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Modelling carbon and nitrogen dynamics in paddy rice system: productivity and greenhouse gas emissions

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ABSTRACT

The main challenge of modern agriculture lies in the need of enhancing crop productivity to guarantee food security while achieving the sustainability of cropping systems in a changing climate. In a recent speech to the 21st Conference of Parties to the United Nations Framework Convention on Climate Change (COP21) held in Paris, the president of the United States declared that *for all the challenges we face, the growing threat of climate change could define the contours of this century more dramatically than any other*. This is why He hopes that all the countries in the world, *united in common effort and by a common purpose*, will not *condemn the next generation to a planet that's beyond its capacity to repair*. Agricultural activities deep influence the carbon, water and nutrients cycles at global level, then still play a vital role in the survival of humankind. The need to double food production by 2050 is entrusted to agriculture, which accounts for 14% of greenhouse gases emission and is considered as the economic sector most uniquely susceptible to changes in climate patterns, due to its dependence on the biophysical environment. Standing first among all food grain crops, rice (*Oryza sativa* L.) is in the spotlight due to the projected decrease in production in top producing countries and to the environmental sustainability of rice cropping systems, in light of the use of large amount of water for irrigation and of the contribution to the emission of greenhouse gases (GHGs) at the global level. The improvement of the water and nutrient management in paddy rice cropping systems is then considered as a necessary step to mitigate agriculture's GHG emissions, as reported by the United Nations Foundation. The scaling up of mitigation strategies from farmers' level to national policy makers needs the support of the scientific community, who is in charge to develop research to address these paramount questions. In this framework, the adoption of cropping system simulation models as a reference to assess both the productivity and the environmental impacts of cropping systems under a variety of management and climatic scenarios seems unavoidable, as they are the only available tools to reproduce the nonlinear responses of biophysical processes to boundary conditions. They also represent a viable solution to design and test alternate strategies to mitigate the emission of GHGs and to optimize the use and management of resources in agriculture.

This PhD program enables the scientific community to move forward the integration of available biophysical models to dynamically simulate the different components of the rice cropping system, considering the multiple, mutual interactions among system’s domains which determine rice crop yield and environmental drawbacks. The final achievement is the delivery of a software targeting this purpose, which is documented in the last chapter; the objective of this research product is to give a modelling solution to simulate the comprehensive set of biophysical processes involved with the paddy rice cropping system, considering the crop development and growth, the soil water dynamics, the effects of fertilizers on nitrogen leaching and the emission of greenhouse gases at field scale, considering the impact of alternate farmer management strategies.

During the work some deficiencies in current models were highlighted and solved, such as the unjustified complexity of widely adopted crop simulators or the lack, within them, of algorithms for the simulation of processes which significantly contribute to explain the variability of rice yield.

The output of this work is made available through software components and modular modelling solutions: this choice, representing the state of the art of software engineering science, removes technological bottlenecks which usually prevent advances in agricultural system modelling and fosters international collaborations between research centers while laying the basis for further developments.

Keywords: Rice cropping system, greenhouse gas emission, agricultural management, modelling solution

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INTRODUCTION

1.1. Challenges in rice agriculture: trade-offs between productivity and sustainability

The major challenge of modern agriculture is to improve yields without compromising environmental integrity or public health. By 2050, global population and grain demand are projected to be 50% and 100% larger than at the beginning of the century (Tilman, 2002): doubling yields and sustaining food production at this level is mandatory. Achieving this goal in ways that do not compromise environmental integrity is a greater challenge still, due to the deep influence of agricultural activities on carbon, water and nutrient cycles as well as atmospheric and soil chemistry. In this context, rice (Oryza sativa L.) cropping systems play a key role, providing the primary source of nutrition for over half of the world's population (Juliano, 1993). The main environmental challenges associated with flooded rice cropping systems are the use of large amount of water for irrigation and emission of greenhouse gases (GHGs, Johnson-Beebout, 2009). The shortage of water resources in agriculture is an increasing issue globally (Rijsberman, 2006), as well as its increasing demand and competition among various sectors (urban, industrial, environmental) which will likely exacerbate the impact of climate change on water supply to rice-growing areas (Bouman et al., 2007). Consequently, there is the need to investigate alternate practices in rice-growing regions in order to enhance water productivity (Bouman, 2007) and cropping intensity (Dobermann and Witt, 2000). So far, suggested pathways include the incorporation of non-flooded crops and pastures into traditional rice rotations (e.g., Zeng et al., 2007; Singh et al., 2005), changes in agronomic and irrigation practices (e.g., Li et al., 2011; Belder et al., 2007), and genetic improvement (e.g., Bennett, 2003; Mitchell and Hardy, 2000). The unique water management of irrigated rice makes this cropping system one of the most important source of anthropogenic methane (CH4; Yan et al., 2009) and nitrous oxide (N2O; Akiyama et al., 2005). Currently, much research efforts are pushed to find irrigation methods which would cause the least integrative greenhouse effect by mitigating CH4 and N2O emissions while ensuring high rice yields (Berger et al., 2013). Controlled irrigation practices leaving rice paddies under non-water logged conditions for 40–80 % of the cropping season are under examination (e.g., Peng et al. 2011; Qin et al. 2010; Zou et al. 2007). Such management strategies save water and mitigate CH4 emissions, but can cause stronger N2O emissions due to oscillations in soil oxygen status, soil redox potential, moisture and temperature (Peng et al. 2011; Liu et al. 2010; Johnson-Beebout et al. 2009). The different redox potential conditions required for N2O and CH4 formation and the trade-off pattern of their emissions in rice fields makes it a challenge to abate the production of one gas without enhancing the production of the other, even if a redox window with minimum global warming potential for rice fields was identified under laboratory conditions (Yu and Patrick, 2004). Nevertheless, under field conditions emission of GHGs is determined and modulated by a number of variables, such as environmental factors (e.g., physicochemical properties of soils, organic carbon, water and oxygen availability, temperature; Le Mer and Roger, 2001), rice cultivar and growth dynamics (Neue et al., 1997; van Bodegom et al., 2001) and fertilizer applications (e.g., Gu et al., 2009). In recent years, simulation modelling is becoming a reference tool to quantify the mutual interactions among all these factors and to assess the impact of alternate mitigation strategies (Fumoto et al., 2008; Li et al., 2005).

1.2. State of the art of paddy rice system modelling

1.2.1 Crop models

Crop growth simulation models have been long recognized as valuable tools in agricultural research. They are employed for a wide range of purposes, e.g., to critically test scientific knowledge, to predict yields, to extrapolate experimental findings to wider environments and to support farmers and policy makers decisions, by exploring effects of alternate management strategies and climate change on cropping system performance (Bouman and van Laar, 2006). The global relevance of rice as a staple food led in the last decades to the development of a number of models specifically designed or adapted to simulate the unique traits of this crop. The first attempt of modelling rice goes back to 1983, when the International Rice Research Institute (IRRI) published RICEMOD (McMennamy and O'Toole, 1983); in the following years, rice-specific parameterizations were developed for generic crop simulators such as WOFOST (van Keulen and Wolf, 1986) and MACROS (Penning de Vries et al., 1989). Since then, the international modelling community continued to develop new models, shifting the interest from the detailed simulation of physiological processes characterizing earlier studies, to management-oriented models to support decision-making and integrated assessment of system performance. Currently, the application of crop models is mainly aimed at gaining insight into the magnitude, rate and pattern of climate change impacts on agricultural productivity: in this context, multi-model intercomparison is becoming a standard to deal with uncertainty in model estimates (Rosenzweig et al., 2014). Thirteen major rice models were identified to address this issue, differing in structure, forcing variables and input parameters used to run simulations (Li et al., 2015). They commonly use daily climatic factors such as solar radiation and temperature as input variables to estimate e.g., growth duration, biomass and yield; most of them modulate crop growth considering physiological responses to enriched CO_2 atmospheric concentrations. Phenology, biomass production and spikelet fertility in response to temperature are identified as the most relevant sub-processes to simulate yield responses to climate change. All models consider temperature as the main driver of the progress of developmental stages, using linear on non-linear response functions; some of them individuate an optimum temperature above which developmental rate decreases while temperature raises. Photosynthesis and biomass accumulation is typically driven by solar radiation, with temperature possibly modulating assimilation rates. A range of complexity and empiricism is explored for the simulation of such processes, models principles spanning from canopy radiation use efficiency (Monteith and Moss, 1977), to light response curve of single leaf integrated to the whole canopy (De Wit, 1978) and Farquar biochemical model of leaf photosynthesis (Farquar, 1980). Widening the field of application of crop models required the inclusion of routines not directly linked to crop dynamics. In this process, the international community paid particular attention to soil processes influencing crop growth by limiting availability of water and nutrients (especially in terms of nitrogen), taking advantage of models originally developed by soil hydrologists and biologists. Currently, almost any rice model implements algorithms to simulate soil water balance ¬ or at least actual transpiration ¬ to derive a water stress factor reducing growth. Most of them, moreover, simulate crop nitrogen uptake, which can affect plant processes at different levels, such as photosynthesis, respiration, leaf area development, spikelet number and accumulation of non-structural carbohydrates. Detailed description of these dynamics decidedly improved crop models as tools to elucidate genotype-by-environment interactions determining rice growth and yield (Yoshida and Horie, 2010).

1.2.2 Soil models

Early development of models for agricultural soils has been supported by the need of understanding the processes that determine carbon and nitrogen turnover in soil, in order to shed light on the complex interactions involved with soil organic matter dynamics (e.g., Parton et al., 1994, Coleman and Jenkinson, 1996) and crop nutrition (e.g., Rijtema and Kroes, 1991, Bergström et al., 1991). Processes considered in these models are typically surface application (as fertilizer, manure or slurry, atmospheric deposition and deposition or incorporation of dead plant material), mineralization/immobilization between organic and inorganic forms, nitrification (from ammonium to nitrate), nitrate leaching, denitrification (to nitrous oxide and dinitrogen) and uptake by plants (Wu and McGechan, 1998). Currently, most advanced models simulating carbon and nitrogen additions to rice-based cropping systems account for nitrogen fixation and growth of other non-N-fixing photosynthetic algal biomass, now considered to be critical for sustaining soil organic carbon and soil nitrogen supplying capacity (Gaydon et al., 2012). The increasing awareness that agricultural soils are at the same time one of the major sources of anthropogenic greenhouse gases (GHGs), a significant carbon stock and even a sink for CH_4 and N_2O, drew attention to soil management aimed at carbon sequestration and minimization of GHGs emissions. Abatement and mitigation strategies have been often investigated by means of ecosystem modelling (Blagodatsky and Smith, 2012). Despite the existence of several well-known models for the simulation of GHGs at site level (e.g., DNDC, Fumoto et al., 2008), scientific literature continues to produce new, alternate models, addressing the increasing demand of tools for the assessment and prognosis of environmental changes at different temporal and spatial scales. Simulation of paddy rice soil is no exception, and it even appears more challenging compared to other conditions due to the transition between flooded and non-flooded soil environments, in turn influencing physical characteristics of the medium and biological dynamics. For example, gas transport in submerged soil is complicated by pressure variations and changes in diffusion caused by water blockage: the result is a limited availability of oxygen, affecting microbial and root respirations as well as organic carbon decomposition. In absence of O_2, a number of redox reactions are sequentially triggered in soils, i.e., denitrification, iron, manganese and sulfate reduction and methanogenesis (Kirk, 2004). A number of rice soil models paid particular attention to processes leading to CH_4 emission, focusing either on microbial processes (van Bodegom and Scholten, 2001), their integration with plant growth dynamics (Xu et al., 2007) or the role of water flows (Rizzo et al., 2013). Coupling gas transport models in the soil profile and simulation biological reactions allowed to improve the estimation of GHGs emission from rice soils. The rate of gaseous transport is indeed comparable with the rate of biological reactions: taking denitrification as an example, the final product ratio of N_2O and N_2 emitted from soil surface is strongly influenced by retention time of intermediates in soil; for methane emissions, the slower the diffusion of CH_4 in soil, the higher amount of gas will be oxidized by methanotrophs bacteria, determining the ratio of CH_4 and CO_2 emitted following methanogenesis. Correct simulation of the supply of reaction zones and prediction of the escape pathways for gases is therefore paramount in modelling GHGs emissions: since transport within soil is often a limiting factor in rice paddy fields, most gases are released via plant mediated transport (van Bodegom et al., 2001) and ebullition of gas bubbles (Tang et al., 2010). The spongy tissue of rice plants (i.e., the aerenchyma) serves as a main conduit for oxygen transport from atmosphere to the root zone, and guarantees tissues survival during flooding period; nevertheless, it also provides low-resistance escape pathway for gases produced in soil. Accounting for all the factors which may influence GHGs emission inevitably leads to the construction of very complex models. A possible practical solution is the use of modular structures within model frameworks, allowing to apply different types of mechanistic models ¬ selected among a library of available approaches ¬ according to the leading driving factors and environmental conditions (Blagodatsky and Smith, 2012).

1.2.3 Modelling agricultural management

Many models developed to simulate agricultural production activities target the analysis and evaluation of agricultural management impacts on production and system externalities (Keating et al., 2003; Jones et al., 2003). In this context, efforts were recently addressed at simulating the effects of alternate management strategies on GHGs production and emission, e.g., explaining the significantly different N gas emission and nitrate leaching resulting from different N fertilization rates, fertilizer type and application method (Gu et al., 2009). Concerning rice, simulation studies focused on the impact of water management on the emission of the main GHGs, which is strongly dependent on the oxic/anoxic transitions occurring in paddy soils. Continuous flooding and mid-season drainage ¬ the most representatives water managements in irrigated rice ¬ were compared in terms of regional scale emissions of CH_4, CO_2 and N_2O (Li et al., 2005). Results highlighted heterogeneity of mitigating effects of mid-season drainage across climatic zones and soil types, with a general trend of reduction of aggregated CH_4 and CO_2 emissions partially counterbalanced by enhanced N_2O emissions, sustained by the increased activity of nitrification and denitrification. In order to reproduce farmer management and to test alternate strategies, comprehensive rule-based management systems for supporting agricultural decision making were developed, allowing simulated management events to occur in response to flexible rules and to weather and management induced changes in the cropping system over time and space (Shaffer and Brodhal, 1998). Such systems overcame the limitations imposed by fixed date management events, which did not provide flexibility needed for dynamic development and testing of site-specific agricultural production rules. Description of agricultural management models in rice cropping system is lacking in scientific literature, but principles behind the implementation of management modules within generic crop simulators can definitely apply also to this unique system. For example, the CropSyst model (Stöckle et al., 2003) allow the user to set events on specific dates, on dates relative to planting date, synchronized to the crop phenology or to the occurrence of specified conditions (e.g., low soil moisture triggering automatic irrigation). This flexibility allows CropSyst to be used to model management practices based on crop conditions rather than fixed schedules. Within APSIM, a widely known model framework (Keating et al., 2003), the early recognition that all the possible management configurations could not be explicitly identified and addressed *a priori* led to the development of the "*MANAGER*" module, enabling users to apply simple concepts of states, events, actions and conditional logic to build complex management systems. The increasing demand for modularity and interchangeability in biophysical model development led to the implementation of management simulation models in a component based system, providing an extensible set of “rules” and “impacts” to account for production techniques and their consequences on the cropping system (Donatelli et al., 2006). Rules are a formal way to describe farmer’s behavior, characterized by three main pieces of information, i.e., inputs (states of the system and time), parameters and a model returning a true/false output (if true, an action is triggered). Impacts are sets of parameters to implement the consequences of a management event on the simulated system: such impacts can be recognized by specific models implemented within software components (e.g., a soil component), in turn determining a change in the states of the related domain.

1.3. Recent trends in agricultural system modelling

In the last ten years, the focus of agricultural system modelling has shifted from on-farm crop productivity to the integrated analysis of e.g., greenhouse gas emissions, soil carbon changes, ecosystem services, environmental performances, losses associated with pest and diseases, climate change adaptation and mitigation. In this process, a number of applications were developed to meet the request of tools able to serve particular needs, while few emphasis was placed on model improvement: as a result a large untapped potential in model development still remains, and filling this gap would likely contribute to solve emerging issues in food security, policy assessment, farmer advice and human health and nutrition (Holzworth et al., 2015). Nevertheless, broadening the horizon of cropping system models requires crop simulators to be linked to models belonging to other disciplines, such as hydrology, plant pathology and economics, and current software implementations, often characterized by legacy code and the lack of good software engineering principles, strongly limit cross-domain model integration. Most of models rely on monolithic implementations based on procedural languages (e.g., DSSAT, EPIC), thus needing heavy code maintenance and limited reuse (Holzworth et al., 2015). This is far from limiting the problem to a programming issue, since the use of unsuitable technology for developing complex, integrated system models is likely one of the major factors limiting the formalization of new knowledge in mathematical constructs, resulting in a gap between scientific knowledge and its transfer to simulation models. Reusability and extendibility in agricultural system models ¬ claimed as major objectives of the environmental modelling community (Holzworth et al., 2010) ¬ largely remain goals to be achieved. Many of the models are incompatible with each other with little or no reuse of sub-models, leading to the proliferation of software tools representing a variety of different implementations of the same algorithms. In most cases, these algorithms derive from the reimplementation of very common approaches to simulate crop and soil processes: reimplementation is a time-consuming process which removes resources that could otherwise be available for model improvement and can lead to subtle differences among models that are not immediately apparent. In order to limit this tendency, and to improve the reusability not only of models, but also of I/O procedures and data services, a number of frameworks (i.e., a group of interconnected models with infrastructure to support inter-model communications) were developed: most advanced frameworks embrace component-oriented programming as a common practice (e.g., BioMA, Donatelli et al., 2012; OMS, David et al., 2013; APSIM, Holzworth et al., 2014), in order to isolate knowledge in discrete, extensible and interchangeable software units. Such frameworks promote the development of fine granularity models, which reflect the most common level of detail at which research produces outcomes (i.e., process level). Software industry has long recognized that smaller units of computation are easier to understand and reuse between different projects: they can be aggregated into larger constructions to form what is generally called model, instead of the possibly more appropriate term modelling solution (Donateli et al., 2014). For these reasons, component-oriented programming is becoming an unavoidable prerequisite for the development of agricultural and ecological models (e.g., Papajorgji et al., 2004; Donatelli et al., 2010): the availability of software components fosters the development of modelling solutions that integrate single-disciplines approaches (Bregaglio and Donatelli, 2015). Ideally, each component encloses knowledge on the dynamics of processes belonging to a certain domain and it is kept up-to-date with research outcomes by specialists in the specific sectors. The strength of this approach is that it allows community collaboration around a common ‘trusted’ base, allowing applications to be built on shared knowledge in the form of components.

1.4. Objectives and organisation of the research

The main objective of this doctorate is the development of a modelling solution suitable for the simulation of the rice cropping system, accounting for crop growth and development, the impact of water and nitrogen availability on growth dynamics and the interactions among crop, environment and agricultural management leading to the emission of GHGs. The solution takes advantage of existing software units developed according to the state of the art of agricultural system modelling, i.e., the software components collecting model approaches for the simulation of crop (UNIMI.CropML), soil water (UNIMI.SoilW), soil temperature (UNIMI.SoilT) and agricultural management (CRA.Agromanagement) processes. This allows to concretely explore and exploit the features promoting reuse and extension of such components within the BioMA framework. A large portion of the solution is made up by well-known and tested models, which are interlinked to construct models of increasing complexity without losing transparency in the implementation and ease of maintenance of the code, thus promoting further development of the modelling solution. Some of the model approaches made available via software components, however, require a revision to properly simulate rice growth dynamics; considering the soil domain, moreover, models describing biological processes leading to GHGs emission are not implemented in a software component still. The activities of this research are therefore focused on the extension and development of models covering both crop and soil domains. In the first case, the activities are organized as follows:

- Improvement of the WOFOST model for the simulation of potential production of grain cereals. This task is achieved via (i) the development of specific functions to reduce the information needed to run simulations, increasing the possibility to couple the model with advanced tools for sensitivity analysis and automatic calibration, and (ii) the proposal of an alternative approach to describe the biophysical processes occurring within the canopy, via an explicit representation of the canopy vertical dimension. Changes to the original model are implemented within the component UNIMI.CropML.
- Extension of the components UNIMI.CropML and UNIMI.CropML_WL, encapsulating algorithms for the simulation of crop potential production and constraints to growth and development related to water availability, with the definition of the component UNIMI.CropML_NL. Such component is aimed at collecting available models for the quantification of the impact of nitrogen shortage or luxury consumption on crop productivity.
- Definition and implementation of a model to simulate dynamics of carbohydrate remobilization during rice grain filling, a process that can

contribute up to the 40% of rice yield known to be strongly influenced by water and nitrogen availability. Despite its importance, remobilization is often neglected in available crop simulators: this activities is aimed at filling this gap, in order to improve models capability to (i) predict yield variability and (ii) to support farmers in optimizing crop productivity.

Concerning soil domain, models for the simulation of processes leading to GHGs emission are implemented within a new component (UNIMI.CRONO), collecting modelling approaches to simulate carbon and nitrogen dynamics in agricultural soils. The software library implements models for soil organic matter decomposition, biological mediated reactions in aerobic and anaerobic conditions, transport of molecules in the gaseous and liquid phase, soil-plant interactions at root level and responses to agricultural management practices.

The last activity involves the confluence of available models and advances achieved during the doctorate within a modelling solution to assess the performance of paddy rice cropping system in terms of productivity and environmental impacts. To achieve this aim, the solution simulates the mutual interactions among crop growth and development, biogeochemistry, soil water and temperature dynamics, as modulated by meteorology and farmer management choices. A preliminary evaluation of the agreement between measured and simulated data using field data is performed, and the opportunity of employing the solution to study the effects of alternate management strategies on crop yield, nitrogen leaching, CH_4 and N_2O emissions is explored.

1.5. Synopsis

Chapter 2 presents two new formalizations of WOFOST, which is one of the most widespread model from the SUCROS-type family of models. The first (WOFOST-GT) enhances the usability of the model by markedly reducing the number of parameters of the model, via the substitution of AFGEN tables with functions driven by few parameters with a clear biological meaning. These changes increased the usability of the original version of the model, without compromising the high level of detail in the way biophysical processes are reproduced and without lowering its performances in terms of accuracy. The second version (WOFOST-GT2; extending -GT) is based on an improved representation of the canopy structure, with an explicit consideration of the vertical dimension of the canopy and of the bottom-up dynamic of leaves senescence. This improvement would likely increase the capability of the model to interact with models for the simulation of micrometeorological aspects within the canopy, and with models for the simulation of biotic (e.g., diseases) and abiotic (e.g., pre-flowering thermal shocks) factors affecting crop productions.

Chapter 3 proposes a new modeling approach to give an interpretation of the contribution of carbohydrate redistribution during rice grain filling based on a reanalysis of published information. The model was designed targeting a degree of adherence to physiological processes coherent with the current state-of-the-art of crop models. The result is a set of equations driven by few parameters reflecting crop physiological traits, whose calibration allowed to give reliable estimates of non-structural carbohydrate remobilization in both Indica and Japonica cultivars. The new model can be easily integrated in rice simulators based on the concept of net photosynthesis or simulating the gross assimilation of CO_2 and respiration losses.

