 DOI: 10.22616/RRD.30.2024.036

INTEGRATION OF MODULE OF NITRIFICATION IN SOIL ACTIVE LAYER IN THE CONCEPTUAL HYDROLOGICAL MODEL METQ

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Abstract
In the world, hydrological models are often used in the modeling of ecological components. In the context of the Paris Agreement and the European Green Deal, it is necessary to develop GHG emission modeling capabilities. The development and refinement of the conceptual model METQ is necessary not only for the quantitative analysis of flow, but in addition to its refinement, it is possible to conduct interdisciplinary research in the subfield of ecohydrology, which studies the interaction of water and ecosystems, and in environmental engineering, which addresses the issues of reducing diffuse pollution and reducing greenhouse gas emissions, technology implementation issues, where water content in the soil and groundwater fluctuations play one of the main roles, for example, in the processes of the formation of nitrous oxide emissions. This paper examines potential GHG emission calculation algorithms used to successfully model GHG emissions from soils, with a particular focus on agricultural soils, which contribute one of the largest amounts of GHG emissions in national emission reports for the agricultural sector. Available algorithms for nitrous oxide nitrification calculations are reviewed and possible algorithms that can be used for modeling emissions from soils and integrated into the conceptual hydrological model METQ are discussed. The developed conceptual solutions for modeling GHG emissions from soils will develop a modeling tool that will be used to estimate the volumes of GHG emissions and evaluate the effectiveness of various GHG emission reduction measures, as well as to perform a complex assessment of the soil GHG balance.
Key words: GHG gases, nitrous oxide, hydrological model METQ.

Introduction

GHG emissions from soil are mainly made up of three gases: carbon dioxide (CO_2), methane (CH_4) and nitrous oxide (N_2O). CO_2 fluxes can be divided into three main stages: soil respiration, which includes respiration by roots, anaerobic and aerobic microorganisms (Hanson *et al.*, 2000), respiration of the ecosystem, which also includes the respiration of the above-ground part of plants; ecosystem gas exchange, which is the balance of CO_2 used in photosynthesis and CO_2 released in respiration. Under anaerobic conditions, methane CH_4 is synthesized in the process of methanogenesis, while methane CH_4 is consumed under aerobic conditions, where oxygen and CH_4 are used in the metabolic processes of microorganisms (Dutaur & Verchot, 2007). Nitrous oxide (N_2O) and nitric oxide (NO) emissions arise primarily from two fundamental processes: nitrification and denitrification. Nitrification involves the oxidation of ammonium (NH_4^+) to nitrate (NO_3^-) via nitrite (NO_2^-), while denitrification entails the reduction of nitrate (NO_3^-) to N_2O and ultimately to nitrogen gas (N_2). Notably, N_2O production predominantly occurs during the denitrification process, particularly under anaerobic conditions where micro-scale anaerobic zones are fostered, typically occurring when soil pore filling with water exceeds 50% (Ussiri & Lal, 2012). Nitrification is conventionally conceptualized as a first-order process with respect to soil ammonium (NH_4^+) concentration under aerobic conditions. Furthermore, the production of N_2O during nitrification is typically modeled as a fraction of the overall nitrification rate, reflecting the intricate interplay between microbial activity and environmental factors influencing nitrogen cycling dynamics.

Microbial activity, root respiration, chemical processes involved in the degradation of organic matter, and heterotrophic respiration from soil fauna and mycelia collectively contribute to greenhouse gas (GHG) emissions within soil ecosystems (Chapuis-lardy *et al.*, 2007). The emission rates of these GHGs are intricately influenced by a multitude of environmental factors, including soil moisture, temperature, nutrient availability, and pH levels (Ludwig *et al.*, 2001), as well as the physical characteristics of both vegetation and soil. Consequently, meteorological parameters, climatic conditions, and agricultural soil management practices exert significant influences on GHG emissions. These factors can be further categorized into direct and indirect influences, elucidating the complex interplay between biotic and abiotic components in regulating soil GHG dynamics (Robertson, 1989).

