Special Section: Trace Gases

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Introduction to Production, Transport, and Emission of Trace Gases from the Vadose Zone to the Atmosphere

After a brief introduction of trace gas emissions from the soil to the atmosphere and relevant processes involved, the seven papers dealing with novel modeling approaches, experimental data analysis tools, and improved concepts for the mathematical description of key subprocesses are introduced.

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Rising concerns about global warming as a consequence of increased anthropogenic greenhouse gas emissions have markedly strengthened scientific, political, and even public interest in issues surrounding human-induced climate change. This has resulted in fundamental economic and ecologic debates focusing on greenhouse gas mitigation strategies. Besides H_2O vapor, three major trace gases are primary contributors to the greenhouse effect: CO_2, N_2O, and CH_4 (Intergovernmental Panel on Climate Change, 2007). Such gases occur naturally in the atmosphere and are fundamental for life on Earth. With the onset of the industrial era, however, human activities, e.g., intensification of and changes in land use, industrial production, and burning of fossil fuel, among others, have resulted in the current atmospheric concentration of greenhouse gases significantly exceeding historical levels. In comparison to N_2O and CH_4, most of the CO_2 is emitted by fossil fuel burning. Nevertheless, biogenic CO_2 sources contribute about 17.3% to the total greenhouse gas emissions, whereas the overall emissions of N_2O and CH_4 contribute 7.9 and 14.3%, respectively (Intergovernmental Panel on Climate Change, 2007). Although N_2O and CH_4 represent a small fraction of the total mass of atmospheric greenhouse gases, they are now receiving considerable attention because of their large global warming potentials of about 300 and 25 times that of CO_2, respectively (Intergovernmental Panel on Climate Change, 2007).

Soil organic C also plays a key role in the global C cycle. Globally, 68 to 98 Pg C yr^{-1} is respired in the soil and emitted to the atmosphere (Schimel et al., 1996; Raich and Potter, 1995; Raich et al., 2002; Bond-Lamberty and Thomson, 2010), constituting the second largest C flux between ecosystems and the atmosphere. Thus, even small changes in C stocks or respiration processes directly affect the atmospheric CO_2 content. Accurate prediction of C turnover is therefore critical to address one of the key unanswered questions, namely "Is the soil C reservoir behaving globally as a sink or source of atmospheric C?" (Lal, 2004, 2010).

The atmospheric concentration of N_2O has increased markedly from about 270 ppb in preindustrial times to 319 ppb in 2005, which corresponds to a global total of 1510 Tg N (Intergovernmental Panel on Climate Change, 2007). Nitrous oxide is emitted to the atmosphere from both anthropogenic and natural sources, with a total average emission rate of 18 Tg N yr^{-1} (Intergovernmental Panel on Climate Change, 2007). Anthropogenic sources are mainly due to industrial and agricultural activities, e.g., livestock husbandry, the use of N fertilizers, fossil fuel combustion, and biomass burning. Natural sources comprise soils of temperate and tropical regions and aquatic systems and oceans (Nieder and Benbi, 2008). On a global scale, however, natural and agricultural soils are recognized to be the main source of atmospheric N_2O, with estimated emissions of 6 (3.3–9.7) and 3.3 (0.6–14.7) Tg N yr^{-1}, respectively (Intergovernmental Panel on Climate Change, 2007). Hence, soils contribute about 60% to the global atmospheric N_2O reservoir. In contrast, the only known sink for N_2O in the atmosphere is chemical depletion in the stratosphere. In the last decade, however, temperate upland soils have been identified as able to act, at least temporarily, as N_2O sinks; they nevertheless remain net sources (Chapuis-Lardy et al., 2007; Lamers et al., 2007).

Nitrous oxide is naturally produced in soil mainly as a byproduct of the two microbial processes of nitrification and denitrification. Both processes play a central role in the global N cycle, providing an important link between decomposition of organic matter, release of NH_4^+, and the re-entering of fixed nitrogenous compounds to the atmosphere as N_2 gas. Key environmental factors for N_2O production in the soil by nitrification and denitrification are the availability of O_2 and the presence of NH_4^+ for nitrification and anaerobic conditions, the presence of N oxides, and degradable C compounds for denitrification. The relative importance of each of these controllers, however, varies among natural habitats.