Chapter 4 presents a new software component (UNIMI.CRONO) aimed at collecting models for the simulation of carbon and nitrogen dynamics in agricultural soils. It is designed to maximize usability and extension, as well as the integration in complex modelling solutions. These features overcome some of the limitations affecting current soil models and will likely contribute to update UNIMI.CRONO with the latest outcomes in soil science. Model sensitivity to input parameters was tested in a range of conditions consistent with those characterizing the actual field conditions. Sensitivity analysis was carried out considering GHGs emissions as the main synthetic variables to evaluate system’s performance. This analysis pointed out the high interrelation of underlying processes leading to the emission of CO_2, CH_4 and N_2O, with soil organic matter, agricultural management and soil-plant interactions playing a major role.

Chapter 5 describes the development of a modular modelling solution ¬ explicitly designed for being easily used, composed and extended ¬ aimed at describing multiple aspects of the rice cropping system and their mutual interactions. The solution is built by selecting and linking models belonging to different domains: the design of the project favours the substitution of implemented models with alternate approaches, simplifying its maintenance and further development. Currently, simulation results highlight ¬ after calibration ¬ the suitability of the MS to simulate rice growth dynamics and the emission of CH_4 and CO_2. Nevertheless, evaluation of modelling solution performance against measured data is still preliminary, and more comprehensive datasets are needed to perform an in-depth assessment of the agreement between observations and simulations. The solution demonstrated to be an effective tool for the exploration of management scenarios, allowing to perform *in-silico* experiments to test the impact of alternate agronomic strategies on cropping system productivity and environmental impacts.

Chapter 6 highlights future perspectives after drawing the general conclusions of this work with regard to the development achieved and the realization of specific objectives.

Note

Chapter 2 is published in Environmental Modelling and Software. Chapter 3 is published in Ecological Modelling. Chapter 4 and 5 will be submitted to Environmental Modelling and Software. I would like to acknowledge the editorial boards of Environmental Modelling and Software and Ecological Modelling for their permission to include the papers in this thesis.

MODEL SIMPLIFICATION AND DEVELOPMENT VIA REUSE, SENSITIVITY ANALYSIS AND COMPOSITION: A CASE STUDY IN CROP MODELLING

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2.1. Abstract

Crop models, like many representations of environmental processes, tend to be over-parameterised. A redesign of the SUCROS family of crop models, largely driven by sensitivity analysis, is presented here. In particular, two new versions of WOFOST, the most widespread model from this family, were developed. The first (WOFOST-GT) reduces model complexity through the definition of functions driven by few parameters with biological meaning. The other (WOFOST-GT2) improves canopy representation and senescence. Each version was evaluated for rice and winter wheat. Results highlighted a similar accuracy for the three versions: the original one achieved mean normalized RMSE of 13.75% and 10.75% for winter wheat and rice; corresponding values for the new versions were 14.42% and 10.79% (WOFOST-GT), and 14.38% and 10.85% (WOFOST-GT2). The new versions were considerably less complex, (60% less parameters). These improvements, increasing model usability without compromising its sophistication, can be transferred to other models from the same family.

Keywords*:* AFGEN tables, canopy layers, CropML, WOFOST

Software availability: CropML.WOFOST-GT, CropML.WOFOST-GT2 are distributed free of charge for noncommercial purposes as .NET 4.5 components. The Software Development Kit is supplied on request (cassandra.lab@unimi.it) to interested users, and includes hypertext files documenting algorithms and code, as well as source codes of sample applications.

2.2. Introduction

The formalization of knowledge in agro-environmental models often leads to representations of the underlying systems characterized by a marked tendency towards over-parameterisation (Tremblay and Wallach, 2004). This might be due to different factors, like (i) the need to compose results from researches which targeted different subsystems, (ii) the partial understanding of key processes, that leads to models suitable for accommodating flexible calibrations against sets of observations, and (iii) technological bottlenecks partly preventing the adoption of advanced techniques for analysing and improving model design. To a certain extent, these considerations apply to the widespread crop models belonging to the SUCROS family (Bouman et al., 1996; van Ittersum et al., 2003). The worldwide spread of these models stems from the soundness of the approaches used to reproduce crop growth and by the high level of detail in describing the interactions between plants and environment. These features allowed the successful application of these models across a wide range of climatic (e.g., Supit et al., 2010) and management (e.g., Hengsdijk et al., 2005) conditions, and make them the first choice when a high level of adherence to real systems is needed, as in the case of, e.g., in silico phenotyping studies (Confalonieri et al., 2012), or for analyses in environments with a complex orography (Ferrara et al., 2010). On the other hand, this demands a huge amount of information for their parameterization, in turns increasing the effort for using them operationally (Donatelli and Confalonieri, 2011) and exposing users to risks because of the large number of freedom degrees during calibration. Indeed, the higher the number of parameters, the higher the risk of including site- and season-specific factors affecting observations in the values of parameters, which should instead describe only morphological and physiological plant traits. A portion of the large number of parameters present in SUCROS-type models is explained by the high level of detail used to represent biophysical processes, and should be considered as a positive, intrinsic feature of this family of models. Nevertheless, the main reason for the over-parameterization is the presence of AFGEN (Arbitrary Function GENerator) tables to describe the dependence of some parameters on air temperature or development stage. Especially when parameters are calibrated using observations related to just one state variable (e.g., aboveground biomass), AFGEN tables could allow the user to fit unrealistic functions for the description of plant processes. Therefore, although these functions could potentially lead to a better fit of the outputs during calibration because of their high flexibility, they increase the risks of losing adherence with actual biophysical phenomena. Another critical issue related to the presence of AFGEN tables refers to the difficulty of coupling the crop models to advanced tools for sensitivity analysis and automatic calibration. The reasons are that many of the algorithms implemented in such tools sample the parameters hyperspace by considering parameters as independent, and – for the sampling methods accounting for parameters correlation – it is often very difficult to define a priori the degree of correlation. In case of different parameters defining, e.g., specific leaf area (SLA) in two different development stages, these algorithms iterate sampling combinations of SLA values which could lead to a function without any physiological meaning. Some authors (e.g., Confalonieri, 2010; Ceglar et al., 2011) succeeded in performing Monte Carlo based sensitivity analyses on these models only at the cost of drastically reducing the number of couples defining the AFGEN tables with the aim of minimizing the risks of overlaps among the parameters distributions for different values of development stage code or average air temperature.

Another source of possible inconsistencies in the way SUCROS-type models reproduce the underlying system is represented by their peculiar representation of the canopy structure. They divide the canopy in a fixed number of layers, for which instantaneous gross assimilation rates are calculated. This number appears to be arbitrary, e.g., it is three for WOFOST (van Keulen and Wolf, 1986) and five for SUCROS (van Keulen et al., 1982), apparently with no justification in both cases. Moreover, this number is maintained constant from emergence to maturity, ignoring differences in canopy structure occurring during crop cycle. One of the most critical point in this representation is that the division of the canopy in different layers is explicitly considered only for some processes, e.g., gross photosynthesis. On the contrary, other processes, e.g., leaves death, do not take into account the position of leaf area index (LAI) units within the canopy, neither for aging nor for self-shading. “Dead LAI” (representing leaves no more photosynthetically active) is thus evenly allocated along the canopy profile (i.e., to all the layers). This representation leads to situations where the last emitted LAI units, representing the youngest leaves, die exactly like the oldest ones, and where portions of dead leaves shade green ones (Confalonieri et al., 2012).

In light of the shortcomings highlighted above, two new versions of the WOFOST model were developed. WOFOST is considered as one of the most important representative of the SUCROS family: it is the main crop model used by the European Commission within the MARS Crop Yield Forecasting System (http://mars.jrc.it/mars/Bulletins-Publications), and it is widely used as a tool for analysing yield variability and the effects of climate change on crop productivity (Supit et al., 2012). The new versions and the original version were evaluated and compared using experimental data collected during rice and winter wheat field experiments, by considering their accuracy, robustness and complexity.

Therefore, the specific aims of this study were:

- to simplify WOFOST by substituting AFGEN tables with functions driven by few parameters with a clear biological meaning;
- to improve the usability and applicability of the model, by reducing the information needed to run simulations and increasing the possibility to couple the model with advanced tools for sensitivity analysis and automatic calibration;
- to investigate an alternative approach to describe the biophysical processes occurring within the canopy, via an explicit representation of the canopy vertical dimension.

2.3. Materials and Methods

2.3.1. The WOFOST model

WOFOST is a generic crop simulator for annual field crops, based on a hierarchical distinction between potential and water-limited productions. Crop growth is simulated on the basis of its underlying eco-physiological processes. Among these, phenological development, light interception, gross photosynthesis, transpiration, growth and maintenance respiration, and partitioning of assimilates to the different plant organs play a major role. The appearance of vegetative and reproductive organs, which characterizes crop phenological development, is described as a function of average daily temperature, optionally corrected by a factor accounting for photoperiod. Thermal time accumulated is then normalized to a development stage code (DVS; unitless; 0: emergence; 1: anthesis; 2: maturity) by using two parameters describing the thermal time from emergence to anthesis and from anthesis to maturity. Instantaneous gross CO2 assimilation is estimated in three moments during the day as a function of intercepted radiation and of a photosynthesis-light response curve of individual leaves. Light interception depends on total incoming radiation, on photosynthetic leaf area and on leaf angle distribution. Given that photosynthesis response to light intensity is non-linear, variations in the irradiance level are considered along the vertical profile. This is carried out by splitting the canopy into three horizontal layers and calculating the amount of radiation intercepted by each layer on the basis of the direct and diffuse light transmission through overlying layers. Daily increase in total LAI is estimated using a two-stage approach: using an exponential function driven by temperature during early stages, and from specific leaf area (SLA) and daily increase in leaves dry weight later. LAI is then allocated to the layers according to Gaussian Integration distances. Non-photosynthetically (dead) LAI units are computed daily as a function of self-shading and senescence. Part of the assimilates is consumed by maintenance respiration, depending on the dry weight of the different plant organs and on air temperature, assuming that the different organs have different respiration to dry weight ratios. Daily accumulated carbohydrates remaining after maintenance respiration are converted into plant organs components by considering development-dependent partitioning factors and the different efficiencies of conversion of assimilates into the components of the different plant organs (growth respiration). Potential evapotranspiration is estimated using the Penman approach (Frère and Popov, 1979), and water stress is derived by the actual to potential transpiration ratio.

For this study, the WOFOST version implemented in the Crop Models Library (CropML; http://agsys.cra-cin.it/tools/cropml/help/) was used. The library consists of a framework-independent MS .NET software component where different pure (e.g., WOFOST, CropSyst, WARM, STICS, CANEGRO), hybrid and new modelling solutions for crop growth and development are implemented following a fine level of granularity, according to the software architecture proposed by Donatelli and Rizzoli (2008). All the changes to the model presented and discussed in the following sections were implemented in the same component, as modelling solutions alternative to the original WOFOST.

2.3.2. Decreasing model complexity

The methodology used to reduce the complexity of the original version of WOFOST is based on the substitution of the AFGEN tables (identified in the text by the suffix “TB”) with functions (i) driven by few parameters with a clear biophysical meaning to simplify parameterization activities, and (ii) able to properly formalize the available knowledge on changes in parameter values according to crop development or air temperature. A concrete example of how we proceeded in replacing AFGEN tables is represented by the reduction of the number of pairs [SLA (m^2 kg^{-1}) – DVS] needed to run a simulation. This parameter corresponds to the ratio between area (m^2 m^{-2}) and the dry weight (kg m^{-2}) of a representative sample of leaves. Leaf dry weight can be easily measured after oven-drying the leaves until constant weight, whereas accurate LAI measurements – needed for SLA determination – are time-consuming (Negròn Juarez et al., 2009), since indirect methods (e.g., LAI2000) are not adequate in this case, and direct (i.e., planimetric) methods involving destructive sampling are normally used. Moreover, during crop development the effort required by planimetric methods for LAI determination progressively increases, because of the increasing number of leaves to be processed. In the original WOFOST version, up to ten couples of SLA values have to be provided by the user, together with the corresponding crop development stage starting from emergence to maturity. In this case, the objective of the work aimed at substituting the AFGEN table involved with SLA was to develop a function (Figure 1) driven by SLA values (i) only in two clearly recognizable phenological stages and (ii) with the two stages characterized by a moderate number of leaves per plant, to increase the possibility of easily parameterizing the model for this aspect.

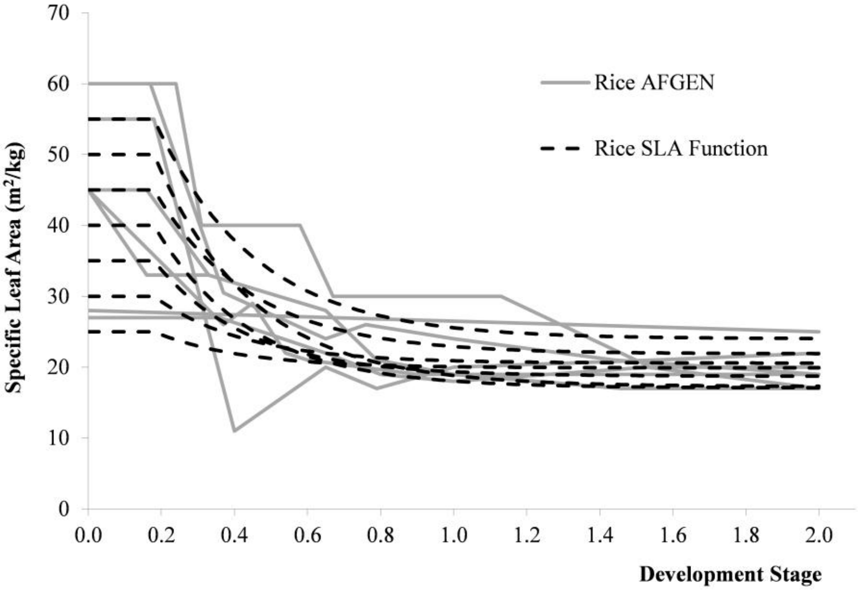

Figure 1. Specific leaf area (SLA) as a function of development stage: grey continuous lines represent AFGEN parameterizations of eight rice cultivars available in the Wofost Control Centre release; black dashed lines show four possible parameterizations of the function that replace the SLA AFGEN table in the new versions of the model.

2.3.2.1 Replacement of AFGEN tables

Two approaches were used to replace AFGEN tables. The first approach involves AFGEN tables which highlighted negligible differences among available WOFOST parameterizations for a group of species (e.g., van Diepen et al., 1988; van Heemst, 1988). In these cases, the tables were substituted with non-editable functions, developed by interpolating the available WOFOST parameterizations for rice and wheat, without introducing any additional parameter. The AFGEN tables replaced according to this approach were those related to specific stem area (SSATB; function of DVS; ha kg^{-1}, replaced by Equation 1), reduction factor of gross assimilation rate (TMNFTB; function of minimum temperature; kg kg^{-1}, Equation 2), dry biomass partitioning to roots (FRTB; function of DVS; kg kg^{-1}, Equation 3) and storage organs (FOTB; kg kg^{-1}, Equation 4), and relative death rates of roots (RDRTB; function of DVS; kg kg^{-1} d^{-1}, Equation 5) and stems (RDRSTB; kg kg^{-1} d^{-1}, Equation 5).

$$SSA = \begin{cases} 0.0003 & DVS < 0.9 \\ -0.00027 \cdot DVS + 0.00054 & DVS \geq 0.9 \end{cases} \tag{1}$$

$$TMNF = \begin{cases} 0.333 \cdot T_{\min} & T_{\min} < 3 \\ 1 & T_{\min} \geq 3 \end{cases} \tag{2}$$

$$FR = \begin{cases} 0.2 \cdot DVS^2 - 0.7 \cdot DVS + 0.5 & DVS < 1 \\ 0 & DVS \geq 1 \end{cases} \tag{3}$$

$$FO = \begin{cases} 0 & DVS < 0.7 \\ \dfrac{1}{1 + 0.5 \cdot \exp\left[\dfrac{-33.3 \cdot DVS + 33.3}{2}\right]} & 0.7 \leq DVS \leq 1.5 \\ 1 & DVS > 1.5 \end{cases} \tag{4}$$

$$RDR = \begin{cases} 0 & DVS \leq 1.5 \\ 0.02 & DVS > 1.5 \end{cases} \tag{5}$$

The second approach to replace AFGEN tables involves cases for which marked differences among parameterizations available in literature were observed. In these cases, the differences were in the values assumed by parameters, whereas the shapes (e.g., monotonic decreasing for partitioning to leaves) of the AFGEN functions proposed by different authors were coherent, since reflecting biological features of the plants. This led to the need of introducing functions driven by editable parameters to allow users to modulate the physiological crop responses to temperature and development stage. A set of functions was therefore developed to interpolate the available AFGEN parameterizations – mainly derived from measurements (e.g., Spitters et al., 1989) – with the aim of minimizing the number of parameters. These parameters were defined providing them with a clear morphological or physiological meaning, in order to ease the attribution of their values through field measurements and/or literature search. This allowed a consistent reduction of the number of parameters without undermining the degree of adherence of the model to real systems.

Temperature effect on thermal time accumulation rate (originally represented by the AFGEN DTSMTB; °C-d) was simulated by using the β function proposed by Yin et al. (1995, Equation 6), driven by the parameters minimum, optimum and maximum temperature for development ($T_{base,dev}$, $T_{opt,dev}$ and $T_{max,dev}$, respectively; °C). The same temperature response function (Equation 6, editable through the parameters $T_{base,gro}$, $T_{opt,gro}$ and $T_{max,gro}$, representing cardinal temperatures for growth) was used for the temperature effects on CO_2 assimilation (AFGEN TMPFTB; unitless), where maximum rate is represented by the parameter A_{max} (kg ha^{-1} h^{-1}). Changes in A_{max} during the crop cycle are now simulated without the need of further parameters.

$$\beta = \begin{cases} 0 & T < T_{base} \\ \left[\left(\frac{T-(T_{base}-a)}{T_{opt}-(T_{base}-a)}\right)\cdot\left(\frac{(T_{\max}-a)-T}{(T_{\max}-a)-T_{opt}}\right)^{\frac{(T_{\max}-a)-T_{opt}}{T_{opt}-(T_{base}-2)}}\right]^{b}\cdot\left(T_{opt}-T_{base}\right) & T_{base} \le T \le T_{\max} \\ 0 & T > T_{\max} \end{cases} \tag{6}$$

where a = 2 and b = 1.8 for thermal time accumulation and a = 0 and b = 1 for the calculation of thermal limitation to gross photosynthesis.

The light use efficiency table (EFFTB; function of daily mean temperature; kg ha^{-1} h^{-1} j^{-1} m^{2} s) was replaced by a linear function between two parameters (EFF_{10} and EFF_{40}; kg ha^{-1} h^{-1} j^{-1} m^{2} s), representing light use efficiency of single leaves at 10°C and 40°C. The original table describing the evolution of the extinction coefficient for diffuse visible light (KDIFTB; function of DVS; unitless) was substituted by Equation 7, driven by the parameter $KDIF_{max}$ (unitless), representing the maximum value of KDIF; changes in this parameter simulate the extinction of light along canopies of different cereal species or cultivars.

$$KDIF = \begin{cases} 0.4 & DVS < 0.65 \\ \left(KDIF_{\max}-0.4\right)\cdot\frac{1}{1+\exp\left[\frac{-\left(57.14\cdot DVS-47.14\right)}{3.3}\right]} & 0.65 \le DVS \le 1 \\ KDIF_{\max} & DVS > 1 \end{cases} \tag{7}$$

The AFGEN table describing the changes in specific leaf area (*SLA*) during crop cycle (SLATB; function of DVS; ha kg^{-1}) was replaced by a function returning SLA values which are constant during early stages and decrease exponentially later (Equation 8). Two parameters are required to adapt this function to different cereal species or varieties: SLA at emergence (SLA_{em}; ha kg^{-1}) and at mid-tillering (SLA_{035}; ha kg^{-1}).

$$SLA = \begin{cases} SLA_{em} & DVS < 0.18 \\ \left(SLA_{em} - SLA_{035} \cdot f\right) \cdot SLA_{em}^{\left[0.7(DVS-0.18)\right]} + SLA_{035} \cdot f & DVS \geq 0.18 \end{cases} \tag{8}$$

where *f* (estimating the ratio between minimum SLA reached by the crop and SLA at mid-tillering) is derived using Equation 9:

$$f = 15936 \cdot SLA_{em}^{\ 2} - 251.22 \cdot SLA_{em} + 1.43 \tag{9}$$

This formulation allows model users to specify the value of SLA at tillering instead of the value reached by the variable at the end of the crop cycle (minimum SLA), the former being easier to measure within field experiments.

Since the changes discussed above led to a non-editable FOTB function and FSTB (the fraction of aboveground photosynthates partitioned to stems; kg kg^{-1}) is – for each DVS – the complement to one of the sum of FOTB and FLTB (the fraction partitioned to leaves), partitioning to the aboveground organs is now completely dependent on the partitioning to leaves (FL, kg kg^{-1}). FL is derived by using a function driven by a single editable parameter: partitioning to leaves at emergence (RIP_{L0}; kg kg^{-1}) (Equations 10 and 11). The same concepts behind this type of representation of allocation patterns to the different plant organs are used in the rice-specific WARM model (Confalonieri et al., 2009b).

$$FL \begin{cases} -0.3 \cdot \dfrac{1 - 1.7 \cdot \exp\left[-\left(16.67 \cdot DVS - 10\right)\right]}{1 + n \cdot \exp\left[-\left(16.67 \cdot DVS - 10\right)\right]} + 0.3 & DVS \leq 1.1 \\ 0 & DVS > 1.1 \end{cases} \tag{10}$$

with:

$$n = \left[0.043 \cdot 0.051^{2.7 \cdot \left(RIP_{L0} - 0.4\right)} + 0.008\right] \cdot 1000 \tag{11}$$

The version of the model with functions replacing AFGEN tables –aimed at reducing model complexity– was named WOFOST-GT.

2.3.3. Improving the representation of canopy architecture

The methodology adopted to improve the representation of senescence dynamics within the canopy was based on the use of phenological development (via DVS) for deriving indirect information on the main variables involved, i.e., LAI and plant height. DVS identifies critical phases closely related to (i) photosynthetic area evolution, e.g., tillering (0.3<DVS<0.6) and flag leaf emission (DVS=0.9), and (ii) stem elongation (0.6<DVS<0.9). In the same way, DVS – via its role in modulating the patterns of assimilates partitioning to the different plant organs – is indirectly related to plant height, since this variable is strictly related to the fraction of photosynthates daily allocated to stems (Confalonieri et al., 2011).