Given the fragmented and sporadic nature of greenhouse gas (GHG) emission measurements from agricultural soils, there is a critical imperative to employ modeling techniques to regionalize such data and compute global GHG emission budgets. In addition to empirical models (Freibauer & Kaltschmitt, 2003), process-based models incorporating fundamental physical and chemical principles are extensively utilized to synthesize acquired field data (Pattey *et al.*, 2007). These modeling approaches facilitate the integration of diverse datasets, enabling analyses across varying spatial scales, ranging from local to global domains (Reimann *et al.*, 2009). Such modeling endeavors play a pivotal role in advancing our understanding of soil GHG dynamics and informing policy decisions aimed at mitigating anthropogenic contributions to climate change.

Daily organic matter decomposition, nitrification, denitrification, ammonia volatilization, CO_2 emissions (including those from soil microorganisms and root respiration), plant nitrogen consumption, and plant growth can be effectively modeled, as demonstrated by Li *et al*. (1994). These models serve as valuable tools for calculating greenhouse gas (GHG) emissions from soil, particularly in agricultural contexts, as evidenced by studies such as those conducted by Abdalla *et al*. (2011, 2020), Gu *et al*. (2014), and Li *et al*. (2012). Input parameters for these models encompass a spectrum of meteorological and soil attributes (e.g., soil structure, pH-value, mass density, organic carbon), alongside factors related to vegetation type and management practices (e.g., tillage, fertilizer application, grain yield) (Abdalla *et al*., 2009). By assimilating such comprehensive datasets, these models facilitate a nuanced understanding of soil GHG dynamics and offer insights crucial for informing sustainable land management strategies.

To understand the complex nature of the N_2O calculation algorithm, it is necessary to understand the main components of the nitrogen cycle, where atmospheric N_2 is reduced to NH_3 through biological or industrial nitrogen fixation, which provides nitrogen fertilizer for plants. However, only 30-50% of the nitrogen used in field fertilization and available in the process of decomposing organic matter, which is in the form of NH_3 and NO_3^-, is used in plant growth processes, while the remaining part is metabolized by soil microorganisms, which has an adverse effect on the environment and climate. The first of these processes, nitrification, refers to the biological oxidation of NH_3, NO_2^- and NO_3^-, which has a high level of immobilization and, under certain conditions, leaches these compounds from the soil, thereby contributing to eutrophication. In the second process of denitrification, NO_2^- and NO_3^- is gradually reduced to N_2O and N_2. Significant volumes of N_2O produced by this process enter the atmosphere, contributing to climate change and ozone depletion (Lehnert *et al*., 2018).

The conceptual hydrological model METQ has been created under the guidance of scientists from the Latvian University of Life Sciences and Technologies and approved for qualitative assessment of flows. The deep integration of the agricultural sector into natural processes requires additional knowledge and opportunities to predict GHG emissions from soil changes under different management scenarios in different soils and in different climatic conditions. This need can be fulfilled using modeling tools. Studying the past experience in the development of tools for calculating GHG emissions, it can be concluded that the models have been developed for different purposes (Colomb *et al*., 2012). Colomb *et al.* in 2012, one of the first classifications of GHG calculators was created, based on the model use approach 'Figure 1'.

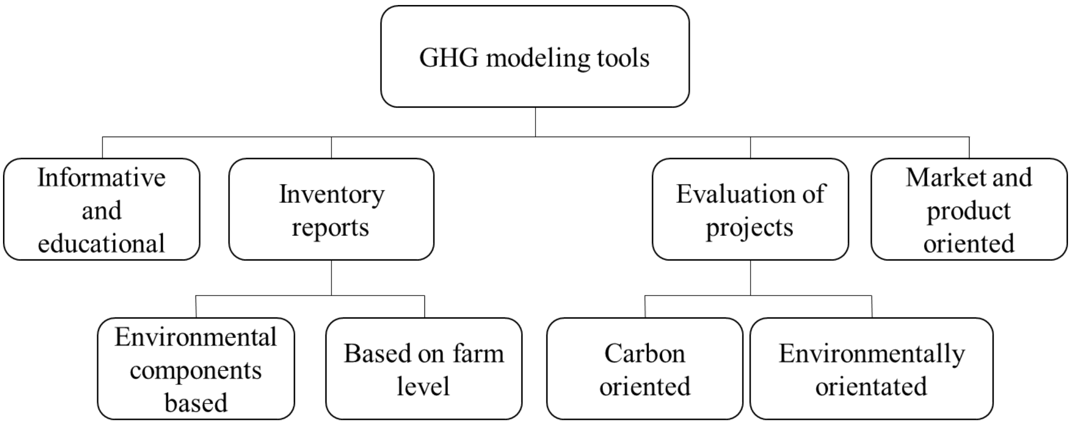

Figure 1. Classification of GHG emission modeling tools.