With more than three decades of intensive research on greenhouse gas production in soil, transport from the soil to adjacent compartments, and emission to the atmosphere, various studies have thoroughly investigated the role of key biophysical and environmental factors, such as substrate availability, soil moisture, and temperature. Most of these studies, however, were performed as single-factor studies, summarized by Dobbie et al. (1999) and Robertson and Grace (2004). A review of these studies revealed that, due to the complexity of interactions between physical and biological state variables and ecological drivers, estimates of greenhouse gas fluxes are still highly uncertain, particularly at larger scales (Hernandez-Ramirez et al., 2009). Therefore, recent research has focused on a detailed description and characterization of linkages between biological and physical variables, ecological drivers, and biophysical processes by means of process-based modeling (e.g., Schaaf et al., 1995; Ingwersen et al., 2008; Herbst et al., 2008; Reichstein et al., 2002a,b; Cervarolo et al., 2011; Stolk et al., 2011; among others). While most of these modeling approaches aimed at capturing and linking the basic biophysical processes within a unique numerical tool, other researchers have improved and further developed algorithms to describe subprocesses, such as gas diffusivity (Moldrup et al., 2004; Thorbjørn et al., 2008; Chamindu Deepagoda et al., 2011).

Besides modeling, novel measurement techniques have also been developed. These techniques are primarily aimed at quantifying in situ concentrations and fluxes of trace gases at high temporal and spatial resolution (Albanito et al., 2009; Lazik et al., 2009). Both modeling and novel measurement techniques contribute to an improved understanding of the processes and environmental factors promoting greenhouse gas emissions from soils, help to reduce uncertainties associated with estimates of greenhouse gas inventories, and encourage the focus of scientific interest on the relevance of soils in the context of climate change.

While trace gas production and consumption is primarily a biochemical process mainly mediated by plant and soil microbes, it has become evident that the spatial and temporal patterns of CO_2, CH_4, and N_2O fluxes cannot be analyzed and explained without taking the soil water budget into account. The soil water not only directly affects microbial activity but also influences gas diffusion and other transport processes, such as convection. Hence, the field of trace gas research is correctly receiving more recognition and attention from the worldwide soil physical and hydrologic scientific community. To account for this growing interest, a new session was provided at the European Geoscience Union (EGU) General Assembly within the Hydrological Sciences Division in 2008. The session was addressed by both experimental scientists and modelers from various disciplines, who discussed their latest research results on greenhouse gas emissions ranging from laboratory to field and regional scales. This led to the idea of presenting the state of the art of European trace gas research to the international scientific community.

The seven studies collected in this special section of the *Vadose Zone Journal* evolved from the EGU meeting in 2009 convened by Lutz Weihermüller, Marc Lamers, and Markus Reichstein. The studies present novel modeling approaches, experimental data analysis tools, as well as improved concepts for the mathematical description of key subprocesses.

In the study of Stolk et al. (2011), the researchers aimed at simulating N_2O fluxes from managed peat soils on a daily time step. Therefore, they linked a novel N_2O module to the extensively tested hydrologic–biogeochemical model combination SWAP-ANIMO. They hypothesized that an accurate simulation of the controlling factors of N_2O production, especially the dynamics of soil water with depth, would imply an accurate simulation of the dynamics of N_2O emissions as well. To test the approach, daily measured N_2O emission records from three sites in the Netherlands were used, with complementary data on soil moisture, mineral N content, and soil N_2O concentrations. Simulation of soil moisture, mineral N, and N_2O concentrations provided reasonably good results. Simulation of daily N_2O emissions, however, was poor, with model efficiencies <0, mainly due to an overestimation of N_2O emissions generated by denitrification in the topsoil. The reason for the overestimation was a result of shortcomings in the representation of the N_2O diffusion process in the topsoil, resulting in an underestimation of the storage time of N_2O in the soil and of the reduction of N_2O to N_2. They linked these shortcomings to the complex peat pore geometry and concluded that the description of the N_2O transport processes in the model is insufficient to accurately simulate daily N_2O emissions from peat soils even when the main controlling factors are precisely simulated. To overcome the shortcomings, they recommend incorporating the effects of (peat) pore geometry on soil moisture and on N_2O production, reduction, storage, and transport.