Starting from WOFOST-GT, a further version of the model (named WOFOST-GT2) was developed, aimed at explicitly considering the vertical canopy profile, via the implementation of a model for plant height (Confalonieri et al., 2011) coupled to a function for deriving the number of canopy layers from DVS (Equations 12 and 13).

$$NumberOfCanopyLayers = \begin{cases} 2 & l < 2 \\ \lfloor l \rfloor & l \geq 2 \end{cases} \tag{12}$$

where the second equation is the floor function of

$$l = \begin{cases} \dfrac{20}{1 + \exp\left(-\dfrac{15 \cdot DVS - 6}{1.5}\right)} & DVS \leq 0.9 \\ 20 & DVS > 0.9 \end{cases} \tag{13}$$

This dynamic simulation of the emission of canopy layers assumes that during early stages (DVS<0.2) the canopy can be adequately described as composed by two layers; as long as the crop is growing, the number of photosynthetic layers increases according to a logistic function, with the maximum rate of emission of new layers set during tillering (DVS≈0.25÷0.35). The emission rate of new layers decreases during stem elongation, and ends with the emission of the flag leaf (DVS=0.9). Leaf senescence is then computed allocating dead LAI units starting from the lowest canopy layer until the dead LAI of the layer is equal to its total LAI. Then, this layer is considered no longer photosynthetically active, and dead LAI units start to be allocated to the layer above. Simulating leaf senescence with such a bottom-up dynamic is coherent with both the drivers for leaves senescence reproduced by WOFOST: the aging of leaves (the bottom layers contains the first emitted leaves) and self-shading (the bottom layers are those which are shaded).

The maximum number of canopy layers is set to 20 and is reached at anthesis. This value represents a compromise between the need to increase the vertical resolution to allow a fine description of leaf senescence dynamics and the need to limit the increase in the computational cost of the simulation, given the frequent adoption of WOFOST in projects requiring simulations against large-area databases. The adoption of two canopy layers at emergence is justified by (i) the pronounced worsening of the performance of the original WOFOST version run with a single canopy layer (data not shown) and (ii) by simulation experiments that revealed that the original WOFOST version markedly changes its behaviour only while increasing the number of canopy layers from one to two (Figure 2). Moreover, coupling the approach for dynamic emission of canopy layers and bottom-up leaves senescence with a model for estimating plant height allows to assign an explicit thickness to each canopy layer and to identify the height above which LAI is photosynthetically active and below which it is represented by senescent tissues. This gives the opportunity to improve the simulation of micrometeorological aspects within the canopy (e.g., dead LAI units do not transpire, thus their temperature is higher), which, in turns, could lead to a more realistic simulation of biophysical processes involved with biotic (e.g., fungal pathogens) and abiotic stressors affecting the crop.

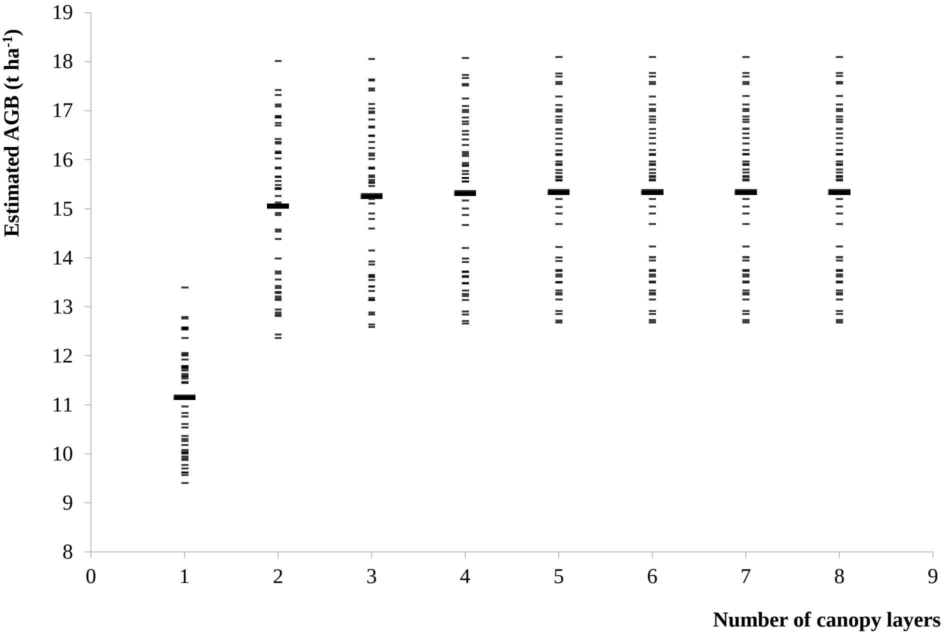

Figure 2. Aboveground dry biomass values simulated with WOFOST by changing the number of canopy layers. Results of 400 simulations (10 nations × five years × eight layers). Thicker points indicate the mean values of the outputs calculated with the number of canopy layers reported on the X-axis.

2.3.4. Testing the WOFOST versions

2.3.4.1. Sensitivity analysis experiments

Sensitivity analysis experiments were carried out for all the three versions of the model. For the original WOFOST version, the sensitivity analysis was carried out twice, with the second run performed by adding the number of canopy layers to the set of parameters investigated. For this parameter, a discrete uniform distribution (values ranging from one to eight) was used. For all sensitivity analysis experiments, aboveground dry biomass at maturity (AGB, kg ha^{-1}) was selected as the output variable, as it is best at synthetizing all the processes involved with crop growth. A two-step sensitivity analysis procedure was carried out: the Morris (1991) screening method (as improved by Campolongo et al., 2007) was first applied to identify a sub-set of relevant parameters, on which the computationally expensive Sobol' variance-based method (Sobol', 1993; Saltelli, 2002) was then applied to better discriminate among their relevance. The Morris method calculates a set of incremental ratios ($\Delta_{output}/\Delta_{parameter}$) when moving across different points of the parameter hyperspace and derives average (μ^*) and standard deviation (σ) of the ratios distribution. The higher the μ^* value, the higher the overall parameter importance, whereas the lower the σ value, the lower the interactions with other parameters. According to Morris method, the most relevant parameters are therefore those achieving high values for both these sensitivity indices. The Sobol' method identifies the relevance of each parameter or group of parameters via the quantification of their contribution to the variance of the model output, providing statistical estimators of partial variances. This method explores the parameters hyperspace via Monte Carlo sampling. In this study, the Sobol' total sensitivity index (S_t) of each parameter was considered, which quantifies the overall effect of the parameter on the output, thus including all the possible interactions with others.

In order to carry out sensitivity analysis while exploring both temporal and spatial variability, 5-year simulations (2005-2009) were performed on different European countries where the crops are intensively cultivated. France, Italy and Spain were chosen for rice, whereas England, Germany and Italy were selected to run the sensitivity analysis experiments for wheat. Within each country × crop combination, the percentage of crop presence within each of the 25 km × 25 km grid cells of the MARS database of the European Commission (Micale and Genovese, 2004) was analysed, and the cell with the highest crop presence was selected for the sensitivity analysis experiments.

The statistical distributions of the parameters of the original WOFOST version were taken from Confalonieri (2010) and Confalonieri et al. (2012) for rice and wheat, respectively (Table 2). For the new versions of the model, distribution parameters were derived from literature and unpublished data (Table 2); in case available data were not enough to reliably test distribution hypotheses, normality was assumed and standard deviations was set to 5% of the mean of available data (Richter et al., 2010).

Table 1. Locations for which sensitivity analysis experiments were performed. Latitude and longitude refer to the centroids of the 25 × 25 km grid cells of the European Commission MARS database (Micale and Genovese, 2004).

		Latitude (degrees)	Longitude (degrees)
Rice	France	43.71 N	4.63 E
	Italy	45.42 N	8.52 E
	Spain	37.04 N	6.11 W
Winter Wheat	Italy	41.43 N	15.56 E
	United Kingdom	53.31 N	0.29 W
	Germany	51.94 N	10.97 E

In order to gain an in-depth understanding of the impact of changes in the number of canopy layers on AGB variability, 400 one-season rice simulations were also run with 50 meteorological data sets (ten sites × five years, including those used for sensitivity analysis experiments) by changing the number of canopy layers from one to eight.

Table 2. Statistical settings used to define the distributions of the parameters involved in sensitivity analyses for WOFOST, WOFOST-GT and WOFOST-GT2. Mean values are derived from literature and unpublished data. Standard deviations of the parameters were set to 5% of the mean in case available data were not enough to test distribution (assumed as normal) and to reliably estimate standard deviation.

		Rice			Winter wheat		
WOFOST	Unit	Mean	St.Dev	Source	Mean	St.Dev	Source
CVL	-	0.5	0.025	f; l; p	0.685	0.03425	a; p
CVR	-	0.5	0.025	f; l; p	0.694	0.0347	a; p
CVS	-	0.5	0.025	f; l; p	0.662	0.0331	a; p
CVO	-	0.5	0.025	f; l; p	0.709	0.03545	a; p
KDIFTB000	-	0.436	0.1	d; f; j; k	0.6	0.03	m; p
KDIFTB100	-	0.625	0.02	d; f	0.6	0.03	m; p
FLTB000	kg kg^{-1}	0.7	0.083	f; l; p	0.65	0.0325	m; n; p
FLTB050	kg kg^{-1}	0.45	0.16	f; l; p	0.5	0.025	m; n; p
FOTB082	kg kg^{-1}	0.2	0.043	f; l; p	0.0001	0.0000001	m; n; p
FOTB100	kg kg^{-1}	0.65	0.083	f; l; p	1	0.05	m; n; p
FRTB000	kg kg^{-1}	0.45	0.058	f; l; p	0.5	0.025	m; n; p
FRTB100	kg kg^{-1}	0.25	0.042	f; l; p	0.02	0.001	m; n; p
LAIEM	m^2 m^{-2}	0.01	0.005	e	0.1365	0.006825	m; p
SPAN	days	35	3.5	l	35	1.75	a; p
EFFTB10	kg ha^{-1} h^{-1} J^{-1} m^2 s	0.55	0.04	l; p	0.45	0.0225	c; p
EFFTB30	kg ha^{-1} h^{-1} J^{-1} m^2 s	0.35	0.04	l; p	0.45	0.0225	c; p
TBASE	°C	9	1.5	l	0	0.05	m
AMAXTB000	kg ha^{-1} h^{-1}	40.24	5	g; i; q	35.83	4.4785	m
AMAXTB200	kg ha^{-1} h^{-1}	40.24	5	f; l; p	4.48	0.224	m; p
RGRLAI	m^2 m^{-2} day^{-1}	0.00855	0.000482	f	0.00817	0.0004085	m; p
TMPFTB14	-	0.2	0.08	f; l; p	0.92	0.046	m
TMPFTB23	-	0.8	0.02	f; l; p	1	0.05	m
Q10	-	1.8	0.1	f; l; p	2	0.1	a; m; p
RML	kg kg^{-1} day^{-1}	0.028	0.0004	f; l; p	0.03	0.0015	a; p
RMR	kg kg^{-1} day^{-1}	0.012	0.0011	f; l; p	0.015	0.00075	a; p
RMS	kg kg^{-1} day−1	0.018	0.001	f; l; p	0.015	0.00075	a; p
RMO	kg kg^{-1} day^{-1}	0.01	0.0005	f; l; p	0.01	0.0005	a; p
SLATB035	ha kg^{-1}	0.0035	0.000525	j	0.00212	0.000106	m; p
SLATB045	ha kg^{-1}	0.00262	0.0002128	j	0.00212	0.000106	m; p
SLATB065	ha kg^{-1}	0.0023	0.000276	j	0.00212	0.000106	m; p
SSATB030	ha kg^{-1}	0.000919	0.000269	f	0	0	p
SSATB120	ha kg^{-1}	0.000216	0.00003	f	0	0	p
SSATB150	ha kg^{-1}	0.000335	0.000009	f	0	0	p
NumberOfCanopyLayers	Discrete (from 1 to 8)						
WOFOST-GT / -GT2	Unit	Mean	St.Dev	Source	Mean	St.Dev	Source
$T_{base,gro}$	°C	12	0.6	h	0	0.05	s
CVL	-	0.5	0.025	f; l; p	0.685	0.03425	a; p
CVR	-	0.5	0.025	f; l; p	0.694	0.0347	a; p
CVS	-	0.5	0.025	f; l; p	0.662	0.0331	a; p
CVO	-	0.5	0.025	f; l; p	0.709	0.03545	a; p
$KDIF_{max}$	-	0.55	0.04	j	0.48	0.022	m; p
LAIEM	m^2 m^{-2}	0.01	0.005	e	0.1365	0.006825	m; p
SPAN	days	35	3.5	l	35	1.75	a; p
BASE	°C	9	1.5	l	0	0.05	m
RGRLAI	m^2 m^{-2} day^{-1}	0.00855	0.000482	f	0.00817	0.0004085	m; p
$T_{max,gro}$	°C	42	2	j	35	1.75	p
$T_{opt,gro}$	°C	28	2	h	19	1	b; o
Q10	-	1.8	0.1	f; l; p	2	0.1	a; m; p
RML	kg kg^{-1} day^{-1}	0.028	0.0005	f; l; p	0.03	0.0015	a; p
RMR	kg kg^{-1} day^{-1}	0.012	0.0011	f; l; p	0.015	0.00075	a; p
RMS	kg kg^{-1} day^{-1}	0.018	0.001	f; l; p	0.015	0.00075	a; p
RMO	kg kg^{-1} day^{-1}	0.01	0.0005	f; l; p	0.01	0.0005	a; p
RIP_{L0}	kg kg^{-1}	0.6	0.1	r	0.65	0.0325	m; n; p
SLA_{em}	ha kg^{-1}	0.0045	0.0003	r	21.2	1.06	m; p
SLA_{035}	ha kg^{-1}	0.0030	0.0002	r	21.2	1.06	m; p
A_{max}	kg ha^{-1} h^{-1}	40.24	5	g; i; q	20.155	1.00775	p
H_{max} *	cm	100	5	r	100	5	r

a: Arora and Gajri (1998); b: Bechini et al. (2006); c: Biernath et al. (2011);d: Boschetti et al. (2006); e: Boschetti (unpublished data); f: Casanova al. (2000); g: Choudhury (2001); h: Confalonieri and Bocchi (2005); i: Da Matta et al. (2001); j: Dingkuhn et al. (1999); k: Kiniri et al. (2001); l: Kro et al. (1994); m: Richter et al. (2010); n: Rötter et al. (2011); o: Slafer and Rawson (1995); p: van Diepen et al. (1988); q: Ziska and Teramura (199 r: unpublished data, collected in northern Italy under the same management conditions of the experiments described in Bechini et al. (2006) wheat and Confalonieri and Bocchi (2005) for rice, *Only for WOFOST-GT2

2.3.4.2. Experimental data

Experimental data used to evaluate the performances of the original and of the new versions of WOFOST come from 20 datasets collected in Italy (rice and winter wheat) and in the United Kingdom (winter wheat) (Table 3). Experiments 1 to 6, carried out in the Po Valley (Northern Italy), are described in detail by Confalonieri and Bocchi (2005) and Confalonieri et al. (2006). Experiments 1 and 2 were aimed at evaluating the production of two japonica-type rice varieties differing in the length of the crop cycle under non-limiting conditions for water and nutrients. During experiments 3 to 6, different rice varieties were grown under flooded conditions and different levels of nitrogen fertilization. For experiment 3, three levels of nitrogen (60, 120, 180 kg N ha−1) were applied as urea in two or three events, in a split-plot design with three replicates. In experiment 4, four nitrogen levels (0, 40, 80, 120 kg N ha−1) were applied in one or two events as urea or calcium cyanamide. Three levels of nitrogen were applied as urea during the experiment 5: 0-70-150 kg N ha−1 and 0-50-110 kg N ha−1 levels were used in two different sites. In experiment 6, two levels of nitrogen (0 and 140 kg N ha−1), split in two events, were tested. Experiments 7 to 9 were aimed at investigating growth dynamics of winter wheat and other grass species (Bechini et al., 2006). During experiment 7, three levels of nitrogen fertilization were used (0-140-210 kg N ha−1). Experiment 8 was aimed at studying the dynamics of biomass accumulation of five species, including winter wheat, under non-limiting conditions for water and nitrogen. In experiment 9, nine nitrogen treatments were evaluated (0, 50, 100 kg N ha−1 in pre-sowing combined with 0, 40, 80 kg N ha−1 top-dressed). Experiments 10 and 11 were conducted by ADAS (former Agricultural Development and Advisory Service, Nottinghamshire, UK) with the aim of measuring – under different irrigation managements (fully irrigated and rainfed) – green area expansion, radiation interception, water uptake and AGB accumulation of six winter wheat cultivars (Foulkes et al., 2001). 180 kg N ha−1 as ammonium nitrate were distributed in two events.

In this study, the three WOFOST versions were run under potential conditions, i.e., with solar radiation and air temperature as the only factors driving crop growth and development. Therefore, in case different water or nitrogen levels were tested during the experiments, only data coming from the non-limiting treatments were used for model calibration and evaluation. For the experiments where fertilization and irrigation were not experimental factors, water and nutrient availability was always adequate in fully satisfying crop needs. All the datasets refer to experimental plots which were kept weed, pest and disease free.

Available data were split in calibration and validation datasets as shown in Table 3.

The weather data used to run the models (daily air maximum and minimum temperature and global solar radiation) came from different sources: a floating micrometeorological weather station placed inside the field for experiments 5-6, automatic weather stations near the fields for experiments 1-4 and 7-9, and ECMWF (European Centre for Medium-Range Weather Forecast; www.ecmwf.int/) ERA-Interim data, with a resolution of one degree latitude × one degree longitude, for experiments 10-11.

Table 3. Datasets used for model calibration and validation. Exp.: experiment number; DOY: day of the year; J: japonica rice; I: indica rice; WW: winter wheat; C: calibration datasets; V: validation datasets.

Exp.	Country	Location	Latitude, Longitude	Years	Crop / Variety Cultivar	Sowing DOY	Flowering DOY	Maturity DOY	Dataset
1	Italy	Vercelli	45°19’ N, 8°25’ E	1989	J Cripto	128	224	249	C
1	Italy	Vercelli	45°19’ N, 8°25’ E	1990	J Cripto	130	209	254	V
1	Italy	Gudo Visconti	45°22’ N, 9°00’ E	1990	J Cripto	104	218	264	V
2	Italy	Castello d’Agogna	45°14’ N, 8°41’ E	1995	J Ariete	130	217	245	C
3	Italy	Castello d’Agogna	45°14’ N, 8°41’ E	1996	J Drago	128	229	273	C
3	Italy	Mortara	45°14’ N, 8°41’ E	1996	J Drago	129	230	273	V
4	Italy	Velezzo Lomellina	45°09’ N, 8°44’ E	1999	I Thaibonnet	91	204	237	V
5	Italy	Vignate	45°29’ N, 9°22’ E	2002	I Sillaro	119	218	279	C
5	Italy	Opera	45°22’ N, 9°12’ E	2002	I Thaibonnet	119	213	264	V
6	Italy	Opera	45°22’ N, 9°12’ E	2004	I Gladio	145	230	262	C
7	Italy	S. Angelo Lodigiano	45°15' N, 9°22' E	1986-1987	WW Gemini	294	145	186	V
7	Italy	S. Angelo Lodigiano	45°15' N, 9°22' E	1987-1988	WW Gemini	298	133	174	V
8	Italy	S. Angelo Lodigiano	45°15' N, 9°22' E	1989-1990	WW Pandas	306	130	191	C
8	Italy	S. Angelo Lodigiano	45°15' N, 9°22' E	1990-1991	WW Centauro	320	141	176	C
9	Italy	S. Angelo Lodigiano	45°15' N, 9°22' E	2001-2002	WW Guadalupe	320	130	184	C
10	UK	Gleadthorpe	55°13' N, 1°6' W	1993-1994	WW Haven	307	175	213	C
10	UK	Gleadthorpe	55°13' N, 1°6' W	1993-1994	WW Soisson	307	168	210	C
10	UK	Gleadthorpe	55°13' N, 1°6' W	1993-1994	WW Rialto	307	175	215	V
11	UK	Gleadthorpe	55°13' N, 1°6' W	1994-1995	WW Mercia	287	165	215	C
11	UK	Gleadthorpe	55°13' N, 1°6' W	1994-1995	WW Riband	287	168	215	V

2.3.4.3. Calibration of the models

The parameters of WOFOST-GT identified as the most relevant during the sensitivity analysis experiments were calibrated to obtain the best agreement between measured and simulated AGB values for rice and winter wheat. Phenology parameters (i.e., growing degree days to reach a certain phase and cardinal temperatures for development) were adjusted to reproduce observed flowering and maturity dates. For processes formalized in the same way in the three versions of the model, the same parameterization was used to increase the comparability among the three WOFOST versions (see, e.g., base temperature for emergence); the same was done for parameters with a clear biological meaning, although included in processes formalized in different ways in the three versions (see, e.g., base temperature for development) (Appendices A, B and C).

The absence of AFGEN tables allowed the calibration of WOFOST-GT parameters using the downhill simplex method (Nelder and Mead, 1965) and root mean square error (RMSE; Fox, 1981; optimum and minimum value = 0, maximum = +∞) as the objective function. A single simplex is a geometrical entity characterized by n+1 vertices moving through the n-dimensional space of the model parameters to calibrate. Each vertex represents a combination of model parameters that leads to a certain value of the objective function. The simplex moves in the parameters hyperspace following a gradient of the objective function until the minimum (or the maximum, according to the objective function selected) is reached. In this study, the evolutionary shuffled simplex method described by Acutis and Confalonieri (2006) was adopted as it (i) lowers the risk of finding local minima and (ii) forces the simplex to explore a region of the hyperspace defined by realistic values of the parameters, since boundaries are defined according to the parameters biophysical range. The calibrations were performed running simultaneously 10 simplexes, with the tolerance for the objective function set to 10-5 and the maximum number of iterations for each of the simplexes fixed at 150.

After calibration, the models were evaluated against independent datasets (Table 3) adopting a multi-metric procedure. The metrics were chosen among those proposed by Bennett et al. (2013), focusing on the ones suitable to test the model ability to reproduce time- and space-dependent data. They are root mean square error (RMSE, optimum and minimum = 0, maximum = +∞, t ha-1), normalized RMSE (NRMSE, corresponding to RMSE divided by the range of variation of measured data, optimum and minimum = 0 and maximum = 100%), modelling efficiency (NSE, Nash and Sutcliffe, 1970, optimum and maximum = 1, minimum -∞) and the coefficient of determination (R^2, optimum and maximum = 1 and minimum = 0).

2.4. Results and discussion

2.4.1. Sensitivity analyses

The results of the sensitivity analysis carried out on the original WOFOST version pointed out the relevance of the parameter "number of canopy layers" according to both the Morris and Sobol' methods. Regardless of the combination location × year, this parameter is the most relevant in explaining the variability of simulated AGB. Indeed, Morris μ* and σ indices for the number of canopy layers are, respectively, three and five times larger than those of the second ranked parameter (CVS, efficiency of conversion into stems; kg kg-1), and – according to Sobol' – 67% of total AGB variance is explained by the number of canopy layers. However, this high sensitivity of the model to the number of canopy layers is almost completely explained by the marked increase in simulated AGB while shifting from one to two layers, as outlined by the results of the simulations presented in Figure 2.

Sensitivity analysis experiments performed on WOFOST without considering the number of canopy layers as a parameter, i.e., by fixing three layers like in the original version, highlighted a different behaviour of the model in terms of parameters relevance between rice and wheat simulations (Figures 3 and 4). These differences were analysed in terms of concordance between the rankings of parameters sorted according to Morris μ* for the two crops and were significant, with a value of the top-down concordance coefficient TDCC (Iman and Conover, 1987) equal to 0.71. The differences were particularly marked for some parameters, like AMAXTB200 and RGRLAI, whose variations explained a large part of rice AGB variability, but were found to be rather irrelevant for wheat. This was both due to the different meteorological conditions characterizing the growing period of the two crops (rice is a summer crop, whereas wheat is a winter one) and to the different parameter distributions used for the sensitivity analysis experiments.