The development and refinement of the conceptual model METQ is necessary not only for the quantitative analysis of flow, but in addition to its refinement, it is possible to carry out interdisciplinary research in the sub-field of eco-hydrology, which studies the interaction of water and ecosystems, and in environmental engineering, which deals with the reduction of diffuse pollution and greenhouse gases issues of implementing emission-reducing technologies, where soil water content and groundwater fluctuations play one of the main roles, for example, in the processes of the formation of nitrous oxide emissions.

Materials and Methods

The structure of the conceptual hydrological model METQ and the possibilities of integration of GHG emission calculation algorithms are evaluated from the prism of conceptuality and four main stages necessary for the successful integration of the GHG emission calculation module into the conceptual hydrological model METQ 'Figure 2' are identified.

In the first stage, it is necessary to evaluate the possibilities of selecting data sets necessary for GHG emission modeling from the intermediate results of the conceptual hydrological model METQ, as well as the need for additional parameters and data rows for GHG emission modeling.

In the second stage, existing algorithms of the conceptual hydrological model METQ should be evaluated and a conceptual solution for the integration of GHG emission modules or the creation of additional algorithms should be created.

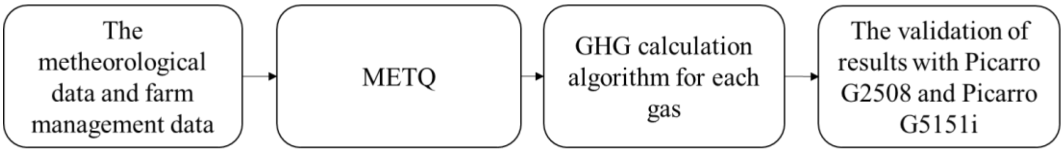

Figure 2. Possibilities of using the conceptual hydrological model METQ in modeling GHG emissions.

In the third stage, a calculation algorithm is created for each GHG gas, which uses the intermediate results of the calculations of the soil active layer of the conceptual hydrological model METQ and additional parameters related to the calculation of GHG emissions. The fourth step is a long-term measure, where gas measurements in field conditions are used in the calibration of the established GHG emission calculation modules. This study will describe the first two steps and describe the conceptual solution for module integration.

The GHG calculation modules should be divided into two groups, the first group of modules is emissions from the soil, where the GHG calculation modules can be connected to the METQ calculation algorithms of the conceptual hydrological model. GHG calculation modules must be created for carbonic acid gas, methane and nitrous oxide separately 'Figure 3'.