Schack-Kirchner et al. (2011) present a new finite-element regression procedure to estimate depth profiles of gas production in soils. To develop this, they divided the soil into homogeneous finite elements consisting of second-order polynomials for the gas concentration and quadratic splines to estimate the derivatives of scattered soil gas data. That allowed fitting integral soil gas concentration profiles that yielded the second derivative required for the estimation of the gas production term in the soil at various depths. They tested their method by means of quantifying the depth profiles of CO_2 and N_2O production in a central European Norway spruce [*Picea abies* (L.) H. Karst.] stand. Furthermore, they used synthetic data sets for re-estimating belowground gas fluxes with the new procedure. The results revealed the superiority of the finite-element method especially for deeper in the soil profile as long as the preconditions are fulfilled. As a future alternative, they suggest an inverse parameter optimization for the respiration rate in numerical solutions of Fick's second law.

The aim of the study of Klier et al. (2011) was to test two modeling approaches for their ability to describe and quantify the seasonal variations of N_2O fluxes in a potato (*Solanum tuberosum* L.)-cropped soil. Whereas one approach neglected N_2O transport in the soil, the other explicitly included a gas transport module. In the case of gas transport simulation, a dynamic N_2O/N_2 ratio for N_2O production was assumed, otherwise a fixed N_2O/N_2 ratio was simulated. Nitrous oxide fluxes were measured above the vegetation for the growth cycle using a closed chamber technique. Data from the first experimental year were used for model calibration and from the second year for model validation. The simulated N_2O emission dynamics showed a smoother transient behavior when using the gas transport module, but generally the observed seasonal dynamics of N_2O emission and peak events after heavy precipitation were described well by both approaches. The variation of N_2O emissions could be explained by assuming denitrification to be the major source for N_2O production. Only extremely high emission rates from the interrow soil of the potato plantation were underestimated by both model approaches. The lower N_2O emissions from the ridge soil were mainly due to unfavorable aeration conditions for denitrification caused by lower soil bulk density and lower water contents. In conclusion, they suggest to test in future studies whether data sets of higher temporal resolution will provide a better basis for model hypotheses testing.

In the study of Weihermüller et al. (2011), the researchers used the physically based water, heat, and gas transport model SOILCO2 (Šimůnek and Suarez, 1993) coupled with the RothC C pool concept (Coleman and Jenkinson, 1996) as proposed by Herbst et al. (2008) to estimate the error of a variable time discretization with regard to temperature input. Within the simulated case study, they demonstrated that averaging input temperature data from hourly to daily and monthly averages led to changes in the predicted C turnover and CO_2 efflux to the atmosphere. The simulations showed differences when changing averaging from hourly to daily to monthly temperatures in both the cumulative CO_2 outflow, which could be >4% yr^{-1} for long-term simulations (5 yr) and the instantaneous fluxes. Differences in instantaneous fluxes could be up to 5 g C m^{-2} d^{-1} depending on the season and temperature. These overestimated fluxes with daily and monthly input values mainly occurred during the nighttime, when hourly temperatures dropped below the average value. Finally, they investigated if different daily amplitudes for the rescaling of the daily temperature pattern would improve the model predictions using daily and monthly averaged temperatures. A comparison with hourly input data showed that the error due to temperature aggregation was not significantly improved. In conclusion, they suggest that the temporal scale of modeling should match the temporal scale of observations to avoid substantial bias of model results.