WOFOST-GT and -GT2 achieved practically the same values for the sensitivity analysis metrics and presented smaller differences in the parameter rankings obtained for rice and wheat (TDCC = 0.87). In fact, top-ranked parameters according to Morris μ* always included – for both rice and wheat – Amax, RIPL0, at least one parameter related to specific leaf area (SLAem and/or SLA035), optimum temperature for growth (Topt,gro) and conversion efficiencies into different organs (CVO, CVS and CVL). For parameterization purposes, the higher concordance between sensitivity analysis results achieved by WOFOST-GT and -GT2 for rice and wheat could allow the identification of a single subset of parameters to calibrate, regardless of the crop simulated. This would increase model usability in case, e.g., parameter sets should be defined for more crops within a modelling study. Apart from conversion efficiencies, all the parameters that achieved the highest Morris μ* values are among those introduced in the new versions of WOFOST to replace AFGEN functions. This confirms that the new formalizations included in the new versions of the model are focused on core processes.

The Sobol' method allowed deeper insight on the relevance of the parameters screened by Morris. For WOFOST-GT and -GT2, the values of Sobol' St confirmed the results of the analyses performed with the Morris method, whereas for the original version of the model the two sensitivity analysis methods led to substantial disagreement in the rankings of the most relevant parameters, especially for wheat. In this case, Sobol' method did not recognize AMAXTB000 as the most important parameter, with the variations of EFFTB10 and CVO achieving the highest St values (Figure 4). The distributions of Sobol' St indexes (Figures 3.a2, 2.b2, 3a2, 3.b2) highlighted a marked variability according to the conditions explored: for each version of WOFOST, only few parameters showed a small range of St values (e.g., the WOFOST-GT2 CVS for both rice and wheat, and the WOFOST parameters Q10 and KDIFTB000 for wheat and rice, respectively).

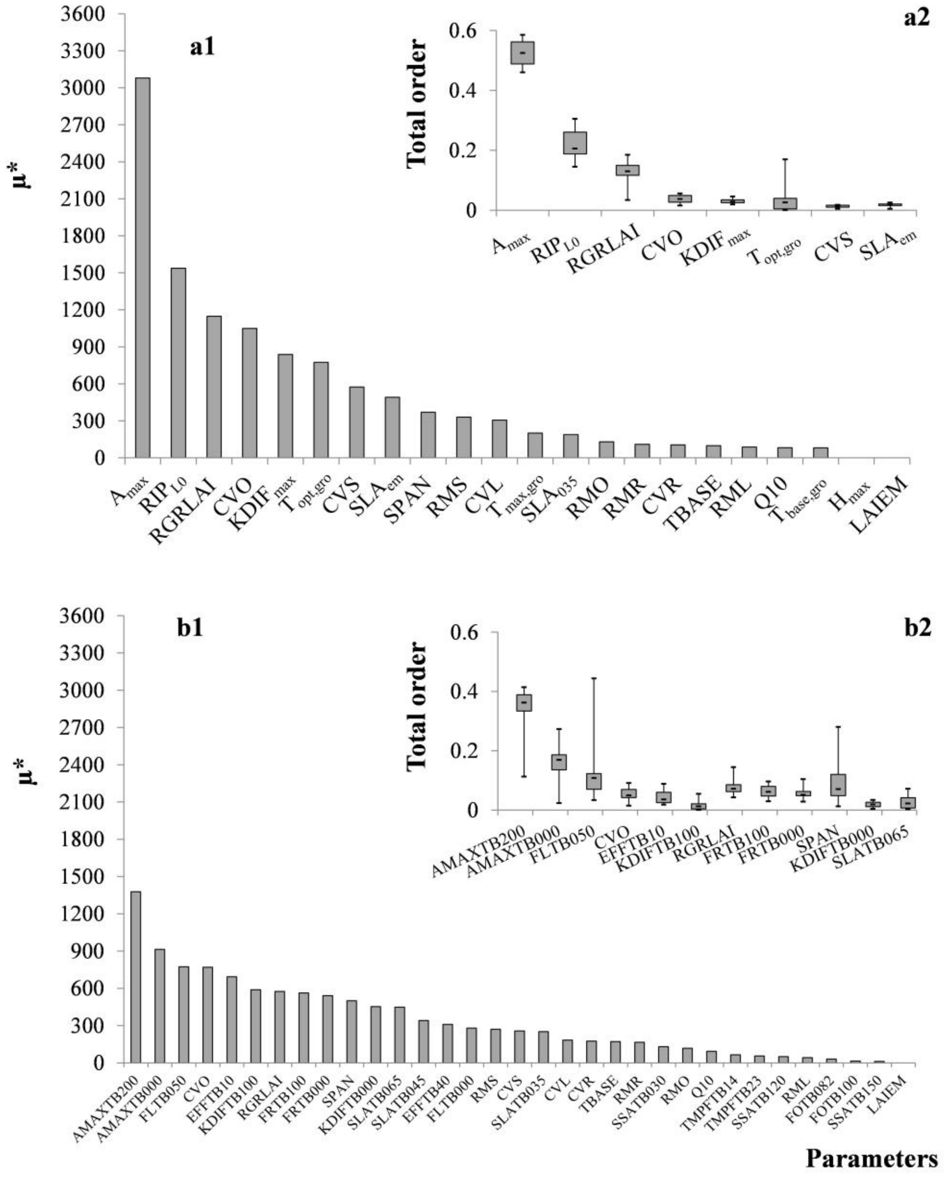

Figure 3. Results of the sensitivity analysis experiments performed for rice. a: WOFOST-GT2; b: WOFOST; 1: Morris Method; 2: Sobol' method. The suffix "TB" identifies a parameter listed in an AFGEN table. The code following "TB" is the value of the independent variable of the AFGEN table. Two digit code: average air temperature (°C); three digit code: development stage (unitless; decimal point after the first digit).

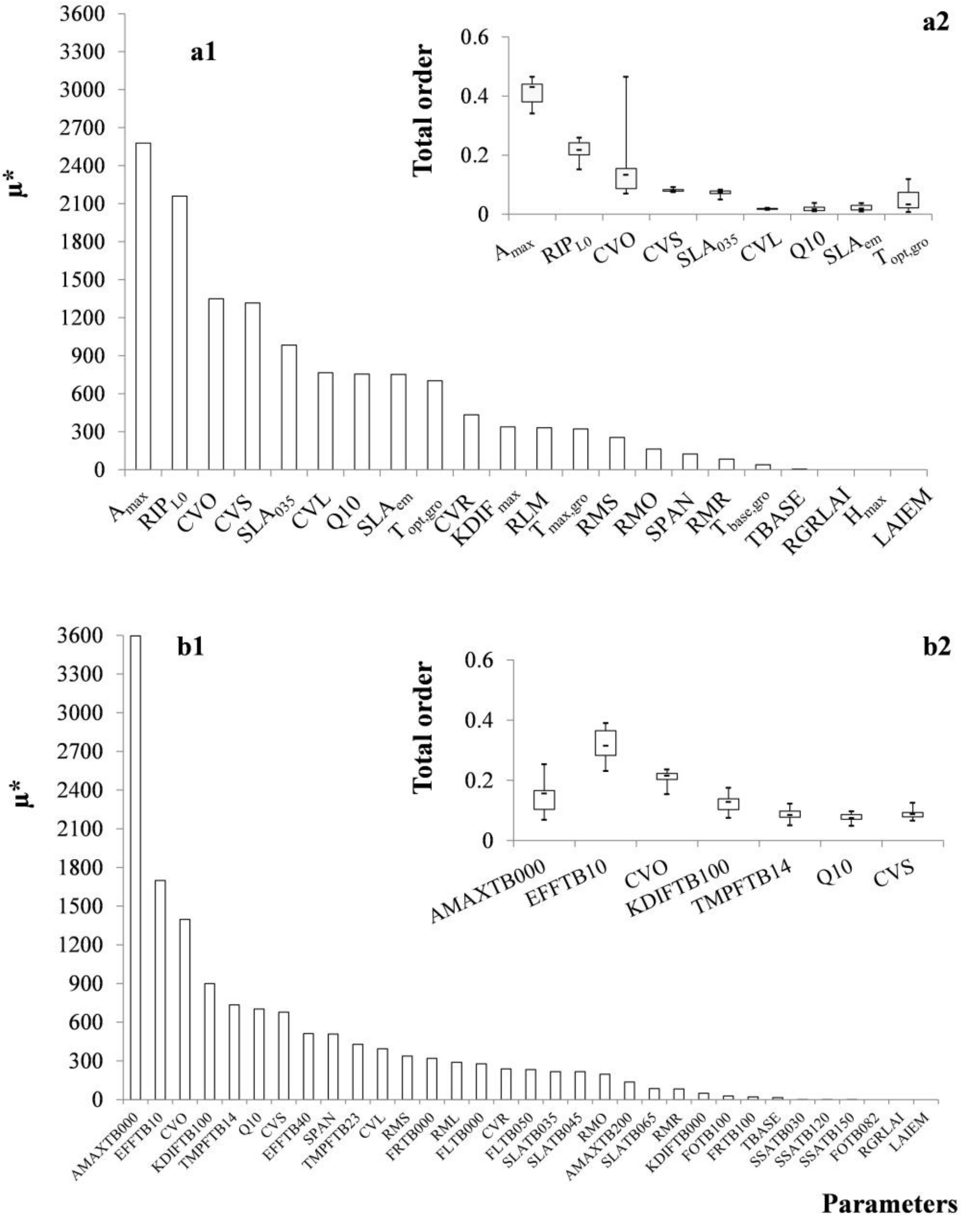

Figure 4. Results of the sensitivity analysis experiments performed for wheat. a: WOFOST-GT2; b: WOFOST; 1: Morris Method; 2: Sobol' method. The suffix "TB" identifies a parameter listed in an AFGEN table. The code following "TB" is the value of the independent variable of the AFGEN table. Two digit code: average air temperature (°C); three digit code: development stage (unitless; decimal point after the first digit).

2.4.2 Calibration and evaluation

For all the versions of the model and for both the crops, calibrated parameters are presented in Appendices A-B (WOFOST) and C (WOFOST-GT and -GT2). Figure 5 shows the growth dynamics of aboveground, leaves, stems and storage organs dry biomass simulated by WOFOST and WOFOST-GT. No sizable differences between the two versions of the model were observed for AGB, leaves and stems dry mass, whereas storage organs biomass simulated by the original version of WOFOST was slightly larger than for WOFOST-GT. The pronounced agreement between WOFOST and WOFOST-GT outputs is explained (i) by the fact that the functions used to replace AFGEN tables were developed with aim of preserving to the full extent the behaviour of WOFOST, and (ii) by the coherence between the parameterization of the two versions of the model. These considerations provide guarantees on the suitability of the partitioning functions implemented in the new versions of the model.

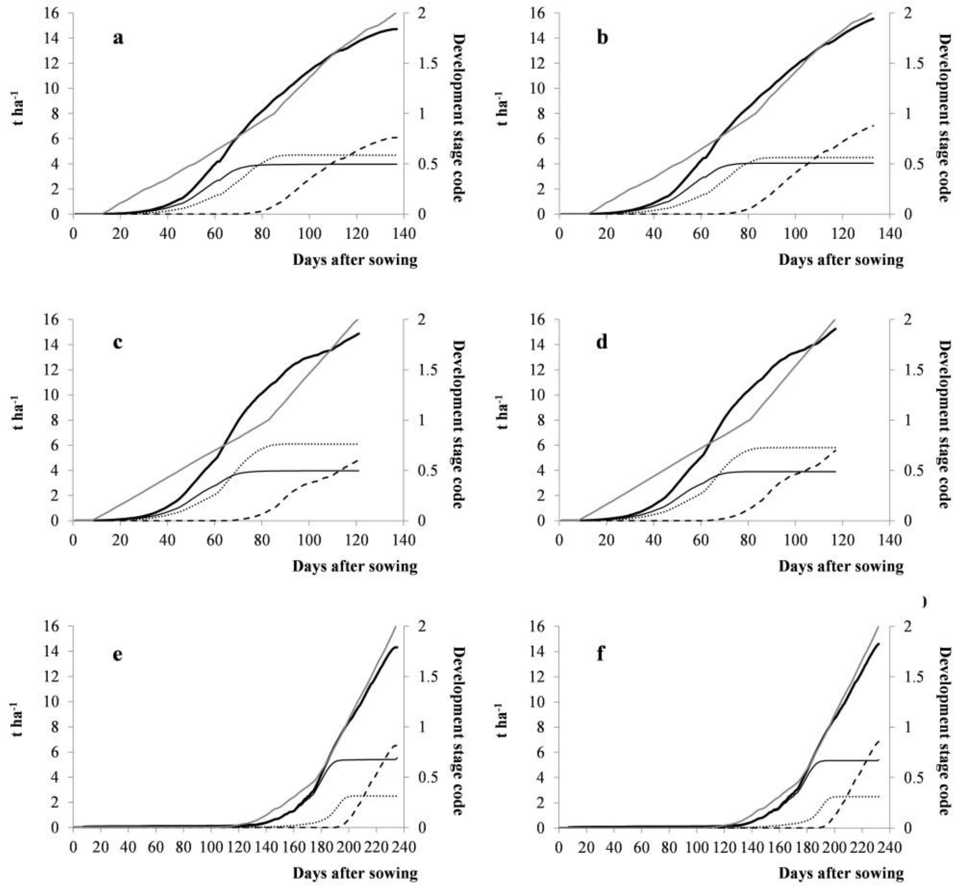

Figure 5. Comparison between WOFOST and WOFOST-GT for the simulation of aboveground biomass (black continuous thick line), leaves biomass (black continuous line), stems biomass (black dotted line), storage organs (black dashed line) and development stage (grey continuous line) for Indica-type rice (a, b), Japonica-type rice (c, d) and winter wheat (e, f). The main y-axis refers to dry biomass values (t ha-1), the secondary one -axis to the development stage code. The x-axis indicates the days after sowing. a) WOFOST, Opera 2004; b) WOFOST-GT, Opera 2004; c) WOFOST, Vercelli 1990; d) WOFOST-GT, Vercelli 1990; e) WOFOST, Sant'Angelo 1989-1990; f) WOFOST-GT, Sant'Angelo 1989-1990.

Figure 6 presents the results of the comparison between measured AGB values and corresponding outputs of WOFOST (circles) and WOFOST-GT (triangles), whereas agreement metrics are shown in Table 4; results for

WOFOST-GT2 are not shown in the figure since very close to those simulated by the -GT version of the model. Under the explored conditions, the three versions of the model achieved similar values for RMSE, NRMSE, NSE and R^2 for both rice and winter wheat (Table 4). In particular, the performances of WOFOST-GT and -GT2 are almost identical to those of the original version of the model for rice, with average RMSE equal to 1.59 t ha-1 for WOFOST and WOFOST-GT, and 1.60 t ha-1 for the -GT2 version of the model. Although the original version of the model achieved the best values for all the accuracy metrics for wheat, differences were also in this case acceptable (average RMSE = 1.80 t ha-1 for WOFOST and 1.94 t ha-1 for the -GT and -GT2 versions). The analysis of NSE, NRMSE and R^2 (the latter higher than 0.90 in 59 out of 62 cases) values confirmed the closeness of the performances of the three WOFOST versions, and the slightly better performances of WOFOST for wheat, although differences were always negligible. These differences are due to small discrepancies between the linear interpolation of the AFGEN tables and the non-linear functions used to replace them.

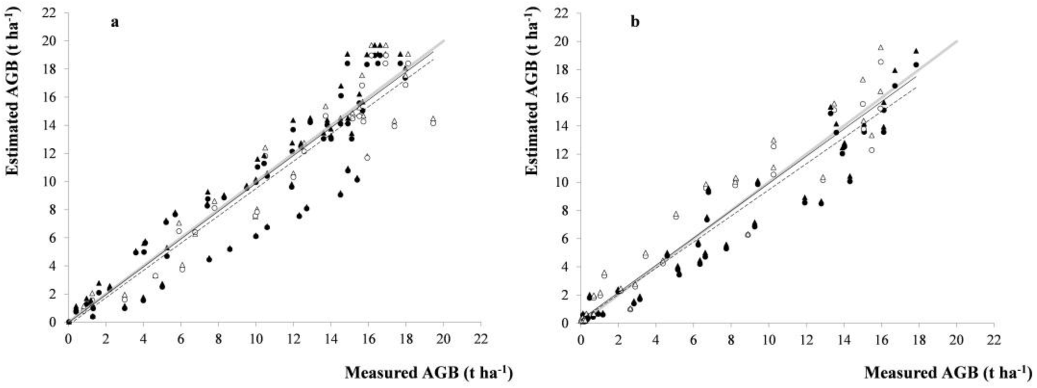

Figure 6. Comparison between measured and simulated aboveground dry biomass values for wheat (a) and rice (b); WOFOST: calibration datasets (black circles), validation datasets (white circles); WOFOST-GT: calibration datasets (black triangles), validation datasets (white triangles). The grey lines are the 1:1 line. Dotted lines are the regression y = 0.9704x - 0.2016 (R^2 = 0.8747) and y = 0.9263x + 0.1974 (R^2 = 0.926) of WOFOST values for wheat and rice, respectively. Continuous lines are the regression y = 0.9899x - 0.0249 (R^2 = 0. 863) and y = 0.9673x + 0.2414 (R^2 = 0. 925) of WOFOST-GT values for wheat and rice, respectively.

Table 4. Indices of agreement between aboveground dry biomass observations and corresponding values simulated by WOFOST, WOFOST-GT and WOFOST-GT2. RMSE: root mean square error; NRMSE: normalized root mean square error (equal to RMSE divided by the range of variation of measured data); NSE: modelling efficiency (Nash and Sutcliffe, 1970) ; R^2: coefficient of determination.

Dataset	RMSE ($\mathrm{t\ ha^{-1}}$)			NRMSE (%)			NSE			R^2		
	W	W-GT	W-GT2	W	W-GT	W-GT2	W	W-GT	W-GT2	W	W-GT	W-GT2
	Winter wheat – Calibration											
Sant'Angelo 89-90	3.56	3.45	3.42	30.7	29.8	29.5	0.376	0.412	0.422	0.841	0.833	0.833
Sant'Angelo 90-91	0.92	1.01	1.04	6.4	7.0	7.1	0.960	0.952	0.950	0.975	0.978	0.978
Sant'Angelo 01-02	1.41	1.20	1.17	10.4	8.9	8.6	0.951	0.965	0.967	0.988	0.987	0.987
Haven 93-94	0.99	1.41	1.46	6.7	9.5	9.8	0.970	0.939	0.934	0.977	0.978	0.978
Soisson 93-94	1.71	2.10	2.16	11.8	14.5	14.9	0.905	0.856	0.848	0.952	0.953	0.954
Mercia 94-95	1.67	2.29	2.35	10.7	14.6	15.0	0.912	0.835	0.826	0.997	0.997	0.997
Mean	*1.71*	*1.91*	*1.93*	*12.8*	*14.0*	*14.2*	*0.846*	*0.826*	*0.824*	*0.955*	*0.954*	*0.954*
	Winter wheat – Validation											
Sant'Angelo 86-87	3.01	2.88	2.77	18.0	18.8	18.7	0.673	0.701	0.724	0.907	0.904	0.904
Sant'Angelo 87-88	2.20	1.90	1.87	23.7	22.7	21.8	0.809	0.859	0.862	0.983	0.983	0.983
Rialto 93-94	0.81	0.98	1.01	13.7	11.8	11.6	0.981	0.973	0.971	0.982	0.982	0.983
Riband 94-95	1.53	2.14	2.20	5.4	6.6	6.8	0.922	0.847	0.839	0.993	0.994	0.994
Mean	*1.89*	*1.98*	*1.96*	*15.2*	*15.0*	*14.7*	*0.846*	*0.845*	*0.849*	*0.966*	*0.966*	*0.966*
	RMSE ($\mathrm{t\ ha^{-1}}$)			NRMSE (%)			NSE			R^2		
	W	W-GT	W-GT2	W	W-GT	W-GT2	W	W-GT	W-GT2	W	W-GT	W-GT2
	Rice – Calibration											
Vercelli 1989	2.01	1.83	1.78	12.5	11.4	11.1	0.899	0.917	0.921	0.961	0.959	0.958
Castello d’Agogna 1995	0.78	0.72	0.71	5.7	5.3	5.2	0.971	0.975	0.976	0.976	0.977	0.978
Castello d’Agogna 1996	1.47	1.83	1.89	8.3	10.3	10.7	0.956	0.932	0.927	0.986	0.989	0.989
Vignate 2002	2.38	2.16	2.13	14.3	13.0	12.8	0.858	0.883	0.886	0.934	0.926	0.927
Opera 2004	1.43	1.24	1.24	10.7	9.3	9.2	0.881	0.910	0.911	0.951	0.952	0.951
Mean	*1.61*	*1.55*	*1.55*	*10.3*	*9.8*	*9.8*	*0.913*	*0.923*	*0.924*	*0.962*	*0.961*	*0.961*
	Rice – Validation											
Mortara 1996	1.94	2.42	2.50	12.3	15.3	15.8	0.907	0.856	0.846	0.989	0.990	0.990
Gudo Visconti 1990	1.49	1.71	1.75	14.6	16.7	17.1	0.827	0.772	0.762	0.978	0.979	0.979
Vercelli 1990	0.90	0.86	0.88	5.7	5.4	5.6	0.978	0.980	0.979	0.979	0.984	0.984
Velezzo Lomellina 1999	1.63	1.45	1.43	10.7	9.5	9.4	0.925	0.942	0.943	0.956	0.963	0.964
Opera 2002	1.87	1.73	1.71	12.7	11.7	11.6	0.893	0.908	0.910	0.947	0.941	0.942
Mean	*1.57*	*1.63*	*1.66*	*11.2*	*11.7*	*11.9*	*0.906*	*0.892*	*0.888*	*0.970*	*0.971*	*0.972*

In general, the reduction of the number of parameters led to a decided improvement of the new versions of WOFOST in terms of complexity, quantified using the Akaike index (Akaike Information Criterion, Akaike, 1974, optimum = 0). The values of the Akaike index of the new versions of the model (Table 5) are in fact 35% and 50% lower – for wheat and rice, respectively – than those calculated for the original version of the model. Besides the obvious advantages deriving from the reduction of the number of parameters, the elimination of the AFGEN tables increases the model usability by lowering the risk of developing incoherent parameter sets while changing parameter values during calibration. The tuning of AFGEN points requires a higher degree of knowledge on plant physiology, since more degrees of freedom are left to the user. On the contrary, the functions used to replace AFGEN tables are forced to reproduce realistic dynamics during the crop cycle. The adherence of these functions to actual physiological processes is enhanced – with our implementation – by smaller biophysical ranges for the parameters (derived from literature). As an example, photosynthates partitioning to leaves in the corresponding WOFOST AFGEN table must range between 0 and values around 0.90, and it is very difficult – in this case – to define bounds to check user-specified values. In the new versions of the model, partitioning to leaves is driven by a single parameter, corresponding to the values at emergence. In this case, bounds can be restricted to 0.40 and 0.90, increasing possibility of performing pre-simulation quality checks of the information provided. All these features increase the model usability even for scientists and technicians not necessarily specialized in crop physiology but interested in analysing agroecosystems (e.g., hydrologists, soil scientists), because the lower the degree of freedom during calibration, the lower the risk of inconsistencies in the parameter sets. Of course, the drawback for crop physiologists or experienced crop modellers is a certain decrease in model flexibility.