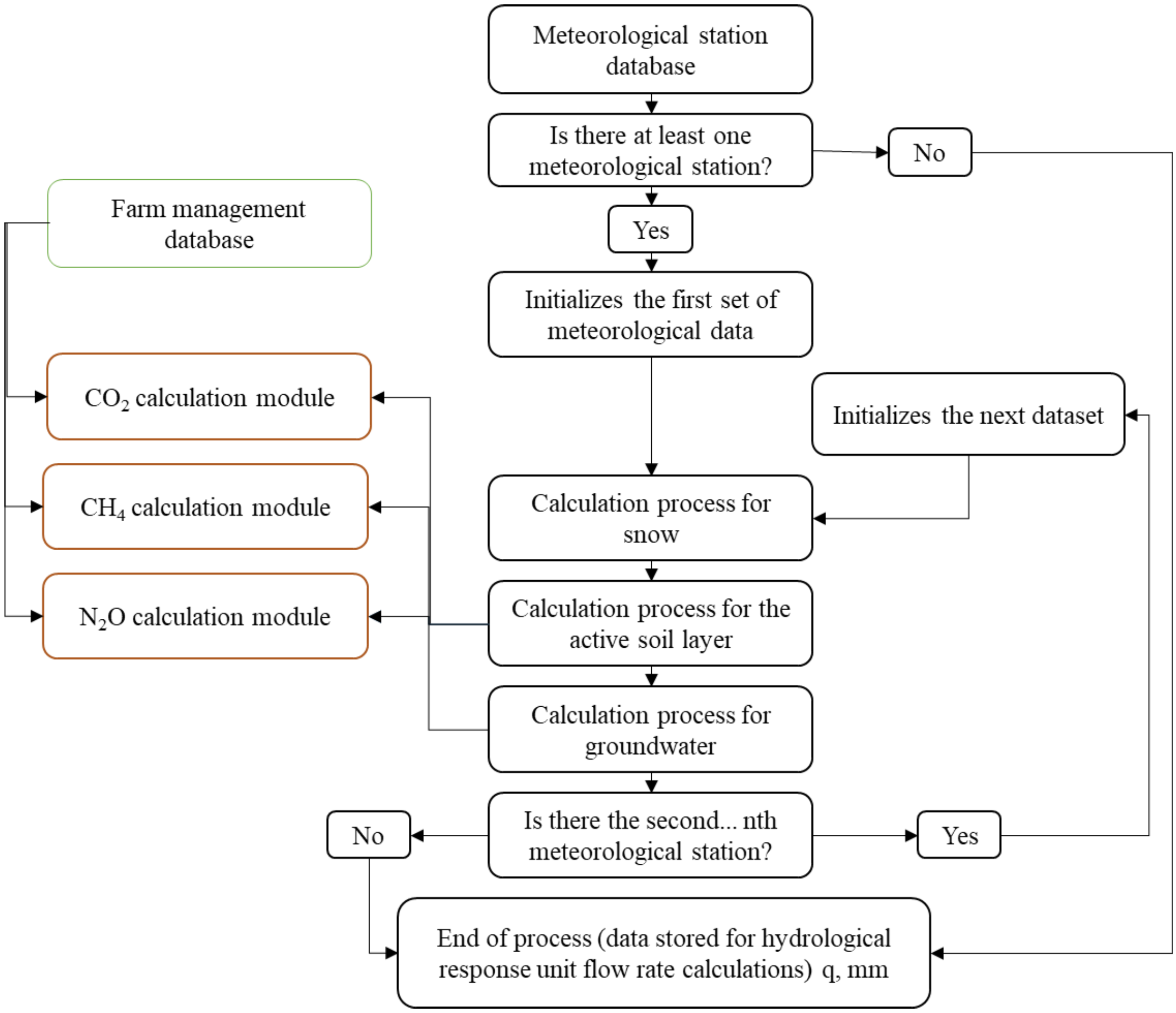

Figure 3. Design model for integration of modules for the calculation of carbon dioxide, methane and nitrous oxide emissions in METQ.

The second group of emission calculation modules is indirect N_2O emissions and methane emissions from water bodies, where it is possible to connect the GHG calculation algorithm to the calculation algorithm 'Figure 4' of the total drainage of the conceptual hydrological model METQ.