The study of Cervarolo et al. (2011) analyzed the effects of dimensionality (one or three dimensions) on modeling field-scale soil CO_2, water, and heat fluxes from heterogeneous and sloping terrain. Specifically, two vegetation dynamic models of different complexity were coupled to a soil–vegetation–atmosphere transfer (SVAT) scheme and to a three-dimensional unsaturated flow and heat diffusion model developed in a macroscopic cellular automata simulation environment, which allowed analysis of heterogeneous soils and vegetation. The two coupled models were validated using half-hour measurements of the leaf area index (LAI) and ground energy and water fluxes from a Mediterranean alfalfa (*Medicago sativa* L.) field (southern Italy) and in a predominantly C_3 grass-covered field in California. Furthermore, some numerical simulations were performed to assess, at the field scale, the effects of model dimensionality on evapotranspiration, CO_2 flux, and LAI with a heterogeneous soil, considering both flat terrain and hillslope, and using either the fully three-dimensional soil water flow model or a simpler model allowing only vertical fluxes. Results showed for one-dimensional modeling a significant underestimation of the simulated quantities with respect to those achieved by the three-dimensional model in flat, heterogeneous terrain, and a less than adequate representation of the gravity effects on soil water redistribution in the hillslope, which also affected the SVAT processes. They pointed out that fully three-dimensional modeling is preferred for a better representation of the physical processes, suggesting the macroscopic cellular automata approach as an aid to reduce the computational efforts because it is directly compatible with parallel programming.

Chamindu Deepagoda et al. (2011) present two density-corrected models for predicting soil gas diffusivity and soil air permeability from total and air-filled porosities based on the measurements from 150 undisturbed soil cores representing a wide range of soil types, density levels, and land uses (urban, agricultural, and forest soils). The new models performed well across different soil types and density levels when compared with existing widely used models. Therefore, two different equations based on the density-corrected and Buckingham (1904) models were combined to account for gas diffusivity in the inter- and intraaggregate regions of the soil. This model was tested on a sieved and repacked highly aggregated Andisol and seems to be a promising tool to predict gas diffusion is such systems.

Graf et al. (2011) present a method to estimate a continuous, fast-response time series of area-averaged soil CO_2 efflux from chamber measurements performed consecutively at different points in space. Such a setup is typical for most field surveys performed by multiplexed automated systems where only one gas analyzer is used for several different chambers, or by repeated manual measurements using closed chamber systems. Usually, such data sets are averaged across all measurement points to obtain an unbiased but slow-response time series of the area average. The simple algorithm presented in this study estimates the fast-response time series using the instantaneous deviations of efflux at each point from the time-stable part of the spatial pattern. For the analysis, different measurement transects located in various crop stands were used. The stability of the spatial pattern, which is a prerequisite for the method, differed considerably between crops; however, the pattern remained stable for at least 1 d. Deviations of single points from this overall pattern could be used to estimate fast fluctuations of efflux. The method could be applied to all data sets including several repetitions per day, and revealed fluctuations of the area average on the subhourly time scale for those days where meteorological boundary conditions such as solar radiation input showed associated fluctuations.

Summary and Outlook

As shown by the contributions to this special section, numerical modeling approaches and experimental data analysis go hand in hand. Additionally, experimental work and field data enhance the evolution of numerical tools for analyzing and understanding biogeophysical and biogeochemical processes related to trace gas emissions. Great care is needed, however, to ensure the use of meaningful input parameters and an appropriate choice of boundary and initialization conditions for numerical models.

In general, the challenge for future research involves the need for a stronger integration and linkage of vegetation with soil biological and physical processes. For example, autotrophic respiration is often described in a very simplistic manner without considering aboveground processes and dynamic changes in rooting densities and depths. To overcome these shortcoming, a close cooperation between the disciplines of soil physics, soil biology, soil chemistry, as well as plant physiology is strongly recommended. Second, C turnover is mainly described using conceptual C pools to facilitate either model initialization or model structure. These C pools, however, do not necessarily reflect the biochemical mechanisms involved in the C turnover itself. Even if some first approaches to account for single biological processes such as enzyme activity are already present in the literature, more effort will be needed to develop algorithms that fully represent these complex systems. On the other hand, it remains a challenge to parameterize the existing models, especially those accounting for lateral and vertical heterogeneity. Therefore, two complementary approaches are conceivable. First, the development and application of fast, and if possible noninvasive, measurement techniques for the characterization of the biological, chemical, and soil physical state variables and parameters, and second, parameter estimation using model–data fusion procedures or data assimilation techniques.

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