Compared to what achieved for WOFOST, the robustness of the new versions of the model decreased for winter wheat, whereas it remained practically unchanged for rice (Table 5). This was partly unexpected, since decreasing the number of parameters should reduce the risk of including season- or site-specific factors in model parameters values. In general, the values calculated for the robustness indicator (Confalonieri et al., 2010, optimum and minimum = 0, maximum = +∞) are more satisfactory for rice (Robustness Indicator = 0.31) than for winter wheat (Robustness Indicator = 1.06). However, a general worsening of the performances of the three WOFOST versions for wheat was, to a certain extent, expected. The reason is that a single parameter set was calibrated here for wheat, despite the large number (nine) of varieties and thus potential differences in the plant traits to be codified in parameter values. This was done because of the absence of objective criteria to cluster the available varieties in groups with similar morphological and physiological features. For rice, the six varieties available were instead equally split into japonica- and indica-type, and two parameter sets were developed for each model. In practice, the impact of simulating different genotypes with the same parameter set was larger for wheat than for rice.

Even if the performances of the three versions of WOFOST were comparable in terms of agreement between measured and simulated AGB values, this study suggests the adoption of the new versions for both wheat and rice because of the substantial reduction of complexity which – however – does not undermine neither model accuracy nor its adherence to plant processes. Concerning WOFOST-GT and WOFOST-GT2, the choice between the two versions should be instead driven by the specific objectives of the modelling study, given that the -GT2 version is more suitable for being coupled with models for processes requiring a fine representation of micrometeorological aspects within the canopy.

Table 5. Robustness indicator (Confalonieri et al., 2010) and Akaike Information Criterion (Akaike, 1974) calculated for WOFOST, WOFOST-GT and WOFOST-GT2.

Crop	WOFOST	WOFOST-GT	WOFOST-GT2
		Robustness Indicator	
Winter wheat	1.16	1.03	1.00
Rice	0.30	0.30	0.33
		Akaike Information Criterion	
Winter wheat	330.9	211.3	213.3
Rice	281.2	144.8	150.1
		Number of parameters under potential conditions	
Winter wheat	104	40	41
Rice	104	38	39

2.5. Conclusions

Although the approaches implemented in the SUCROS family of models are recognized worldwide as conceptually sound and effective in reproducing dynamics related with crop growth, a main constraint to their operational use is represented by the huge effort needed for their parameterization. This is mainly due to the large number of parameters used to reproduce the effect of crop development or air temperature in modulating morphological and physiological plant features (AFGEN tables). Apart from the parameterization effort, this strongly limits the compatibility of SUCROS-type models with advanced tools for sensitivity analysis or automatic calibration. Moreover, the theoretical formalization behind the models belonging to this family remained – to a large extent – identical to what it was in the 80’s, and reveals some inconsistencies with the underlying system, e.g., for the representation of canopy structure and senescence dynamics.

We propose here two new formalizations of WOFOST, which is one of the most widespread model from this family. The first (WOFOST-GT) enhances the usability of the model by markedly reducing the number of parameters of the model, via the substitution of AFGEN tables with functions driven by few parameters with a clear biological meaning. These changes increased the usability of the original version of the model, without compromising the high level of detail in the way biophysical processes are reproduced and without lowering its performances in terms of accuracy. The second version we propose (WOFOST-GT2; extending -GT) is based on an improved representation of the canopy structure, with an explicit consideration of the vertical dimension of the canopy and of the bottom-up dynamic of leaves senescence. This improvement would likely increase the capability of the model to interact with models for the simulation of micrometeorological aspects within the canopy, and with models for the simulation of biotic (e.g., diseases) and abiotic (e.g., frost, pre-flowering thermal shocks) factors affecting crop productions.

The development of the new versions of the model was greatly supported by the software architecture followed to implement the original version of the model in the software component CropML (Crop Models Library; http://agsys.cra-cin.it/tools/cropml/help/). This architecture enhances the extensibility of modelling approaches via the high level of granularity in the way sub-processes are isolated and composed. The redesign of the model also benefited from the use of advanced sensitivity analysis technique, that – despite their pervasive use for understanding model limitations (e.g., Petropoulos et al., 2013; Moreau et al., 2013) – are still rarely used for model redesign. Further developments include the definition of other functions to replace AFGEN tables for other types of crops. This because the functions presented in this study, e.g., assimilates partitioning, are specific for rice and winter cereals, and cannot be considered suitable for other crops. The need for developing specific functions for groups of crops with similar behavior can be considered as a drawback of the elimination of AFGEN tables. Indeed, the AFGEN solution obviously guarantees the highest flexibility during parameterization, since such tables can be customized to draw whatever trend. However, we consider that the benefits deriving from the reduction of model complexity represent an advantage for model users that decidedly overcomes this drawback.

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2.6. Appendices

Appendix A. WOFOST parameters involved with development and growth of winter wheat and rice (Indica and Japonica type). *: calibrated values; parameters excluded from calibration come from Spitters et al., 1989.

Parameter	Units	Value			Description
		Rice Japonica	Rice Indica	Wheat	
Development					
TBASEM	°C	11*	11*	0*	Lower threshold of temperature for emergence
TEFFMX	°C	35*	35*	30*	Maximum effective T for emergence
TSUMEM	°C-days	80*	90*	60*	Temperature sum from sowing to emergence
IDSL	–	–	–	2	Pre-anthesis development based on temperature (=0), day length (=1), both (=2)
DLO	h	–	–	14*	Optimum daylength for development
DLC	h	–	–	10*	Minimum daylength for development
TSUM1	°C-days	1050*	1055*	800*	Temperature sum from emergence to anthesis
TSUM2	°C-days	520*	595*	750*	Temperature sum from anthesis to maturity
DTSMTB	°C; °C-days	0.0; 0.0	0.0; 0.0	0.0; 0.0	Daily increase in temperature sum as a function of average temperature
		9.0; 0.0*	9.0; 0.0*	10.0; 10.0*	
		15; 8.0*	15; 5.0*	18.0; 20.0*	
		20; 13	22; 14*	24.0; 24.0*	
		24; 15	26; 17*	28.0; 21.0*	
		29; 12	29; 14*	30.0; 13.0*	
		38; 0.0	31; 0.0*	31.0; 0.0*	
		40; 0.0	40; 0.0*	40.0; 0.0*	
DVSI	–	0	0	0	Development stage start simulation
DVSEND	–	2	2	2	Development stage at harvest
Growth					
TDWI	kg ha^{-1}	100	100	210	Initial total crop dry weight
LAIEM	ha ha^{-1}	0.15	0.15	0.1365	Leaf area index at emergence
RGRLAI	ha ha^{-1}	0.009	0.009	0.00817	Maximum relative increase in LAI
SLATB	–; ha kg^{-1}	0.0; 0.0023*	0.0; 0.0021*	0.0; 0.00231*	Specific leaf area as a function of development stage
		0.18; 0.0023*	0.18; 0.0021*	0.18; 0.00231*	
		0.42; 0.0018*	0.37; 0.0018*	0.42; 0.00215*	
		0.7; 0.00175*	0.7; 0.00178	0.70; 0.00208*	
		2.0; 0.0017*	2.0; 0.00175*	2.0; 0.00206*	
SPA	ha kg^{-1}	0	0	0.0	Specific pod area
SSATB	ha kg^{-1}	0.0; 0.0	0.0; 0.0	0.0; 0.0	Specific stem area as a function of development stage
		2.0; 0.0	2.0; 0.0	2.0; 0.0	
SPAN	days	35*	35*	29.5*	Life span of leaves growing at 35 °C
TBASE	°C	8	8	0.0	Lower threshold temperature for ageing of leaves
KDIFTB	–	0.0; 0.4*	0.0; 0.4*	0.0; 0.4*	Extinction coefficient for diffuse visible light as a function of development stage
		0.65; 0.4*	0.65; 0.4*	0.65; 0.4*	
		1.0; 0.6*	1.0; 0.6*	1.0; 0.65*	
		2.0; 0.6*	2.0; 0.6*	2.0; 0.65*	
EFFTB	kg ha^{-1} h^{-1} J^{-1} m^2 s	0.0; 0.6*	0.0; 0.6*	0.0; 0.6*	Light-use efficiency single leaf as function of daily mean temperature
		40; 0.36	40; 0.36	40.0; 0.36	
AMAXTB	–; kg ha^{-1} h^{-1}	0.0; 26*	0.0; 24*	0.0; 20*	Maximum leaf CO2 assimilation rate as function of development stage
		2.0; 26*	2.0; 24*	2.00; 20*	
TMPFTB	°C; -	0.0; 0.0*	0.0; 0.0*	0.0; 0.0*	Reduction factor of AMAX as function of average temperature
		12; 0.0*	12; 0.0*	12.0; 0.7*	
		14; 0.4*	14; 0.4*	17.0; 0.9*	
		17; 0.8*	18; 0.8*	23.0; 1.0*	
		22; 1.0*	23; 1.0*	28.0; 0.9*	
		26; 0.9*	27; 0.9*	31.5; 0.6*	
		28; 0.0*	38; 0.0*	33.0; 0.0*	
TMNFTB	°C; -	0.0; 0.0	0.0; 0.0	0.0; 0.0	Reduction factor of gross assimilation rate as function of low minimum temperature
		3.0; 1.0*	3.0; 1.0*	3.0; 1.0*	

Appendix B. WOFOST parameters involved with respiration, partitioning, organs death and rooting of winter wheat and rice (Indica and Japonica type). *: calibrated values; parameters excluded from calibration come from Spitters et al., 1989.

Parameter	Units	Value			Description
		Rice Japonica	Rice Indica	Wheat	
Respiration					
CVL	kg kg^{-1}	0.754	0.754	0.685	Efficiency of conversion into leaves
CVO	kg kg^{-1}	0.684	0.684	0.709	Efficiency of conversion into storage organs
CVR	kg kg^{-1}	0.754	0.754	0.694	Efficiency of conversion into roots
CVS	kg kg^{-1}	0.754	0.754	0.662	Efficiency of conversion into stems
Q10	–	2	2	1.5*	Reletive increase in respiration rate per 10 °C
RML	kg CH$_2$Okg^{-1} day^{-1}	0.02	0.02	0.03	Relative maintenance respiration rate for leaves
RMO	kg CH$_2$Okg^{-1} day^{-1}	0.003	0.003	0.01	Relative maintenance respiration rate for storage organs
RMR	kg CH$_2$Okg^{-1} day^{-1}	0.01	0.01	0.015	Relative maintenance respiration rate for roots
RMS	kg CH$_2$Okg^{-1} day^{-1}	0.015	0.015	0.015	Relative maintenance respiration rate for stems
RFSETB	–; –	0.0; 1 2.0; 1.0	0.0; 1 2.0; 1.0	0.0; 1.0 2.0; 1.0	Reduction factor for senescence as function of development stage
Partitioning					
FRTB	–; kg kg^{-1}	0.0; 0.5 0.1; 0.5 0.2; 0.4 0.35; 0.22 0.4; 0.17 0.5; 0.13 0.7; 0.07 0.9; 0.03 1.2; 0.0 2.0; 0.0	0.0; 0.5 0.1; 0.5 0.2; 0.4 0.35; 0.22 0.4; 0.17 0.5; 0.13 0.7; 0.07 0.9; 0.03 1.2; 0.0 2.0; 0.0	0.0; 0.5 0.1; 0.5 0.2; 0.4 0.35; 0.22 0.4; 0.17 0.5; 0.13 0.7; 0.07 0.9; 0.03 1.2; 0.0 2.0; 0.0	Fraction of total dry matter to roots as a function of development stage
FLTB	–; kg kg^{-1}	0.0; 0.6* 0.5; 0.6* 0.65; 0.54* 0.85; 0.1* 1.0; 0.01* 2.0; 0.0*	0.0; 0.65* 0.5; 0.65* 0.65; 0.58* 0.85; 0.1* 1.0; 0.01* 2.0; 0.0*	0.0; 0.9* 0.5; 0.86* 0.65; 0.73* 0.85; 0.1* 1.0; 0.01* 2.0; 0.0 *	Fraction of aboveground biomass to leaves as a function of development stage
FSTB	–; kg kg^{-1}	0.0; 0.4* 0.0; 0.4* 0.65; 0.46* 0.75; 0.65* 0.85; 0.78* 0.9; 0.68* 1.0; 0.25* 1.1; 0.08* 1.22; 0.02* 2.0; 1.0*	0.0; 0.35* 0.5; 0.42* 0.65; 0.42* 0.75; 0.65* 0.85; 0.78* 0.9; 0.68* 1.0; 0.25* 1.1; 0.08* 1.22; 0.02* 2.0; 1.0*	0.0; 0.1* 0.5; 0.14* 0.65; 0.3* 0.75; 0.65* 0.85; 0.78* 0.9; 0.68* 1.0; 0.25* 1.1; 0.08* 1.22; 0.02* 2.0; 0.0*	Fraction of aboveground biomass to stems as a function of development stage
FOTB	–; kg kg^{-1}	0.0; 0.0* 0.75; 0.0* 0.9; 0.2* 1.0; 0.67* 1.1; 0.9* 1.22; 1.0* 2.0; 1.0*	0.0; 0.0* 0.75; 0.0* 0.9; 0.2* 1.0; 0.67* 1.1; 0.9* 1.22; 1.0* 2.0; 1.0*	0.0; 0.0* 0.75; 0.0* 0.9; 0.2* 1.0; 0.67* 1.1; 0.9* 1.22; 1.0* 2.0; 1.0*	Fraction of aboveground biomass to storage organs as a function of development stage
Death rates					
PERDL	–	0.01	0.01	0.01	Maximum relative death rate of leaves due to water stress
RDRRTB	–; kg kg^{-1} day^{-1}	0.0; 0.0 1.5; 0.0 1.5001; 0.02 2.0; 0.2	0.0; 0.0 1.5; 0.0 1.5001; 0.02 2.0; 0.2	0.0; 0.0 1.5; 0.0 1.5001; 0.02 2.0; 0.2	Relative death rate of roots as a function of development stage
RDRSTB	–; kg kg^{-1} day^{-1}	0.0; 0.0 1.5; 0.0 1.5001; 0.02 2.0; 0.2	0.0; 0.0 1.5; 0.0 1.5001; 0.02 2.0; 0.2	0.0; 0.0 1.5; 0.0 1.5001; 0.02 2.0; 0.2	Relative death rate of stems as a function of development stage
Rooting					
RDI	cm	10	10	10	Initial rooting depth
RRI	cm day^{-1}	1.2	1.2	1.2	Maximum daily increase in rooting depth
RDMCR	cm	80	80	125	Maximum rooting depth

Appendix C. WOFOST-GT and WOFOST-GT2 parameters. * calibrated values; a parameter only for WOFOST-GT. Parameters excluded from calibration come from Confalonieri et al., 2009a and from Spitters et al., 1989 for rice and winter wheat, respectively.

Parameter	Units	Value			Description
		Rice Japonica	Rice Indica	Wheat	
Development					
$T_{base,em}$	°C	11*	11*	0	Lower threshold of temperature for emergence
$TEFF_{max}$	°C	35	35*	30	Maximum effective temperature for emergence
$T_{sum,em}$	°C-days	80*	90*	60	Temperature sum from sowing to emergence
IDSL	–	0	0	2	Pre-anthesis development based on temperature (=0), day length (=1), both (=2)
DLO	h	–	–	14	Optimum daylength for development
DLC	h	–	–	10	Minimum daylength for development
T_{sum1}	°C-days	1050*	1055*	800	Temperature sum from emergence to anthesis
T_{sum2}	°C-days	520*	595*	750	Temperature sum from anthesis to maturity
$T_{base,dev}$	°C	9*	9*	0	Lower threshold of temperature for development
$T_{opt,dev}$	°C	24*	26*	24	Optimum temperature for development
$T_{max,dev}$	°C	38*	31*	33	Maximum threshold of temperature for development
DVS_{end}	–	2	2	2	Development stage at harvest
Growth					
TDWI	kg ha^{-1}	100	100	210	Initial total crop dry weight
LAIEM	ha ha^{-1}	0.15	0.15	0.1365	Leaf area index at emergence
RGRLAI	ha ha^{-1}	0.009	0.009	0.00817	Maximum relative increase in LAI
SLA_{em}	m^{2} kg^{-1}	23*	21*	23.1*	Specific leaf area at emergence
SLA_{035}	m^{2} kg^{-1}	17*	18*	22*	Specific leaf area at tillering
SPA	ha kg^{-1}	0.0	0.0	0.0	Specific pod area
SPAN	days	35	35	29.5	Life span of leaves growing at 35 °C
TBASE	°C	8	8	0	Lower threshold temperature for ageing of leaves
$KDIF_{max}$	–	0.6*	0.6*	0.65*	Maximum extinction coefficient for diffuse visible light
EFF_{10}	kg ha^{-1} h^{-1} J^{-1} m^{2} s	0.54	0.54	0.54	Light-use efficiency single leaf as function of daily mean temperature
EFF_{40}	kg ha^{-1} h^{-1} J^{-1} m^{2} s	0.36	0.36	0.36	Light-use efficiency single leaf as function of daily mean temperature
A_{max}	kg ha^{-1} h^{-1}	26*	24*	20*	Maximum leaf CO2 assimilation rate
NDGP	–	3	3	3	Number of instants in a day for which gross photosynthesis is estimated
$T_{base,gro}$	°C	12	12	0	Lower threshold of temperature effects on CO2 assimilation
$T_{opt,gro}$	°C	22*	23*	23*	Optimum temperature effects on CO2 assimilation
$T_{max,gro}$	°C	38	38	33	Maximum threshold of temperature effects on CO2 assimilation
H_{max}[a]	M	100	100	100	Maximum plant height
Respiration					
CVL	kg kg^{-1}	0.754	0.754	0.685	Efficiency of conversion into leaves
CVO	kg kg^{-1}	0.684	0.684	0.709	Efficiency of conversion into storage organs
CVR	kg kg^{-1}	0.754	0.754	0.694	Efficiency of conversion into roots
CVS	kg kg^{-1}	0.754	0.754	0.662	Efficiency of conversion into stems
Q10	–	2	2	1.5*	Relative increase in respiration rate per 10 °C
RML	kg CH_2Okg^{-1} day^{-1}	0.02	0.02	0.03	Relative maintenance respiration rate for leaves
RMO	kg CH_2Okg^{-1} day^{-1}	0.003	0.003	0.01	Relative maintenance respiration rate for storage organs
RMR	kg CH_2Okg^{-1} day^{-1}	0.01	0.01	0.015	Relative maintenance respiration rate for roots
RMS	kg CH_2Okg^{-1} day^{-1}	0.015	0.015	0.015	Relative maintenance respiration rate for stems
Partitioning					
RIP_{L0}	–	0.6*	0.65*	0.9*	Partitioning of assimilates to leaves at emergence
Rooting					
RDI	Cm	0	0	10	Initial rooting depth
RRI	cm day^{-1}	1.2	1.2	1.2	Maximum daily increase in rooting depth
RDM	Cm	80	80	125	Maximum rooting depth

A MODEL TO SIMULATE THE DYNAMICS OF CARBOHYDRATE REMOBILIZATION DURING RICE GRAIN FILLING

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3.1. Abstract

The remobilization of carbon reserves accumulated in stems during vegetative growth is known to significantly contribute to yield formation in many cereals, and to be modulated by water and nitrogen availability during grain filling. However, despite the extensive use of crop models to support irrigation and fertilization plans, current knowledge on carbohydrate remobilization is rarely formalized in the available simulation tools. This paper presents a model to simulate carbohydrate remobilization in rice, based on the balance between source (i.e., the carbon reserves in stems) and sink (i.e., the grains) strength and on the impact of water stress and nitrogen luxury consumption. The new approach was included in the WARM model and evaluated using data from published experiments where two cultivars were grown under two nitrogen fertilization levels and two irrigation strategies. Results highlighted the model effectiveness in reproducing the amount of remobilization under non stressed conditions ($R^2 = 0.99$), as well as the impact of water and nitrogen availability (average $R^2 = 0.97$) for Indica and Japonica rice cultivars. The proposed model can be easily plugged into available rice simulators to increase their adherence to the underlying system.

Keywords: Grain filling; non-structural carbohydrates; remobilization; source-sink relationship; WARM.

3.2. Introduction

Carbon (C) supply in cereal kernels at maturity depends both on the photosynthates produced during grain filling and on the remobilization of assimilates from vegetative tissues (Schnyder, 1993). For rice, the contribution of the reserves remobilized from stems can reach up to 40% of final yield (Yoshida, 1972), depending on the interaction between the genotype and the environmental and management conditions. These reserves are mostly represented by non-structural carbohydrates (NSC) in the parenchyma cells of culms, and are constituted by starch and soluble sugars synthetized during the vegetative phase (Slewinski, 2012). The amount of NSC can reach up to 4 t ha^{-1} in rice culms at heading (Fu et al., 2011), and a significant portion remains in straw at maturity (Park et al., 2011). Enhancing the efficiency of remobilization could therefore lead to an increase in final yield (Yang and Zhang, 2010a), and this encouraged many authors to investigate the dynamics between source and sink strength (e.g., Yang et al., 2001a, Yang et al., 2003) and the impact of alternate management practices (e.g., Yang and Zhang, 2010a; Pan et al., 2011). Most of available studies agree on considering all these factors as strongly interconnected: low activity of the key enzymes involved in C metabolism (Yang and Zhang, 2010b) and reduced sink size (Fu et al., 2011) may explain the reduced NSC remobilization and the poor filling of inferior spikelets, especially in modern rice cultivars. Other studies underlined how the NSC remobilization from stems – associated with α-amylase activity (Yang et al., 2001a) – is triggered by senescence (Gan and Amasino, 1997; Noodén et al., 1997). As a consequence, factors delaying senescence, like excessive nitrogen (N) fertilization or the adoption of “stay green” cultivars, can decrease the contribution of NSC remobilization to crop production (Yang et al., 2001b). Under these conditions, Yang and Zhang (2010a) demonstrated that a controlled water stress during grain filling can favor NSC remobilization and, in turn, increase water and N use efficiency, harvest index and even yield.