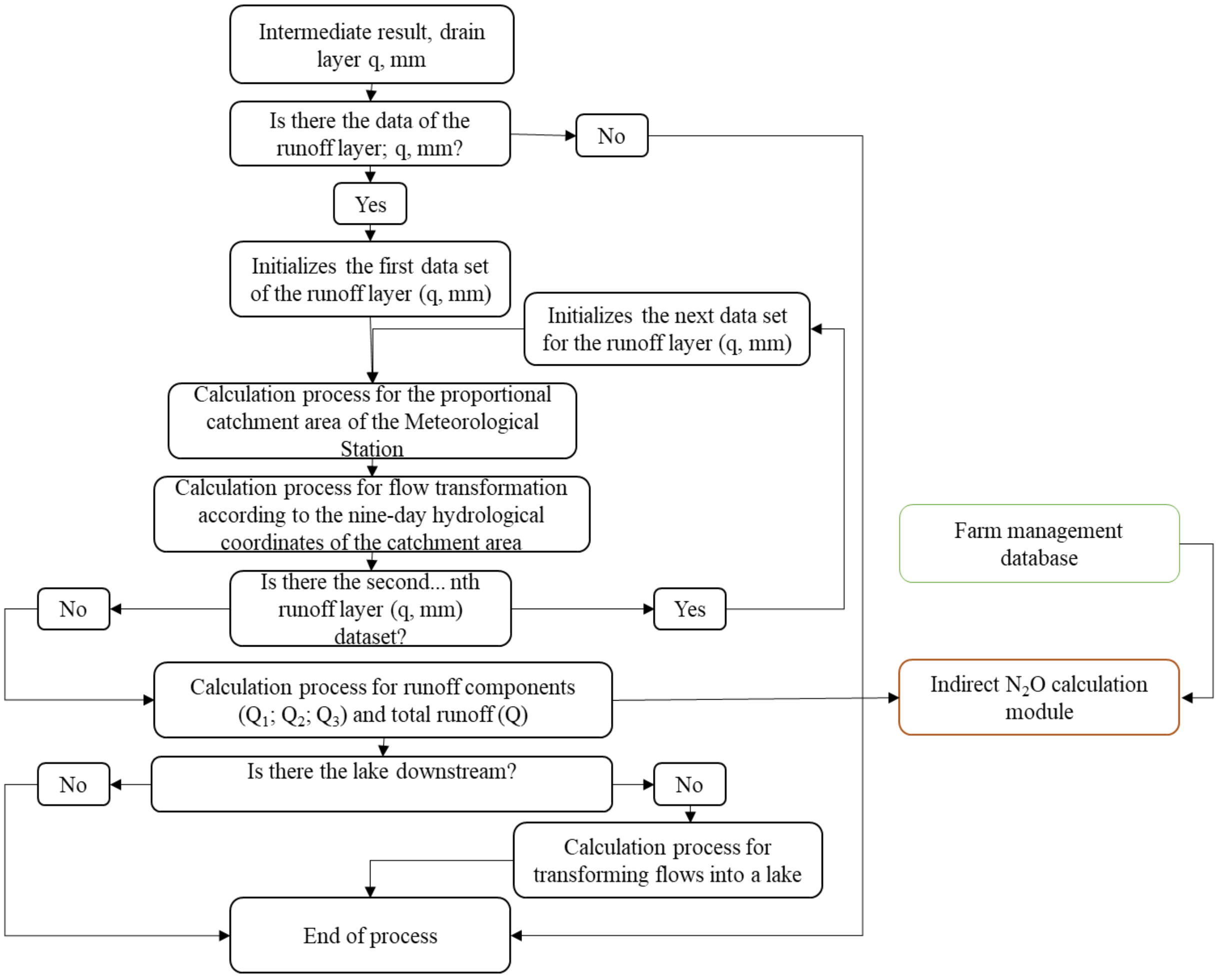

Figure 4. Design model for integration of modules for calculating indirect nitrogen oxide emissions in METQ.

By analyzing information from available statistical databases and the results of scientific studies, it is currently possible to create an N_2O calculation module using existing agricultural drainage monitoring data reflecting farm Management practice and calculate indirect N_2O emissions for the calculation algorithm of components of the conceptual hydrological model METQ drainage.

Results and Discussion

The design platform of THE conceptual hydrologic model METQ allows the use of intermediate results of model calculations such as end-of-day groundwater level, capillary take-off, total evaporation, etc. required in GHG emission calculation algorithms.

The METQ algorithms of the conceptual hydrological model are well documented and allow the integration of GHG emission calculation modules for the calculation of carbon dioxide, methane and nitrous oxide emissions from soil. However, it is necessary to create additional parameter input options for each GHG emission from soil calculation module.

Integration of the GHG calculation into the conceptual hydrological model METQ requires the reprogramming of the existing modelling platform and the creation of an open platform for the addition of new calculation modules. For GHG modelling from agricultural soils based on nitrification and denitrification processes in soil as well as indirect GHG modelling from watercourses based on nitrogen leakage and nitrification and denitrification processes in water.

The connection between nitrous oxide calculation algorithms and conceptual hydrological model METQ is presented in 'Figure 5'.

