3. Conclusions

This literature study presents a short survey of approaches that have been or could be used in modelling N_2O emissions at the field scale. Deterministic regression models for N_2O fluxes at the field scale have been formulated. They are simple, but their explanatory power is restricted and they are site-specific. Regression models taking into account stochasticity have been developed for denitrification rates, but not for N_2O fluxes. Deterministic, process based models predicted field scale N_2O emission pulses observed after wetting, but do not account for spatial variability. Stochastic, process based models were developed to describe the denitrification rates in the soil. However, such an approach was not yet applied to account for the variability of field scale N_2O fluxes.

4. Acknowledgements

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Approaches in field scale modelling of nitrous oxide emission from grassland soils

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1. Introduction

The increase of atmospheric nitrous oxide (N_2O) is one of the causes of global climatic change. The depletion of the stratospheric ozone layer as well as the enhanced greenhouse effect are partly attributed to this gas. Soils are responsible for about 50% of the emissions [2].
The factors that affect N_2O emissions from soils have been intensively investigated, but badly quantified. Quantification is a prerequisite for assessment of future emissions depending on environmental and management scenarios. Models are a tool in quantification. The purpose of this paper is to illustrate and briefly discuss approaches that have been or could be used in modelling N_2O emissions from grassland soils at the field scale.

2. Approaches to model nitrous oxide emissions

2.1. THE NOTION OF INTEGRATION LEVEL

We distinguish six levels of integration in modelling N_2O emission: (i) chemical/physical level, (ii) aggregate level, (iii) soil column level, (iv) rhizotron level, (v) field level, and (vi) regional and national level. The main explaining variables will be different at different levels. However, we postulate that gross N_2O production and consumption are *eventually* determined by the occurrence of denitrifying conditions (simultaneous occurrence of very low partial oxygen pressures, denitrifiers, nitrate, water and easily degradable organic compounds, at preferably $pH \geq 5$ and temperature ≥ 5 °C). These conditions should determine the considered state variables to a high degree, irrespective of the integration level.

2.2. THEORETICAL BACKGROUND OF MODELLING

Modelling is a part of systems analysis [3, 10]. A *system* is a bounded part of reality. It is characterised by entities and relations between them. A *model* is a representation of a system. Here, we consider only mathematical models. The choice of the aspects modelled depends on the purpose of the model and the nature of the system. *Regression models* are used, if the purpose is to describe the considered system in terms of a simple input/output relation based on measured data. These models describe the system as a black box, and do not consider causal relationships between the entities. Regression models can be used to determine which part of the output variability can be explained by input variability or for assessment of the relative

importance of input quantities with respect to the output. *Process based models* are used to more fully understand and explain the behaviour of the system from knowledge of the underlying processes. In comparison with regression models, these models consider the entities within the black box and relate them via causal relationships. These models may be used to explore the expected behaviour of comparable systems under different conditions. *Deterministic models* are used to describe systems of which the relevant behaviour can be acceptably described by model output that is univocally determined by the input. *Stochastic models* are used if the relevant system behaviour can not be described in a deterministic way. On the basis of above-mentioned considerations, we distinguish four classes of models:

1. deterministic regression models,
2. stochastic regression models,
3. deterministic, process based models,
4. stochastic, process based models.

2.3. DETERMINISTIC REGRESSION MODELS

Velthof and Oenema [12] monitored N_2O fluxes from grassland plots on four soil types. They related the fluxes to supposed main determining factors, via the regression equation:

$$\ln(N_2O\ flux) = c_0 + c_1 * \ln(N_{min}) + c_2 * \theta_g + c_3 * temp, \qquad (1)$$

with:

N_2O flux	= N_2O flux from the plot,
N_{min}	= soil mineral N contents in the 0-0.3 m layer,
θ_g	= gravimetric moisture contents of the 0-0.05 m layer,
temp	= soil temperature at 0.05 m depth,
c_0, c_1, c_2, c_3	= (site-dependent) regression coefficients.

(1) accounted for not more than 50% of the flux variability, like in several other studies [5]. Models like (1) are simple and describe experimental results in a compact way. In principle, fluxes could be predicted from knowledge of a few variables. In regression analysis one obtains an impression on the relative importances of the different factors with respect to N_2O fluxes, which could give a clue for emission reduction strategies.
However, the low explained variances deserve attention. They can presumably be attributed to: (i) intrinsic stochastic nature of underlying processes, (ii) nonlinear nature of several underlying processes, and (iii) interaction between the studied factors. Also an improper choice of analysed factors, or inadequate formulation of the model could lead to low explained variances. In our vision a formulation of an *additive* regression equation for N_2O fluxes would be incorrect, since transformations of N_2O only occur if several conditions are simultaneously met, which leads to a *multiplicative* formulation (Leffelaar and Rappoldt, *unpublished*).

Extrapolation of regression models is tricky: the regression coefficients, or even the best fitting regression model, will be site and condition specific.

2.4. STOCHASTIC REGRESSION MODELS

We are not aware of stochastic regression models for N_2O emissions. Parkin and Robinson [9] formulated a stochastic regression model for denitrification. They simulated the probability density function for denitrification rates of cores from the field as determined by the C_2H_2 block technique, by using observed probability density functions for denitrification enzyme activities and CO_2 production rates. A comparable approach in modelling N_2O emissions would probably result in higher explained variances than deterministic regression modelling.

2.5. DETERMINISTIC, PROCESS BASED MODELS

N_2O dynamics was studied in deterministic microscale denitrification models (e.g. [7]). The purpose of these models was to more fully understand the dynamics of denitrification from nitrate to molecular nitrogen by designing an accurate description of the involved microbiological transformations. These models do not account for transport of substances. Recently, denitrication models were coupled with models for water transport [8], respectively water and gas transport [6]. The models reproduced observed field scale N_2O emission pulses upon wetting of the soil (rainfall, respectively melting of snow) fairly well. Their performance under other conditions should be further investigated. Both models describe the time courses of *total* N_2O emissions, but do not account for *spatial variability* observed at the field scale [4]. Process based modelling increases knowledge of the processes underlying N_2O fluxes and the relevant factors. In this way, tailored suggestions to reduce emissions might be formulated and evaluated. Development and use of detailed process based models may be limited by the availability of suitable parameter sets and overall measurements. Rigid validation is difficult: several models may be able to approximate the same set of experimental data.

2.6. STOCHASTIC, PROCESS BASED MODELS

We are not aware of stochastic, process based models for N_2O emissions. The aim of these models would not only be to describe fluxes via their underlying processes, but also to explain their variability. Explanation of the variability is especially important for the identification of conditions causing peak emissions, which could give a clue for emission reduction measures. Smith [11] and Arah [1] developed the "hot-spot" model to account for the distribution of denitrification rates within a soil matrix. The aerobic respiration potentials of these "hot-spots" follow a log-normal probability density function of their radii. The distribution of denitrification rates was deduced from the distribution of aerobic respiration potentials.
Extension of analogous concepts to model field scale N_2O fluxes will involve even larger data sets than deterministic, process based modelling. The distributions characterising the sources of the stochastic behaviour of the system also have to be investigated.