The formalization of the available knowledge on such processes in simulation models would contribute to the interpretation of experimental data (Pan et al., 2007), to enhance models’ ability to predict crop performance at field level, and to better support crop management. Remobilization of C reserves during grain filling was addressed by crop models specific for different crops, such as wheat (Asseng and Herwaarden, 2003), tomato (Wilson et al., 1986) and rice. For the latter, Wu and Wilson (1998) proposed an approach based on the balance between C demand and supply, with NSC remobilization exploited to meet the possible difference between these components, whereas Oryza2000 (Bouman et al., 2001) calculates the remobilization of stem reserves from flowering as the ratio between the simulated weight of stems and a time coefficient. More detailed approaches are currently implemented within functional structural plant models, which aim to explain the relationships between source-sink balances and the impact of environmental constraints on plant C use, morphogenesis and production (Pallas et al., 2013). However, most of available models – including rice specific ones – do not consider the processes involved in NSC remobilization. Nevertheless, most rice models dynamically simulate photosynthates partitioning and the effects of water and N availability on crop growth and development (Li et al., 2015). This means that they provide suitable simulation environments where algorithms specific for C remobilization can be plugged in. The accurate simulation of NSC remobilization would increase the adherence of rice models to real systems and this, in turn, would enhance their suitability as supporting tools for water and N management at field/farm level and for in silico analyses to evaluate management scenarios under different agro-climatic conditions.

We present here a new model simulating NSC remobilization during grain filling of rice, able to respond to water and nitrogen availability and coherent with the level of detail used in rice models to reproduce processes involved with growth and development.

3.3. Materials and methods

3.3.1. A novel model for NSC remobilization in rice

The model for NSC remobilization is based on the balance between sink and source strengths (g NSC m^{-2} d^{-1}), defined as the product of *size* and *activity* of sink and source organs (Venkateswarlu and Visperas, 1987; Ho, 1988). Size represents (i) the physical restraint to remobilization for sink organs ($Sink_{size(d)}$, g grains m^{-2}; a proxy of the number of cells and cell size of the endosperm; Eq. 1) and (ii) the amount of NSC in source organs ($Source_{size(d)}$, mainly in stems for rice; g NSC m^{-2}; Eq. 1). Activities represent the physiological constraint limiting the import/export of C from a source to a sink organ. Source activity ($Source_{activity(d)}$, g g^{-1} NSC d^{-1}; Eq. 1) is here defined as the relative amount of NSC available for translocation in a given time step, whereas sink activity ($Sink_{activity(d)}$, g NSC g^{-1} grains d^{-1}; Eq. 1) refers to the relative demand of NSC per unit of grain dry matter.

During the reproductive phase, the daily rate of carbohydrate remobilization from stems ($NSC_{rate(d)}$, g m^{-2} d^{-1}) is obtained as the minimum, i.e., the most limiting factor, between source and sink strengths (Eq. 1). The transport path between source and sink is not accounted for in the model as phloem does not limit translocatory flux (Marcelis, 1996).

$$NSC_{rate(d)} = \min\left(\left(Source_{size(d)} \cdot Source_{activity(d)}\right), \left(Sink_{size(d)} \cdot Sink_{activity(d)}\right)\right) \qquad (1)$$

$NSC_{rate(d)}$ is used to reduce the total amount of NSC in culms(i.e, the source size) from anthesis (Eq.2).

$$Source_{size(d)} = Source_{size(d-1)} - NSC_{rate(d)} \qquad (2)$$

Respiration losses during remobilization and translocation influence the efficiency of the process, which falls in the range from 65 to 80% (Cock and Yoshida, 1972). This term (i.e., η, Eq. 3) should be accounted for in the estimation of the amount of remobilized NSC effectively used for grain filling (i.e., $NSC_{grainfill(d)}$, Eq. 3).

$$NSC_{grainfill(d)} = NSC_{rate(d)} \cdot \eta \qquad (3)$$

$Source_{activity}$ at day d ($Source_{activity(d)}$, Eq. 4) is a function of the main factors modulating NSC remobilization from stem storage parenchyma (Eq. 4), i.e., the genetic component associated to the "stay-green" trait (α, unitless, 0 – 1), and the effects of water (W_{effect}, unitless) and N (N_{effect}, unitless) availability on the enzyme activity. The gradual effect of plant senescence on $Source_{activity}$ is reproduced via the S-shape of the function (Eq. 4).

$$Source_{activity(d)} = Source_{activity(d-1)} + \alpha \cdot \left(1 + W_{effect} + N_{effect}\right) \cdot Source_{activity(d-1)} \cdot \left(\frac{Source_{activity(\max)} - Source_{activity(d-1)}}{Source_{activity(\max)}}\right) \qquad (4)$$

$Source_{activity(d)}$ is initialized at 0.001 g g^{-1} NSC d^{-1} at flowering; a maximum value of 1 g g^{-1} NSC d^{-1} is set ($Source_{activity(max)}$). The term W_{effect} is calculated according to Eq. 5:

$$W_{effect} = \beta \cdot \psi_{soil} \qquad (5)$$

where β (MPa^{-1}, -30 – 0) is an empirical parameter representing the cultivar sensitivity to water stress, and ψ_{soil} (MPa) is the soil water potential. This term can be derived as a function of the actual to potential transpiration ratio, commonly used by crop models to compute the daily water stress factor. Consistently with available data, in this study the soil water potential was adopted; the conversion between ψsoil and the relative transpiration can be performed according to the approach proposed by Wopereis et al. (1996).

The daily value of N_{effect} is computed according to Eq. 6:

$$N_{effect} = \gamma \cdot \left(N_{status} - 1 \right) \quad (6)$$

where γ (unitless, -5 – 0) is an empirical parameter used to discriminate between the susceptibility of different cultivars to non-optimal (insufficient availability or luxury consumption) N availability, and N_{status} (unitless) is the ratio between actual and critical N concentration in shoots. With critical N concentration, we mean here the concentration below which the plant is stressed and above which the plant experiences luxury consumption (Sheehy et al., 1998). Thus, a value of N_{status} higher than 1 indicates N luxury consumption, whereas values below 1 convey the degree of N stress sensed by the crop. According to our approach, high values of W_{effect} and N_{effect} cause a steep increase of source activity: in other words, negative values of β and γ parameters favor NSC remobilization under insufficient water and N availability and reduce it under N luxury consumption.

Sink size is mainly determined by the number of cells and the cell size in the endosperm (Fu et al., 2011). The cumulated grain weight (g m^{-2}) is used here as a proxy for sink size, given that it is dynamically simulated by most rice crop models.

The value of $Sink_{activity}$ at day d ($Sink_{activity(d)}$, g NSC g^{-1} grains d^{-1} Eq. 7) is dependent upon the metabolism of carbohydrates in developing the rice endosperm. This process is regulated by 33 major enzymes (Nakamura et al., 1989), with sucrose synthase and adenine diphosphoglucose pyrophosphorylase playing key roles. The pattern of their activities observed during grain filling (Yang et al., 2003; Fu et al., 2011) highlights an exponential decay after early development of rice endosperm, leading to the following expression (Eq. 7):

$$Sink_{activity(d)} = Sink_{activity(\max)} \cdot \exp\left(-DPA \cdot \varepsilon \right) \quad (7)$$

where $Sink_{activity(max)}$ (g NSC g^{-1} grains d^{-1}) is set to 1 and ε (unitless, 0 – 0.3) is a cultivar-specific parameter; high values of ε reflect low activities and/or gene expressions of enzymes involved in the conversion of sucrose to starch, which have been observed especially in inferior spikelets of modern rice cultivars (Yang et al., 2010b), such as “super” hybrid rice (Cheng et al., 2007) and New Plant Type (Peng et al., 1999). The tendency to overestimate the sink activity at low *DPA* can be considered negligible because – according to the model proposed – NSC remobilization in the early grain filling phase is mostly limited by source activity and sink size.

Fig. 1 shows the functions used to reproduce size and activity of source and sink organs; the parameterization is the one obtained in this study for Japonica cultivar after model calibration.

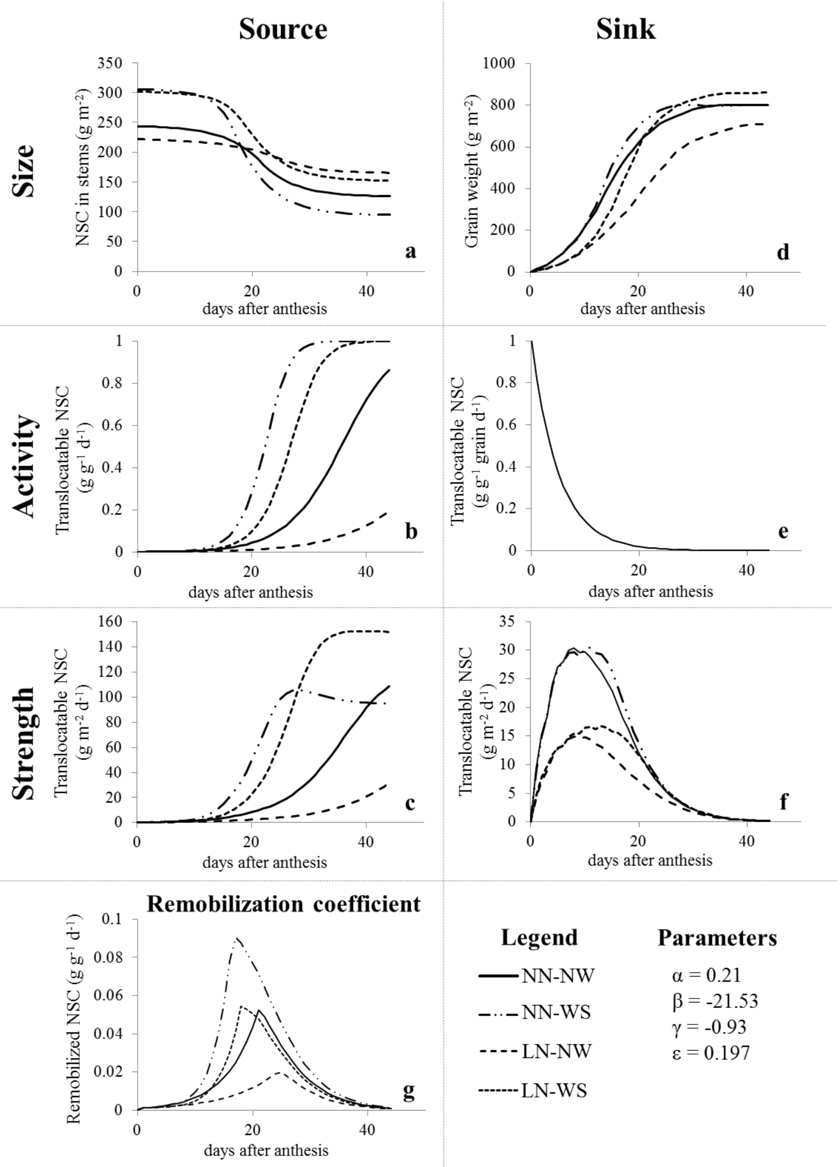


Figure 1. Functions used to describe remobilization during rice grain filling. a: source size; b: source activity; c: source strength; d: sink size; e: sink activity; f: sink strength; g: remobilization coefficient (i.e., the ratio between daily remobilization and source size). NN: normal amount of nitrogen (N_{status}=1); LN: luxury nitrogen (N_{status}=1.4); NW: normal irrigation (ψ_{soil}=0); WS: controlled water stress (ψ_{soil}=-0.05). a, b, c, f and g refer to the parameters used for Japonica rice (see legend). Dynamics of grain filling in d (moisture content = 0%) are interpolated from data points and information provided by Yang et al. (2001b) and Yang et al. (2001c). Solid line in e refers to all the treatments.

3.3.2. Model calibration and verification

Data used for model calibration and verification comes from the work of Yang et al. (2001b), who measured the dynamics of NSC in stems (culms + sheats) during the reproductive phase of rice. Eight treatments were arranged in a randomized block design with three factors (cultivar, N fertilization, soil moisture) and two levels for each factor: cultivar Wuyujing 3 (Japonica) and Yangdao 4 (Indica), normal N (NN) and luxury N (LN), fully irrigated (NW) and water stressed (WS). N was incorporated in soil as urea before transplanting (60 kg ha^{-1}), and applied at mid-tillering (40 kg ha^{-1}) and panicle initiation (25 kg ha^{-1}). NN and LN treatments were top-dressed at initial heading with 50 and 100 kg N ha^{-1}, respectively. Water stress in WS treatments was applied nine days after anthesis. Each treatment i.e., cultivar × nitrogen level × soil moisture level is characterized by 11 measured data points (15-20 plants were sampled every 4 days from anthesis to maturity for the measurement of NSC). Details about experimental approach, plant material and rice growth conditions are provided by Yang et al. (2001b).

The datasets were employed for a stepwise calibration of model parameters as follows: for each cultivar, three experimental datasets were used for model calibration and one for model verification. The treatment with normal application of nitrogen and water (NN-NW) was used for the calibration of the cultivar-specific parameters α (Eq. 4) and ε (Eq. 7), driving the functions to simulate the source and sink activities. The water stressed treatment (NN-WS) was used to calibrate the parameter β (Eq. 5), which modulates the effect of water availability on source activity; similarly, luxury N treatment (LN-NW) was used to calibrate the parameter γ (Eq.6), representing the cultivar attitude to decrease NSC remobilization under high nitrogen contents. The treatment with water stress and luxury nitrogen (LN-WS) was instead used as an independent data set for model verification, to assess the model ability in reproducing NSC remobilization dynamics as influenced by both factors simultaneously. The values of N_{status} (Eq. 6, i.e., 1 and 1.4 in the treatments with normal and luxury nitrogen, respectively), ψ_{soil} (Eq. 5, i.e., 0 and -0.05 MPa in the fully irrigated and water stressed treatments, respectively) and the NSC contents (i.e., source size) at flowering to initialize the model were derived from Yang et al. (2001b).

Model performances were evaluated using the following evaluation metrics (Loague and Green, 1991), both for calibration and verification: mean absolute error (MAE, g m-2, 0 to +∞, best 0), modelling efficiency (EF, unitless, -∞ to 1, best 1), coefficient of residual mass (CRM, unitless, -∞ to +∞, best 0; if negative, it indicates model overestimation, and vice versa), coefficient of determination of the linear regression equation between simulated and observed data (R^2) and the two-tailed t test for significance.

3.4. Results and Discussion

Fig. 2 shows the agreement between measured and simulated stem NSC content during ripening for Indica and Japonica cultivars. The overall satisfactory model performances are confirmed by the values of the evaluation metrics, always close to their optimum (Table 1). The mean absolute error ranged from 2.38 g m^{-2} (Indica, LN-NW) to 12.89 g m^{-2} (Japonica, LN-WS), and coefficient of residual mass does not indicate any tendency of the model to systematically over- or underestimate stem NSC content across treatments. Among the calibration datasets, the worst performances were achieved for the NN-WS treatment, regardless of the cultivar used, suggesting that further model improvements should focus on the impact of water availability on remobilization of NSC reserves. Water stress is known to modulate sink activity (Yang et al., 2003); however, this effect was not included in the model given its higher impact in modulating source activity via the stimulation of α-amylases metabolism in stems (Yang et al., 2001a).

Fig. 2.c refers to data sets used to calibrate parameter γ and shows the ability of the model in properly simulating the effect of the LN treatment on the reduction of remobilization rates, with the ratio NSC at maturity to NSC at flowering equal to 0.75 and 0.6 for Japonica and Indica cultivars, respectively. Even if low nitrogen supply is known to increase translocation of NSC to developing grains (Pan et al., 2011), no adequate data were found to test the model under such conditions. On the contrary, Fig. 2.b (i.e., data sets used to calibrate *β* parameter) highlights the model ability in reproducing the high NSC remobilization rates due to water stress, with the ratio NSC at maturity to NSC at flowering being 0.26 and 0.17 for Japonica and Indica cultivar, respectively. The accuracy of the new model in modulating the remobilization of NSC in stems as a function of both water

stress and excess of nitrogen is confirmed by its application on independent verification data sets (Fig. 2.d), especially for Indica cultivar. The values of NSC at anthesis markedly differed in most cultivar × treatment combinations, suggesting that the accumulation of NSC in stems during the vegetative phase is not constant.

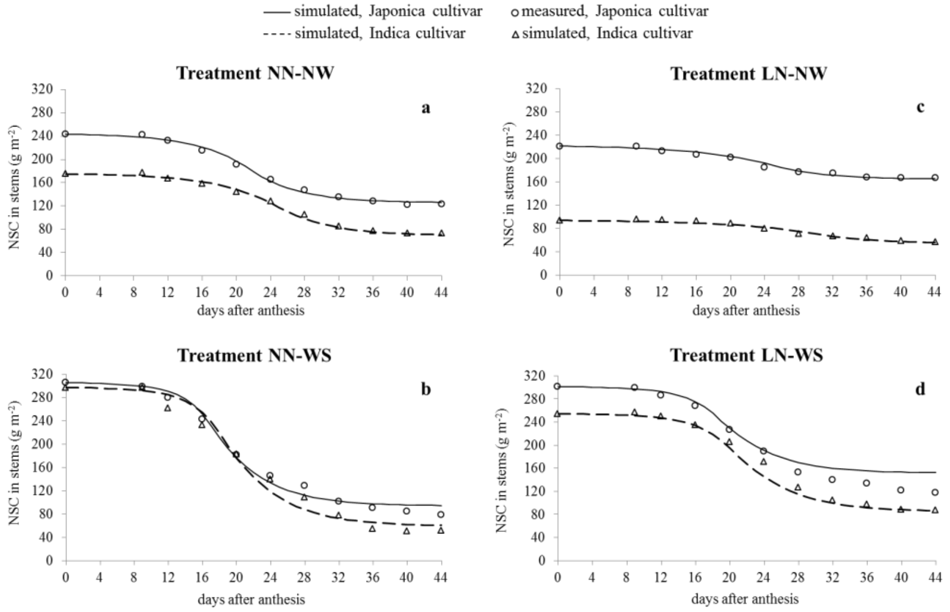


Figure 2. Measured and simulated non-structural carbohydrate content in rice stems during grain filling. Circles and solid lines refer to Japonica cultivar, triangles and dashed lines to Indica cultivar. NN: normal amount of nitrogen (N_{status}=1); LN: luxury nitrogen (N_{status}=1.4); NW: normal irrigation (ψ_{soil}=0); WS: controlled water stress (ψ_{soil}=-0.05). After calibration, parameter values for Japonica cultivar were: α = 0.21, β = -21.53, γ = -0.93, ε = 0.197; for Indica cultivar: α = 0.19, β = -23.15, γ = -0.93, ε = 0.186.

The Akaike Information Criterion (AIC, unitless, 0 to +∞, best 0; Akaike, 1974) was applied to justify the addition of response functions for water and N availability to the base model in terms of model complexity. Four versions of the model were derived by activating/deactivating the algorithms for the effects of water and N on $Source_{activity(d)}$ (Eq. 4). Version A had no effect of water and N, and was characterized by two parameters (α and ε); version B had only the effect of water (3 parameters: β added to parameters of version A); version C had only the effect of nitrogen (3 parameters: γ added to parameters of version A); version D had both water and N effects (4 parameters, complete model). Fig. 3 shows the AIC values computed for the four model versions and the four combinations of water and nitrogen treatments, highlighting that the best performance of the complete model in LN-WS treatment, and similar values in the others. The apparent good trade-off between complexity and accuracy for the version A of the model in LN-WS treatment – proved by a low value of AIC – is due to the counterbalancing effects of water stress and luxury N. Further, the complete model led to the smallest variability of AIC among treatments, thus justifying the inclusion of the effects of both factors in driving NSC remobilization. This suggests the application of the complete model for field scale studies, where environmental conditions and management practices can deeply influence water and nitrogen availability.

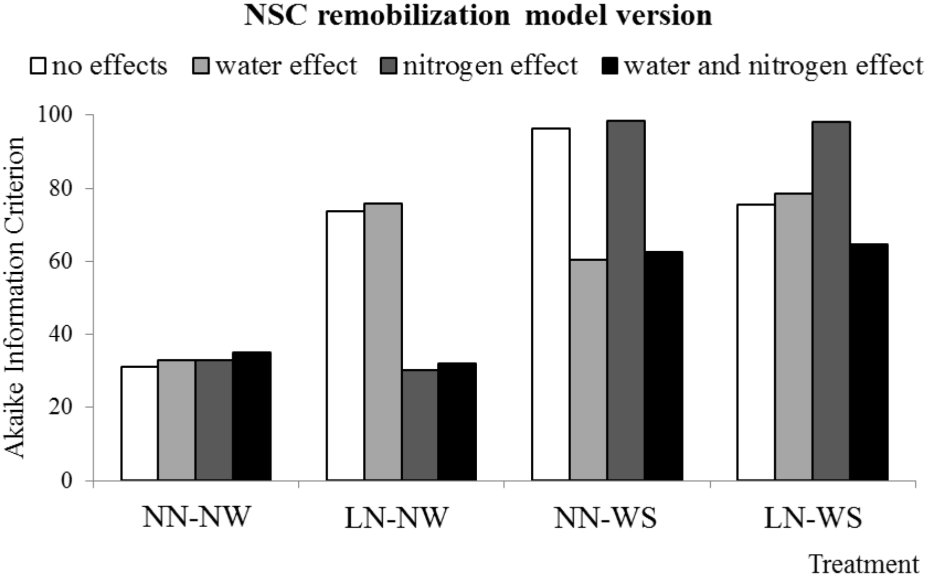


Figure 3. Values of the Akaike Information Criterion (AIC = n · log(MSE)+2 · T; n = number of couples measured-simulated data; MSE = mean square error; T = number of parameters) obtained for different model versions and datasets. The versions differ for the presence/absence of water stress and/or nitrogen effect. Plotted results are the average AIC achieved for Indica and Japonica cultivars.

Table 1. Indices of agreement between measured and simulated non-structural carbohydrate contents in stems: mean absolute error (MAE, g m^{-2}, 0 to +∞, best 0), modelling efficiency (EF, unitless, -∞ to 1, best 1), coefficient of residual mass (CRM, unitless, -∞ to +∞, best 0), correlation coefficient (R^2) and p-value (two-tailed t test).

Cultivar type	Nitrogen level	Water level	Calibrated parameters	Evaluation metrics				
				MAE	EF	CRM	R^2	p-value
Japonica	normal	normal	α, ε	3.000	0.994	-0.003	0.994	0.980
	luxury	normal	γ	2.584	0.976	-0.003	0.980	0.952
	normal	stress	β	8.013	0.987	-0.009	0.987	0.966
	luxury	stress	verification	12.885	0.940	-0.062	0.990	0.678
		Average values		6.621	0.974	-0.019	0.988	0.894
Indica	normal	normal	α, ε	2.484	0.994	0.004	0.995	0.980
	luxury	normal	γ	2.378	0.964	0.014	0.971	0.863
	normal	stress	β	12.181	0.976	-0.008	0.978	0.977
	luxury	stress	verification	6.509	0.979	0.038	0.989	0.834
		Average values		5.888	0.978	0.012	0.983	0.913

3.5. Concluding remarks

The remobilization of carbon reserves from stems to storage organs plays a key role in determining final rice yield. Often ignoring or providing an oversimplified description of such process within simulation models potentially undermines their reliability under a variety of conditions, given that remobilization is non-linearly regulated by irrigation and fertilization rates. However, knowledge on this topic is much more advanced compared with available formalizations in several crop models. The modelling approach proposed here gives an interpretation of the contribution of carbohydrate redistribution during rice grain filling based on a reanalysis of published information. The model was designed targeting a degree of adherence to physiological processes coherent with the current state-of-the-art of crop models. The result is a set of equations driven by few parameters reflecting crop physiological traits, whose calibration allowed to give reliable estimates of NSC remobilization in Indica and Japonica cultivars. The new model is currently included in the WARM model (Confalonieri et al., 2009), but can be easily integrated in other rice simulators based on the concept of net photosynthesis or simulating the gross assimilation of CO_2 and respiration losses. The explicit description of NSC in different plant organs would allow to refine the simulation of their mutual source–sink relationships. Currently our remobilization model does not account for such complex interactions, and considers NSC in stems as a source pool exploited during grain filling. Further, our model would benefit from a finer integration of senescence and remobilization processes and from a process-based description of the influence of soil water and plant nitrogen availability.

