185–204, doi:10.1007/s11027-010-9212-7.

Tonitto, C.; David, M.B.; Drinkwater, L.E. Modeling N2O flux from an Illinois agroecosystem using Monte Carlo sampling of field observations. *Biogeochemistry* **2009**, *93*, 31–48, doi:10.1007/s10533-008-9271-y.

Smith, P.; Davies, C.A.; Ogle, S.; Zanchi, G.; Bellarby, J.; Bird, N.; Boddey, R.M.; McNamara, N.P.; Powlson, D.; Cowie, A.; et al. Towards an integrated global framework to assess the impacts of land use and management change on soil carbon: Current capability and future vision. *Global Change Biology* **2012**, *18*, 2089–2101, doi:10.1111/j.1365-2486.2012.02689.x.

Basche, A.D.; Miguez, F.E.; Kaspar, T.C.; Castellano, M.J. Do cover crops increase or decrease nitrous oxide emissions? a meta-analysis. *JOURNAL OF SOIL AND WATER CONSERVATION* **2014**, *69*, 471–482, doi:10.2489/jswc.69.6.471.

van Kessel, C.; Venterea, R.; Six, J.; Adviento-Borbe, M.A.; Linquist, B.; Jan van Groenigen, K. *Climate, duration, and N placement determine N2O emissions in reduced tillage systems: A meta-analysis*, 2013. *Global Change Biology*, *19*.

N, V.; Follador, M.; Ratto, M.; Leip, A. A comparison of eight metamodeling techniques for the simulation of N2O fluxes and N leaching from corn crops. Environmental Modelling and Software 2012, 51–66, doi:10.1016/j.envsoft.2011.05.003.

Robertson, G.P.; Paul, E.A.; Harwood, R.R. *Greenhouse Gases in Intensive Agriculture: Contributions of Individual Gases to the Radiative Forcing of the Atmosphere*, Science **2000**, 289(5486), 1922-5, https://doi.org/10.1126/science.289.5486.1922

Del Prado, A.; Crosson, P.; Olesen, J.E.; Rotz, C.A. *Whole-farm models to quantify greenhouse gas emissions and their potential use for linking climate change mitigation and adaptation in temperate grassland ruminant-based farming systems*, 2013. *Animal : an international journal of animal bioscience*, *7 Suppl 2*.

Louhichi, K.; Kanellopoulos, A.; Janssen, S.; Flichman, G.; Blanco, M.; Hengsdijk, H.; Heckelei, T.; Berentsen, P.; Lansink, A.O.; Van Ittersum, M. FSSIM, a bio-economic farm model for simulating the response of EU farming systems to agricultural and environmental policies. *Agricultural Systems* **2010**, *103*, 585–597, doi:10.1016/j.agsy.2010.06.006.

Shang, L.; Wang, J.; Schäfer, D.; Heckelei, T.; Gall, J.; Appel, F.; Storm, H. Surrogate modelling of a detailed farm-level model using deep learning. *Journal of Agricultural Economics* **2023**, doi:10.1111/1477-9552.12543.

Cann, D.J.; Hunt, J.R.; Malcolm, B. Long fallows can maintain whole-farm profit and reduce risk in semi-arid south-eastern Australia. *Agricultural Systems* **2020**, *178*, doi:10.1016/j.agsy.2019.102721.