Falloon & Smith (2012) expanded the repertoire of models available for simulating carbon (C) and nitrogen (N) emissions from soil. Meanwhile, Butterbach-Bahl *et al.* (2004) conducted comparative analyses between model predictions and field measurements across agricultural and forest ecosystems. Their findings suggest that while modeling approaches generally yield higher quality estimates, discrepancies between model outputs and empirical data may manifest at both micro and macro scales. Nonetheless, according to these studies, the mean error associated with soil emissions is typically low (Butterbach-Bahl *et al.*, 2004; Hastings *et al.*, 2010), instilling confidence in the utility of modeling data for various applications.

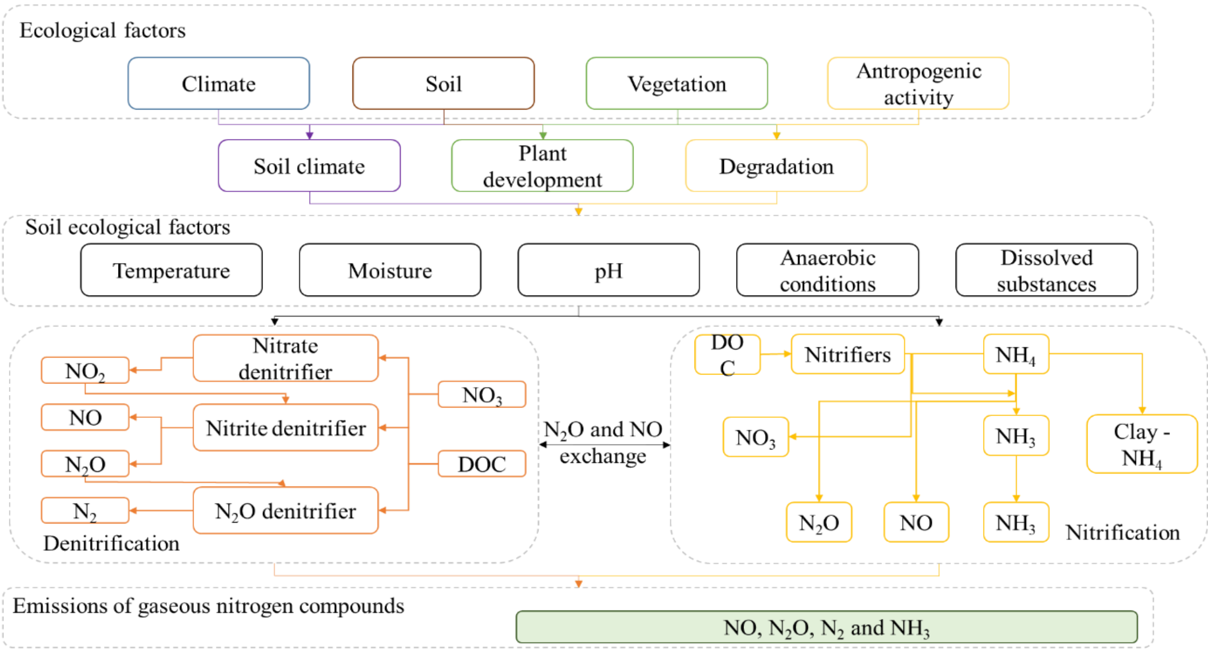

Figure 5. The GHG module connection to conceptual hydrological model METQ and farm management data.

Conclusions

1. In the modeling of hydrological processes, several hundred models are actively used, which can be divided into two main groups, conceptual and physical. The use of conceptual models gives more accurate results for catchments with an area of more than 5 km^2. Newly built modeling tools are used in the modeling of GHG emissions, but hydrological models with an additional algorithm are successfully used, which allows for the modeling of gas emissions and stands out with greater accuracy in the modeling of nitrous oxide in the temperate climate zone, where soil freezing is observed in the winter period;
2. The METQ modeling platform of the conceptual hydrological model allows you to save and use in the calculation algorithm the intermediate results of the model calculations, such as the groundwater level at the end of the day, capillary rise, total evaporation, etc., which are needed in the GHG emissions calculation algorithms;
3. The integration of the GHG calculation into the conceptual hydrological model METQ requires reprogramming the existing modeling platform and creating an open platform for adding new calculation modules. For GHG modeling from agricultural soils, where the calculation is based on nitrification and denitrification processes in plants, as well as indirect GHG modeling from watercourses, where nitrogen leaks and nitrification and denitrification processes in water are taken as a basis.

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