A FRAMEWORK-INDEPENDENT SOFTWARE LIBRARY FOR SIMULATING CARBON AND NITROGEN DYNAMICS IN AGRICULTURAL SOILS: COMPOSITION AND SENSITIVITY ANALYSIS OF IMPLEMENTED MODELS

Tommaso Stella, Nicolò Frasso, Simone Bregaglio, Roberto Confalonieri

4.1. Abstract

We present a new software component (UNIMI.CRONO), which collects modelling approaches to simulate carbon and nitrogen dynamics in agricultural soils. The software library implements models for soil organic matter decomposition, biological mediated reactions in aerobic and anaerobic conditions, transport of molecules in the gaseous and liquid phases, soil-plant interactions at root level and responses to agricultural management practices. UNIMI.CRONO allows users to compose models according to specific applications and research questions. As a case study, a modelling solution is presented, which implements processes for modulating plant nitrogen availability and greenhouse gas emissions in a rice paddy. The behavior of the modelling solution was analyzed using Morris sensitivity analysis method, with factors represented by model parameters. Outputs considered were the simulated dynamics of CO_2, CH_4 and N_2O emissions. Results highlighted the tight relationships between carbon and nitrogen cycles, plant growth and development, and management practices. The software architecture allows easily extending the UNIMI.CRONO library with alternate modelling approaches, and its use within integrated simulation environments targeting a variety of cropping systems and different research and operational contexts.

Keywords: Greenhouse gases, model composition, Morris method, paddy rice soil, sensitivity analysis

Software availability: UNIMI.CRONO is distributed free of charge for noncommercial purposes as .NET 4.5 library. The Software Development Kit is supplied on request (cassandra.lab@unimi.it) to interested users and includes hypertext files documenting algorithms and code, as well as source codes of sample applications.

4.2. Introduction

Agriculture involves about 12% of global land surface and is responsible for ecosystem processes such as carbon (C), nitrogen (N) and nutrients cycling (McLauchan, 2006). A key role in modulating these cycles is played by agricultural soils, in turn affected by land use and farmer management practices (Ogle et al., 2005). In the last decades, several models were developed to understand processes determining C and N turnover in soil, in order to shed light on the complex interactions involved with soil organic matter (SOM) dynamics (e.g., Parton et al., 1994, Coleman and Jenkinson, 1996), the emission of biogenic greenhouse gas (GHG; e.g., Li, 2000, Xu et al., 2007) and crop N nutrition (e.g., Bergström et al., 1991; Rijtema and Kroes, 1991). Available models are the result of a multi-domain research, often leading to an imbalance in the level of detail biochemical reactions and transport are reproduced, potentially undermining models' ability in reliably predicting the emission of GHGs (CO_2, N_2O and CH_4) from soils (Blagodatsky and Smith, 2012). Relationships among the processes leading to GHG emissions (e.g., microbial community dynamics, production and consumption of GHGs in soil, transport and exchange of compounds between gaseous and liquid phases) are very tight. For this reason, the only viable solution to manage the complexity involved in soil physics and biology is the adoption of a modular system, allowing to discretize the models implementation and to successively couple domain specific models. In agricultural science, this approach represents the state-of-the-art of modelling studies (e.g., APSIM, Holzworth et al., 2014; BioMA, 2014), and led to the development of extensible and reusable software units, which can be easily maintained and further extended with alternate approaches for the simulation of specific processes (Bregaglio and Donatelli, 2015). The fine-granularity of model implementation also facilitates the composition of multiple modelling solutions, which can be evaluated in parallel in different pedo-climatic and management contexts (Donatelli et al., 2014). Moreover, component-oriented programming increases the capability of interfacing models with external tools, such as those performing sensitivity analysis, a technique commonly used to support model development (Jakeman et al., 2006) and to investigate model sensitivity to input and parameters (Bennet et al., 2013).

This paper presents a new software component (i.e., UNIMI.CRONO), which is a library of models describing the main processes involved with agricultural soils i.e., SOM dynamics, the biological processes influencing N availability to plants and GHGs production and consumption, the mobility of chemical compounds and interactions among crop, soil, and the impacts of management practices. UNIMI.CRONO is explicitly designed for being extended by first and third parties with the addition of alternate modelling approaches. The fine-granularity of model implementation favors their composition and evaluation. The library can be coupled to external components simulating other aspects of the cropping system (e.g., crop growth and development, management practices, soil water dynamics) in order to develop modelling solutions suitable for the simulation of the cropping system as a whole. This study aimed at presenting the UNIMI.CRONO library and at demonstrating its potential via the development of a complex modelling solution for paddy rice, used here to investigate the sensitivity of the models implemented in UNIMI.CRONO to inputs and parameters using the Morris method (Morris, 1991) and focusing on GHGs emissions.

4.3. Materials and Methods

4.3.1. CRONO: A model library of soil CN dynamics in agricultural soils

4.3.1.1 Software component architecture

The software design of UNIMI.CRONO follows the BioMA framework (BioMA, 2014), thus promoting reusability by limiting dependencies and providing semantically rich, public interfaces. The component encloses a library of algorithms implemented in discrete units (i.e., the *strategies*) to simulate processes in the soil domain. More specifically, a *simple strategy* is the atomic unit of algorithm representing a process (or sub-process) for which alternate modelling approaches can be defined. *Simple strategies* are composed into entities of increasing complexity (i.e., *composite strategies*), which are in turn subject to composition. This pattern leads to a hierarchical structure where each *composite strategy* manages the call of lower level *strategies* and the resulting modelling solution is encapsulated within a top-level *composite strategy*. This *composite strategy* (i.e., CRONO_C in this study) represents one of the possible model realization of the combination of the *strategies* in UNIMI.CRONO. *Strategy* composition is aimed at isolating processes at different levels of detail. Let us consider, for example, biological methanogenesis in soil: two different *simple strategies* calculating methane production are implemented, using either acetate or H_2 as electron donor for the redox reaction, respectively. These two *strategies* are aggregated within a single *composite strategy* addressing the estimation of methanogenesis, which represents – with other strategies (e.g., those related to denitrification) – a *composite strategy* describing anaerobic processes in soils. In this way, the soil model can be accessed and modified at different levels of granularity, starting from the finest (i.e., the *simple strategy*). This architecture facilitates both model developers and third parties to extend the component by adding new *strategies* simulating processes of interest or to reuse *simple* and/or *composite strategies* for the definition of new modelling solutions.

The implementation of the bridge pattern allowed to separate model algorithms from data-types structures (*Domain Classes*, DCs) in two independent and reusable software units (Donatelli and Rizzoli, 2008), i.e., UNIMI.CRONO and UNIMI.CRONO.Interfaces. The DCs describe the biophysical domain by including *strategies* inputs and outputs with their attributes, whereas the ontology of the parameters, being related to the specific modelling representation and not to the domain, is made available via the related *strategies*. The coherence of input, output and parameter values with their ontology can be verified via pre- and post-conditions tests, according to the design-by-contract approach (Meyer, 1997). The bridge pattern allows the deletion/substitution/addition of *strategies*, which are non-unique by definition, without changing the description of the biophysical domain. Figure 1 shows the Unified Modelling Language (UML) diagram of the UNIMI.CRONO component, highlighting the main functionalities of each software unit. *Strategies*, DCs and programming interfaces can be inspected via an external application named Model Component Explorer (http://agsys.cra-cin.it/Tools/MCE/help/). UNIMI.CRONO can be coupled to other available components for the simulation of, e.g., crop growth and development (UNIMI.CropML, http://www.cassandralab.com/components/1), soil water balance (UNIMI.SoilW, http://www.cassandralab.com/components/6) or agro-management practices (CRA.Agromanagement, http://agsys.cra-cin.it/tools/agromanagement/help/).

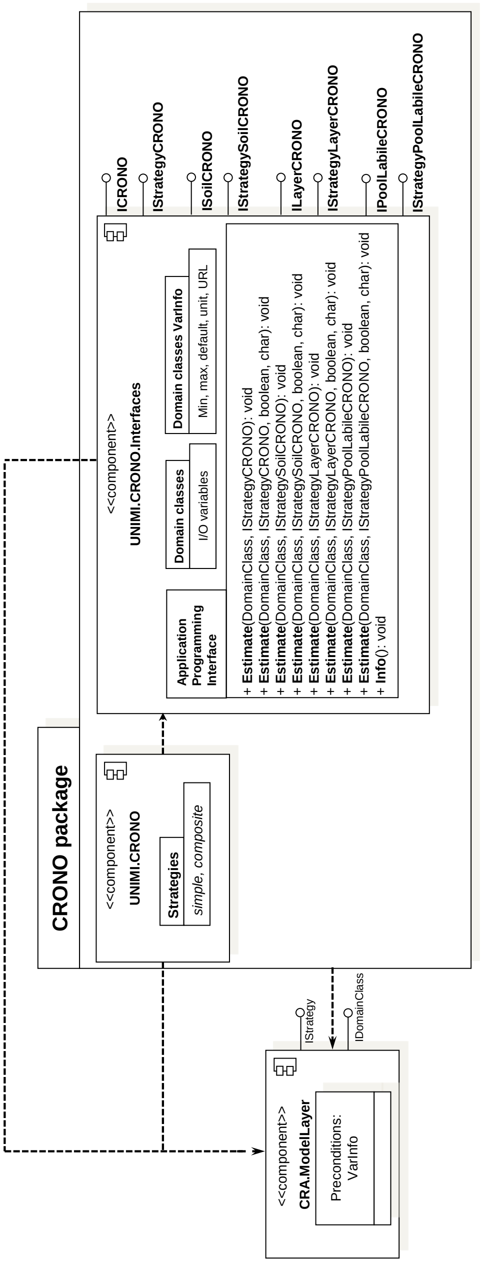


Figure 1. Unified Modelling Language diagram of the software components UNIMI.CRONO and UNIMI.CRONO.Interfaces. UNIMI.CRONO has a dependency to the UNIMI.CRONO.Interfaces component, and both the software units have a dependency (arrow dotted line) to CRA.Core.ModelLayer. The interfaces (circle and solid line) implemented by each component are reported.

4.3.1.2 Representation of soil domain: namespace UNIMI.CRONO.Interfaces

UNIMI.CRONO.Interfaces contains the DCs storing the variables which describe the simulated soil system, i.e. *States* (state variables), *Rates* (rates variables), *Auxiliary* (intermediate variables), *Exogenous* (driving variables), *ExternalStates* (states variables for domains other than soil) and *ExternalRates* (rates variables for domains other than soil). Additional layers of DCs are defined to give a proper description of the domain (Figure 2), as it actually can be further split into subdomains, i.e., flood water, soil layers, SOM pools, rhizosphere and roots. A hierarchical organization of DCs is then realized, with system DCs pointing to soil and flood water DCs, the latter being instantiated for the simulation of agricultural soils characterized by periods of submersion (e.g., in rice cropping systems). Soil DCs in turn collect a list of classes aimed at describing the properties of the soil layers. Since each soil layer is considered a homogeneous entity, an undetermined – both in number and thickness – set of layers allows to account for vertical heterogeneity along the soil profile. A soil layer is divided into compartments, i.e., the soil organic matter (SOM) pools, which are a list of DCs storing variables related to the added organic matter (e.g., litter or manure), and the rhizosphere DC, corresponding to the soil portion influenced by the activity of the root system. Finally, the rhizosphere contains DCs used to represent the roots; each DC can be extended with the addition of variables. UNIMI.CRONO.Interfaces provides programming interfaces (API) which allow models to access different set of DCs, according to the processes simulated. A model for a process which deals with the whole soil, for example, may read and write values from soil DCs (via ISoilCRONO interface), whereas more specific models may directly access layer or organic pools DCs (via ILayerCRONO and IPoolCRONO interfaces, respectively).

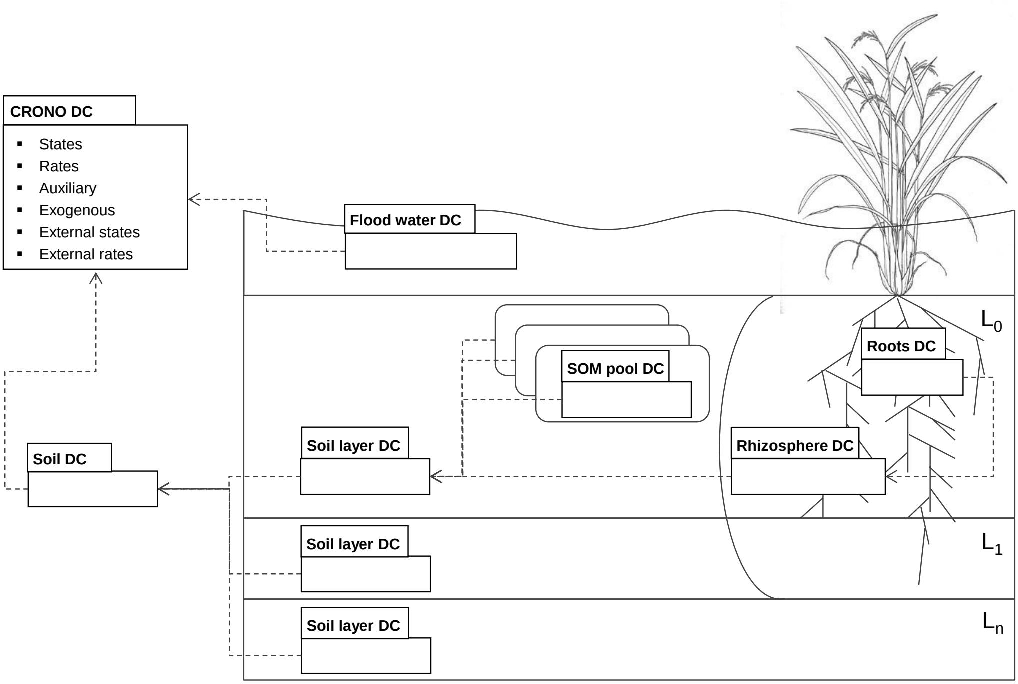


Figure 2. Comparison of domain classes (DCs) organization with a schematic representation of a rice-cropped soil (flooded). Dotted line indicate the encapsulation of classes, arrows point at outer class. The scheme shown in the uppermost soil layer (L_0) is replicated in each underlying layer.

4.3.1.3 Implemented models: namespace UNIMI.CRONO

The current release provides modelling approaches – derived from literature – for the simulation of the main soil biophysical processes and it is designed to be further extended by first and third parties with the addition of alternate models (*strategies*). Implemented approaches simulate the dynamics of SOM decomposition, the main redox reactions mediated by soil microorganisms in aerobic and anaerobic conditions, solute and gas transport in soil and interactions between crop and soil. A set of strategies in also made available for the simulation of the impacts of farmers management practices. A composite strategy, i.e., CRONO_C, links the implemented models within a soil model, which is meant to be one of the possible realization of the combinations of UNIMI.CRONO models.

SOM decomposition

The general principles driving soil organic matter decomposition link carbon and nitrogen processes, with carbon (C) transformations regulating nitrogen (N) mineralization and immobilization, according to the approaches adopted by other soil C-N models (e.g. Wu and McGechan, 1998). Organic matter is divided into different pools, namely one describing slow-cycling organic matter (often called humus in modelling studies) and an undetermined number of pools describing fast cycling organic matter such as incorporated crop residues or manure. Decomposition of such pools is described as a first-order rate process, meaning that degradation is proportional to a decomposition coefficient and the amount of material remaining in the pool. This process is then modulated by temperature (via a Q_{10} expression) and soil moisture response functions. In the first case, the higher the temperature, the faster the SOM degradation, whereas the latter assumes an optimal range of soil water content which does not limit SOM decomposition (Eq. 1).

$$C_{PoolRate} = k \cdot f\left(T\right) \cdot f\left(\vartheta\right) \cdot C_{Pool} \tag{1}$$

where $C_{PoolRate}$ stands for the amount of C in pool which is subject to transformations during the time step, k is the reference decomposition coefficient of a specific pool, $f(T)$ and $f(\vartheta)$ are temperature and soil moisture response functions, respectively and C_{Pool} quantifies the amount of C characterizing the pool.

Microbial biomass is not explicitly simulated in the model, being included in SOM pools, but it ideally controls C flows across pools (Jansson and Karlberg, 2004). During decomposition, an efficiency factor (f_e) determines the amount of C cycling in SOM pools: a fraction (f_h) of this C is converted into humus (Eq. 2), whereas the remaining carbon (i.e., $1 - f_h$ fraction) is transferred back to the SOM pool, reflecting the amount of C assimilated by microbial biomass.

$$C_{Pool->Humus} = C_{PoolRate} \cdot f_e \cdot f_h \tag{2}$$

Where $C_{Pool \rightarrow Humus}$ is the carbon flux to humus (humification process), $C_{PoolRate}$ is calculated according to Eq. 1, f_e is the microbial use efficiency and f_h is the isohumic coefficient. The fraction of $C_{PoolRate}$ which is not directed either to humus or to internal pool recycling is lost during the process as CO_2 (in aerobic conditions) or a mixture of acetate and CO_2 in absence of oxygen. These molecules, together with H_2, represent final products deriving from SOM mineralization and decomposition of complex organic substances during anaerobic processes (van Bodegom and Scholten, 2001).

Dynamics of the slow cycling humus pool are described by the same set of equations, but since this pool is considered as the final destination for organic matter, humus C can be only recycled within the pool or lost as CO_2 or Acetate/CO_2.

Nitrogen flows associated with carbon fluxes depend on the considered pool. Humus decomposition always causes a net N mineralization (i.e., ammonification): according to the C lost by this pool and its C/N ratio, a proportional amount of N is released in soil as ammonium. Carbon flow from SOM pools to humus, microbial use efficiency and the relative values of C/N ratio regulate N mineralization or immobilization associated with SOM cycling in each pool (Eq. 3):

$$N_{PoolRate} = C_{PoolRate} \cdot \left(\frac{1}{CN_{Pool}} - \frac{f_e}{CN_{Humus}} \right) \tag{3}$$

Where $N_{PoolRate}$ represents the N flow (positive and negative values reflect N mineralization and immobilization, respectively), $C_{PoolRate}$ is calculated according to Eq.1, f_e is the microbial use efficiency, CN_{Pool} and CN_{Humus} are the CN ratios of the considered SOM pool and humus.

Redox reactions in soil

UNIMI.CRONO provides *strategies* accounting for alternative electron acceptors that may be involved in soil microbial processes, namely O_2, NO_3^-, Mn(IV), Fe(III) and SO_4^{2-}. This allows to compose models suitable for the simulation of a range of soils spanning from well drained ones to those characterized by alternation of submersion periods. If soil (or a soil compartment) is adequately aerated, the reactions are dominated by oxidations with oxygen as the terminal electron acceptor. In this condition, SOM degradation leads to CO_2 production, ammonium is nitrified and the reduced forms Mn(II), Fe(II) and HS^- are oxidized. Nitrification and oxidation of reduced species is simulated according to the models proposed by Xu et al. (2007), i.e., dual-monod (Eq. 4) and second-order kinetics respectively.

$$V = V_{\max} \cdot \frac{\left[e^-{}_{donor}\right]}{K_{Md} + \left[e^-{}_{donor}\right]} \cdot \frac{\left[e^-{}_{acceptor}\right]}{K_{Ma} + \left[e^-{}_{acceptor}\right]} \tag{4}$$

V (mol m^{-3} water s^{-1}) is the substrate conversion rate, V_{max} (mol m^{-3} water s^{-1}) the potential conversion rate of electron acceptor, $[e^-{}_{donor}]$ and $[e^-{}_{acceptor}]$ the concentration of electron donor and acceptor (mol m^{-3} water), respectively and K_{Md} and K_{Ma} affinity constants (mol m^{-3} water) for electron donor and acceptor. During nitrification, a fraction of ammonium is not completely oxidized to nitrate and N_2O and NO are produced. Such fraction is corrected for temperature and soil moisture response functions to estimate N_2O release; a pH response function is added for NO release (Jansson and Karlberg, 2004).

In absence of O_2, SOM decomposition involves acetate and H_2 production, which serve as electron donor for the reduction of alternative electron acceptors (van Bodegom and Scholten, 2001). Substrate conversion rates are calculated with Eq. 4; in order to simulate the competition among different micro-organisms for common substrates, electron acceptors are sequentially depleted and threshold concentrations define cutoff values below which the next most energetically favorable electron accepting process is allowed to proceed. The order of utilization of electron acceptor is O_2, NO_3^-, Mn(IV), Fe(III) and SO_4^{2-} (Xu et al., 2007). The path of NO_3^- reduction (i.e., denitrification) implies the sequential formation of NO_2, NO, N_2O and N_2. When SO_4^{2-} concentration is below a certain threshold, acetate and H_2 are depleted by methanogenesis, described by a monod equation. This process is partially or completely inhibited by NO, N_2O and HS^-, depending on their concentrations; the latter compound also inhibits denitrification (van Bodegom and Scholten, 2001).

Mobility of chemical compounds

UNIMI.CRONO includes models for the simulation of transport of molecules in liquid and gaseous phase. The liquid transport is driven by diffusion and mass flow according to water infiltration, and the gaseous transport by diffusion. In case of soil water saturation, dissolved gas can move by ebullition. Models to simulate plant-mediated transport are included in UNIMI.CRONO to assure compatibility with the simulation of diffusive gas transport in flooded rice systems. Diffusive transport is modelled via the Fick's law; diffusion coefficients in soil are corrected for temperature, soil porosity, water saturation and clay fraction (Schjønning et al., 2003). Plant-mediated diffusion through stems and root aerenchyma, which is a significant pathway for gas transport in rice cropping systems, is simulated according to van Bodegom et al. (2001a), who divided the soil-plant-atmosphere continuum in compartments characterized by different transport parameters. Partitioning of gas between liquid and gas phase is calculated according to Henry's law (Wilhelm et al., 1977). A pressure-based algorithm (Tang et al., 2010) is implemented to simulate ebullition, which is triggered when the pressure of water-dissolved gases exceeds the hydrostatic pressure imposed by soil water, flooding water and atmospheric pressure. Compounds in the liquid phase are transported by water percolation; an adsorption isotherm is used to estimate the relative amount of ammonium adsorbed to soil particles and dissolved in solution circulating in the soil (Vogeler et al., 2011).

Soil-plant interactions

A set of *strategies* simulates belowground plant related processes, i.e., development and growth of root system, exudation of organic compounds and N uptake. The growth of the root system is defined as rooting depth extension, increase of root biomass and variation of root length density in each soil layer. Root depth and root biomass are considered as external variables (*ExternalStates* DC), whereas routines for the dynamic simulation of root length density (Ritchie, 1988) convert biomass increments partitioned to roots into root length increase. Root decay is accounted for reducing root length density by a parameter, corresponding to the percentage of decrease in the time step; dead roots constitute a SOM pool. Root length density is a driving variable for the estimation of the extent of rhizosphere and the calculation of root exudation, the latter performed according to Personeni et al. (2007) and assumed to release acetate in the rhizosphere (van Bodegom et al., 2001b). Root length density is then used as input to calculate N uptake, which is dependent on the mass flow caused by transpiration stream and N diffusion to the root surface (Abrahamsen and Hansen, 2000).

Response to agricultural management events

UNIMI.CRONO implements *strategies* able to react to farmer management practices to simulate their effects on agricultural soils. Management events are triggered by an external component (i.e., CRA.Agromanagement; Donatelli et al., 2006), quantifying the impact of the agro-management event via a set of parameters. Currently, UNIMI.CRONO provides models to handle fertilization events, the effect of harvest on root activity and tillage. The latter causes the mixing of rhizosphere with bulk soil and a redistribution of SOM along the soil profile.

4.3.2. Testing models for greenhouse gases emission from paddy rice

4.3.2.1 Simulation environment

A modelling solution was set up to investigate the behavior of the models implemented in UNIMI.CRONO when dynamic inputs are used and to evaluate the interactions between soil C-N models and other domains of the system. This modelling solution is composed by models implemented in independent software components and allows to simulate responses to alternate farmer management strategies, the impact of irrigation and fertilizations events on soil carbon and nitrogen dynamics and the mutual interactions between crop growth and soil processes. Models included in the modelling solution are implemented in the following components according to the domain (in brackets) they belong to:

- UNIMI.CropML (crop; Confalonieri et al., 2012) collects algorithms for the simulation of crop growth and development. The library is extended by UNIMI.CropML_WL and UNIMI.CropML_NL components, respectively adding approaches for the simulation of water and nitrogen uptake and related stresses.
- CRA.Agromanagement (farmer management; Donatelli et al., 2006) triggers events – e.g., sowing, harvest fertilization and irrigation – via a set of rules based on the state of the system, constraints of resources availability and physical characteristics of the system.
- CRA.CLIMA (meteorology; Carlini et al., 2006) provides the modelling solution with models for the estimation of reference evapotranspiration, hourly air temperature and solar radiation.
- UNIMI.CRONO (Soil C and N) simulates C and N transformations in soil, gas and solutes transport across soil layers and at the interface between simulated system and atmosphere.
- UNIMI.SoilW (soil water; Acutis et al., 2007) calculates water infiltration and redistribution among soil layers and crop water uptake.
- UNIMI.SoilT (soil temperature; Donatelli et al., 2014) estimates surface and soil temperature at different soil depths.

The modelling solution is implemented as a Microsoft C# class library project managing the interactions between the I/O data produced by the models of biophysical processes belonging to the different software components. Dedicated classes create the instances of the I/O structures implemented in each component as domain classes (i.e., *DataTypes* classes) and call the models implemented in the components in dynamic simulation runs (*Adapters* classes). The input data from different sources (e.g., meteorological data, pedological information) and the scheduling of the management practices is managed via data structures isolated in dedicated file classes. The logic to perform dynamic simulation is managed via the

Adapters classes; methods of these classes are called by the RunnerAPI class, which represents the entry point of the modelling solution. This project has a dependency on the CRA.ModelFramework.ModelRunner component, which is an application allowing to handle the links between I/O data of the different components and to save simulation outputs.

4.3.2.2 Sensitivity analysis

Sensitivity analysis experiments were carried out to investigate the response of UNIMI.CRONO models – namely those called by CRONO_C *composite strategy* – to the variation of input variables and parameters. The modelling solution described in Section 4.3.2.1 was used to simulate dynamics occurring in a paddy rice environment. The unique water management of this cropping system allowed aerobic and anaerobic conditions to occur and to explore the different emission dynamics of the gases produced in soil. Moreover, the adoption of an integrated, dynamic simulation environment allowed to expose the soil to boundary conditions consistent with those characterizing the actual cropping system. Simulations were performed within a 2 × 2 km grid cell located in Northern Italy, in the main European rice district. Meteorological data in the period 1991-2010 were analyzed to select extreme years for cumulated precipitations (1994, the highest, and 2003, the lowest) and mean temperature (1993, the highest, and 2010, the lowest) during the rice cropping season. For each of the selected years, simulations were run from 1st January to 31st December; a soil organic matter pool was initialized to simulate rice straw incorporation. A fixed scheduling of agricultural management operations could not be defined given the variability in the meteorological conditions during the cropping seasons. Farmer management practices were then customized according to the following rules, to avoid marked stress due to water and/or N scarcity, and are in the range of typical management of rice fields in Northern Italy (Zavattaro et al., 2008):

- Sowing was performed on 1st May;
- 200 kg N ha^{-1} (as urea) were applied and split in three events: 46 kg N ha^{-1} at sowing (N0), 74 kg N ha^{-1} at mid-tillering (Nt) and 78 kg N ha^{-1} at panicle initiation (Np);
- Flood water level was forced to 5 cm height and maintained (i) for 10 days starting from 20 days before sowing (false sowing practice), (ii) from

sowing until 7 days before Nt, (iii) from Nt until 7 days before Np and (iv) from Np until 20 days before harvest;

- Harvest was triggered one week after crop physiological maturity was reached.

The cumulated emissions of CO_2, CH_4 and N_2O were selected as the output variables for all sensitivity analysis experiments, as they synthetize most of the processes involved with soil C-N transformations. These outputs were cumulated in different periods i.e., fallow and during cropping season; the latter being split between dry (cropped-dry) and flooded (cropped-flooded) periods.

Sensitivity analysis was carried out using the Morris (1991) screening method (as improved by Campolongo et al., 2007) to identify the subset of relevant parameters for each output variable. This method calculates a set of incremental ratios (Δoutput/Δparameter) when moving across different points of the parameter hyperspace and derives average (μ^*) and standard deviation (σ) of the ratios distribution. The higher the μ^* value, the higher the overall parameter importance, whereas the higher the σ value, the higher the presence of non-linearities and/or interactions with other parameters. According to Morris method, the most relevant parameters are therefore those achieving high values for μ^* and σ. Table 1 shows the parameters under sensitivity and their reference values. Due to the scarcity of information reported in literature, sensitivity analysis was carried out sampling parameters from a uniform distribution. For each parameter, upper and lower bounds of the distributions were defined as the reference value ±10%, respectively. Morris method was parameterized with five trajectories and six levels, thus requiring 520 runs for each year (number of trajectories multiplied by the number of parameters minus one). For each parameter, μ^* indices related to an output variable were cumulated for the different periods of the year (i.e., fallow, cropped-dry and cropped-flooded) to rank parameters' overall relevance. The unilateral Grubbs' test for outliers (significance level 10%) was applied to group the subset *k* of relevant parameters among all the *n* parameters. The method was then iteratively applied on the (*n* *k*) parameters to isolate groups of parameters which display comparable influence on model outputs.

Table 1. Parameters under sensitivity analysis grouped according to the process of interest, average value, units and reference. Description of each parameter is provided in Appendix A.

Process	Sub-processes	Parameter	Avg value	Units	Reference
Soil-plant interactions	Rhizosphere extent	RhizoThick	0.0005	m	2
	Root exudation	C_EffluxRateApex	4.5	µg C cm^{-2} h^{-1}	2,5
		PowerPar	0.44	unitless	5
		RelativeInflux	0.31	cm h^{-1}	5
	Root length density development	RLDExtCoeff	-0.06	cm^{-1}	7
		RL_RootMass	16700	cm g^{-1}	7
	Aerenchyma gas transport	RootPorosity	0.295	m^{3} air m^{-3} root	1
		ShootPorosity	0.39	m^{3} air m^{-3} shoot	1
		ShootRadius	0.0032	m	1
		RootShootCond	0.0001225	m^{3} gas m^{-2} tiller min^{-1}	1
		ShootAtmCond	0.42	m gas min^{-1}	1
		RootSurfaceGasExch	0.9	unitless	1
SOM decomposition	Microbial community influence	Q10_AeroMin	2.85	unitless	4
		Q10_AnaeroMin	2.85	unitless	4
		MicroCUseEff	0.5	unitless	8,12
	Humification	IsohumicCoeff	0.2	unitless	8
	Slow-cycling pool decomposition	HumusDecCoeff	0.026	year^{-1}	8
		HumusC	2	%	13
		HumusCN	10	unitless	8
	Fast-cycling pool decomposition	LitterC0	4000	kg ha^{-1}	13
		LitterCN	30	unitless	11,12
		LitterDecCoeff	0.02	d^{-1}	8,9,10,12
	N immobilization	NO3_MaxImmo	0.00333	unitless	8
		NH4_MaxImmo	0.00333	unitless	8
Aerobic reactions	Nitrification	Vmax_NH4_O2	29.52	mol m^{-3} h^{-1}	4
		Q10_Nitrification	2	unitless	13
		NO_MaxNitrification	0.004	unitless	6
		N2O_MaxNitrification	0.0006	unitless	6
	Acetate oxidation	Vmax_Ac_O2	0.468	mol m^{-3} h^{-1}	4
	Temperature response	Q10_Resp	4.6	unitless	13
	H2 oxidation	Vmax_H2_O2	0.468	mol m^{-3} h^{-1}	4
	Methane oxidation	Vmax_CH4_O2	74.52	mol m^{-3} h^{-1}	4
		Q10_CH4Ox	2.85	unitless	4
Anaerobic reactions	Methanogenesis	MinNOConcInhibCH4	0.0018	mol m^{-3}	3
		MaxNOConcInhibCH4	0.01	mol m^{-3}	3
		MinN2OConcInhibCH4	0.063	mol m^{-3}	3
		MaxN2OConcInhibCH4	0.21	mol m^{-3}	3
		Q10_CH4genesis	4.6	unitless	4
		Vmax_CH4genesis_Ac	0.108	mol m^{-3} h^{-1}	3
		Vmax_CH4genesis_H2	0.23616	mol m^{-3} h^{-1}	3
	Denitrification	Vmax_Ac_NO3	0.468	mol m^{-3} h^{-1}	3
		Q10_Denitr	2	unitless	13
		Vmax_H2_NO3	0.468	mol m^{-3} h^{-1}	3, 4
		Vmax_Ac_NO2	0.3096	mol m^{-3} h^{-1}	13
		Vmax_H2_NO2	0.3096	mol m^{-3} h^{-1}	13
		Vmax_Ac_NO	0.3096	mol m^{-3} h^{-1}	3
		Vmax_H2_NO	0.3096	mol m^{-3} h^{-1}	3
		Vmax_Ac_N2O	0.3096	mol m^{-3} h^{-1}	3
		Vmax_H2_N2O	0.3096	mol m^{-3} h^{-1}	3
Fertilizer degradation		UreaHydrolysisCoeff	0.2	d^{-1}	
		Q10_UreaHydrolysis	2	unitless	

1: van Bodegom et al. (2001a); 2: van Bodegom et al. (2000); 3: van Bodegom and Scholten (2001); 4: Xu et al. (2007); 5: Personeni et al. (2007); 6: Jannson and Karlberg (2004); 7: IRRI (1985); 8: Acutis et al. (2006); 9: Pal and Broadbent (1975); 10: Chen and Avnimelech (1986); 11: Ye et al. (2014); 12: Devevre and Horvath (2000); 13: this study

4.4. Results and Discussion

4.4.1. Model sensitivity to parameters uncertainty

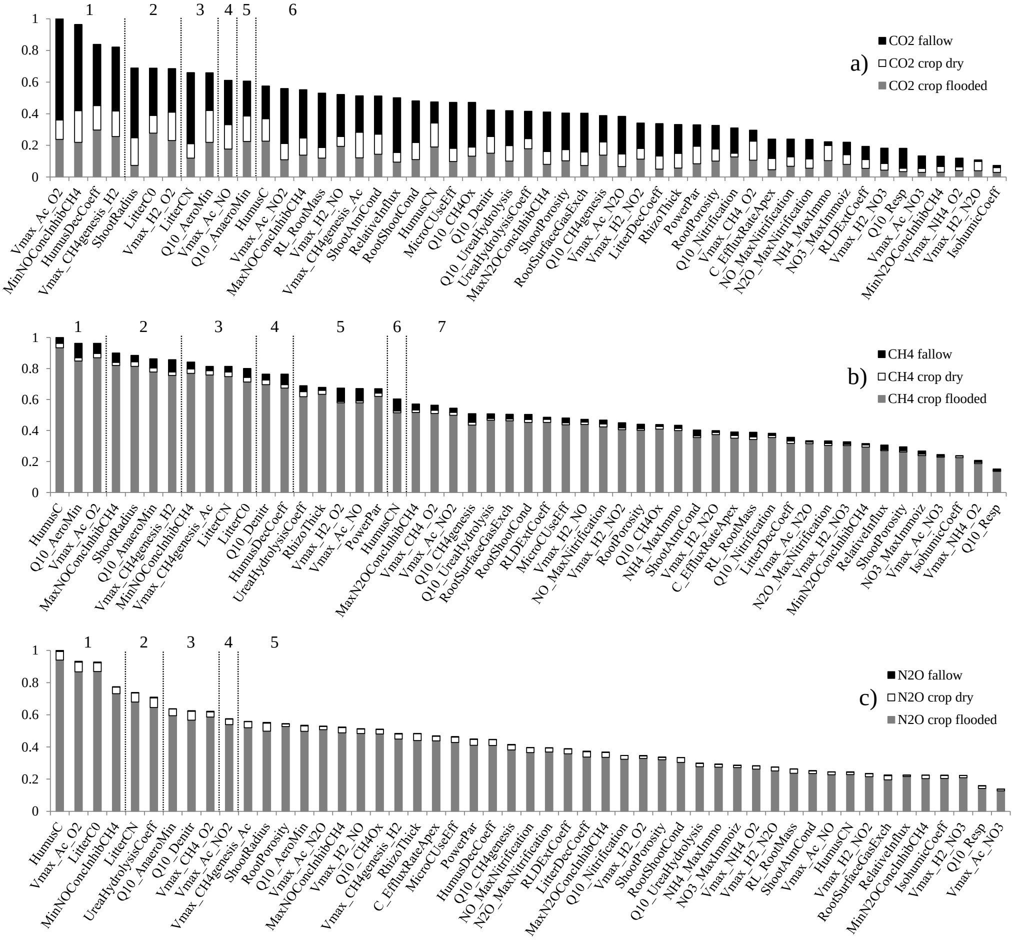


Figure 3. Normalized Morris μ* indices ranking parameters' relevance for different output variables, i.e., CO_2 (a), CH_4 (b) and N_2O (c) emission cumulated in different periods of the year (i.e., fallow, cropped-dry and cropped-flooded). For each parameter, the index results from the average μ* calculated in four simulated years (1993, 1994, 2003 and 2010).

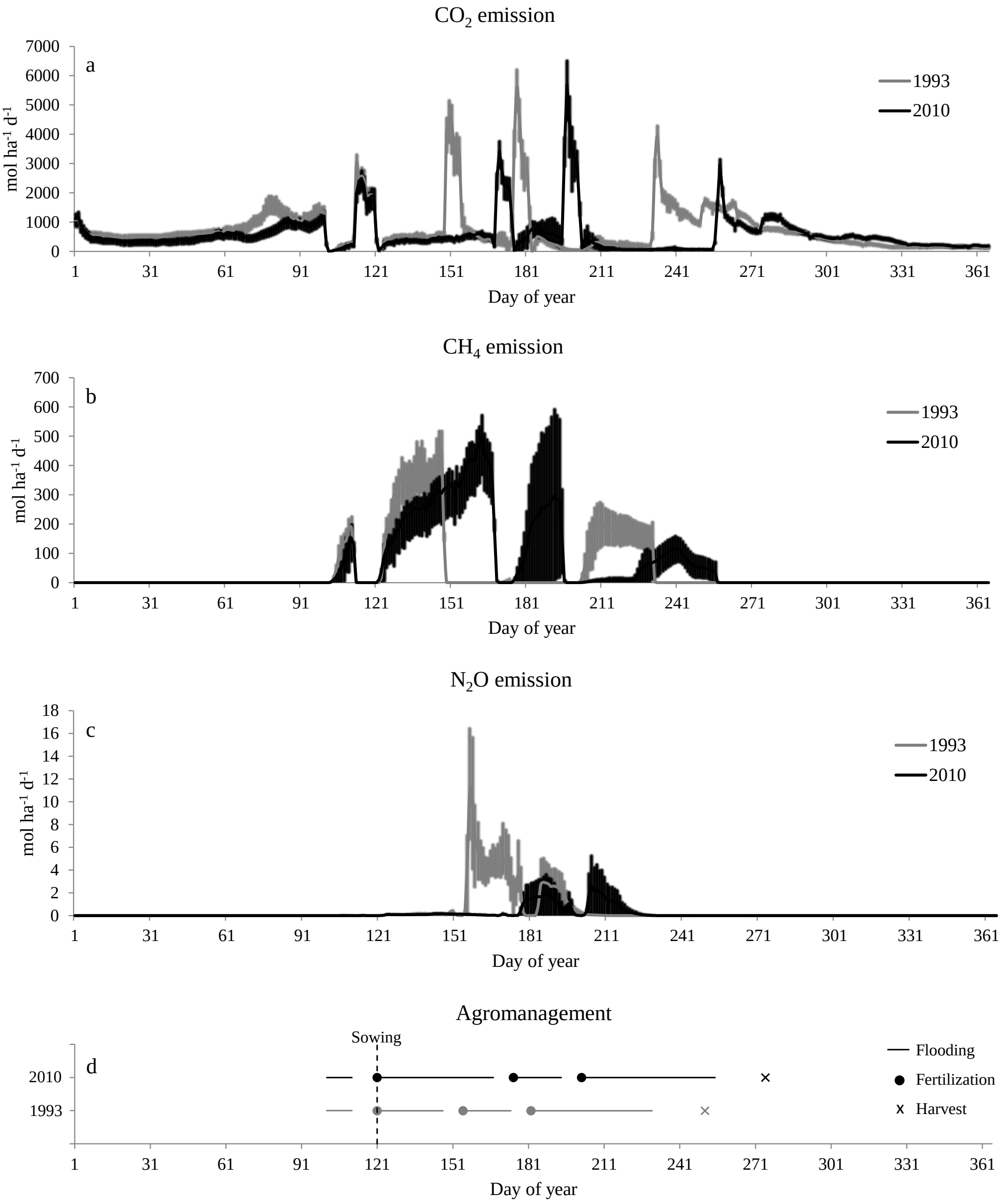
Model sensitivity to variations in input and parameters values is shown in Figure 3, reporting the normalized values of μ* indices averaged in the analyzed cropping seasons (i.e., 1993, 1994, 2003 and 2010). The contribution of fallow and cropped periods to the overall parameters relevance depends on the considered output: concerning CH_4 and N_2O cumulated emissions, the cropped season especially when the field is flooded is of paramount importance whereas, for the emission of CO_2, model sensitivity relies on all the situations identified (i.e., fallow, cropped-dry and cropped-flooded). This can be explained by the emission pattern of the studied gases during the year (Figure 4): on the one hand CH_4 and N_2O emissions occur only during the cropping season, since they strongly depend on crop management (i.e., flooding and N fertilization), on the other hand CO_2 is produced in soil during the whole year, the rate being modulated both by environmental conditions (e.g., soil temperature and moisture) and agricultural management. Sensitivity analysis confirms the dependence of CH_4 production and emission on flooding events: for each parameter, the value of μ* mainly rely on the cropped-flooded period. The contribution of the cropped-dry period is due to the emissions occurring immediately after flooding, when diffusion of methane remaining in soil is not limited by submergence, whereas the residual contribution of the fallow period depends on emissions occurring during pre-sowing flooding (Figure 4b and 4d). N_2O is instead produced both in aerobic and anaerobic conditions, via nitrification and denitrification pathways, respectively. The relative contribution of cropped-flooded and cropped-dry periods to total emission depends on the length of flooding and dry period and by the timing of fertilizations, which occur close to flooding events and are followed by a peak of emission. In such conditions, most of the N_2O emitted derives from denitrification: only a minor part can originate from NH_4 oxidation in bulk soil before the establishment of anaerobiosis or in the rhizosphere. Fertilization at sowing does not trigger significant emission, suggesting a marked response of N_2O production to fertilization rates. CO_2 emission diminishes with flooding (Figure 4a and 4d), due to the decline in SOM degradation in anaerobic conditions, the stimulation of denitrification and methanogenesis pathways and the lower diffusion of the gas in solution. Parameters' μ* indices, however, partially mask this clear pattern since they are related to cumulated emissions and the dry period is relatively short during the rice cropping season.

The Grubbs' test allowed to isolate groups of parameters characterized by the highest μ* indices. Results highlight the relevance of parameters related to SOM decomposition in regulating the emission of all the studied gases. Considering CO_2 emission, this class of parameters is represented in most of the groups of relevant parameters (Figure 3a): the standard decomposition coefficient of slow cycling organic matter (HumusDecCoeff) is found in group 1, whereas parameters describing the amount of organic matter incorporated in soil with plowing (LitterC0) and its quality (LitterCN) belong to groups 2 and 3, respectively. Temperature dependence of SOM decomposition appears crucial in explaining variability among sensitivity analysis simulations as well, with Q10 parameters for aerobic and anaerobic mineralization in groups 3 and 5, respectively. Group 1 also includes two parameters related to methanogenesis, probably due to the substrate competition among the pathways leading to CO_2 and CH_4 emission.

Focusing on CH_4 total emission (Figure 3b), model sensitivity to parameters confirmed the importance of those describing SOM decomposition (both slow cycling – groups 1, 4 and 6 – and fast cycling organic matter – group 4), which provides the electron donors for C reduction to methane. The C/N ratio of organic matter (defined by LitterCN and HumusCN) plays a more important role in determining CH_4 emission compared to that of CO_2, because of the mineralized nitrogen can provide a more favorable alternate electron acceptor and it can be converted in compounds inhibiting methanogenesis (Klüber and Conrad, 1998). This point is consistent with the presence of (i) parameters modulating NO inhibitory effect on methanogenesis in groups 2 and 3 (MaxNOConcInhibCH4 and MinNOConcInhibCH4, respectively) and (ii) a parameter influencing NO consumption in soil in group 5 (Vmax_Ac_NO). The role of denitrification as a process outcompeting methanogenesis for electron donors is further remarked by the presence of the parameter defining its response function to temperature (Q10_Denitr) in group 4 and the standard hydrolysis coefficient of urea in group 5. The interactions among N compounds and methanogenesis can probably explain the lag time between instauration of submergence and CH_4 emission following Nt and Np (Figure 4b and 4d) and contribute to the high variability of CH_4 emission among sensitivity analysis simulations (Figure 4b). Relevant for CH_4 emission are also kinetic parameters modulating methanogenesis (Vmax_CH4genesis_H2 and Vmax_CH4genesis_AC in groups 2 and 3) and some parameters describing soil-plant interactions. The latter include shoot radius (group 2), influencing gas transport through plant aerenchyma: the larger its value, the lower the resistance for methane emission and oxygen transport from atmosphere to the rhizosphere, where it can stimulate methane oxidation. Two more parameters of group 5 belong to soil-plant interactions, i.e., rhizosphere thickness (RhizoThick) and a parameter related to root exudation (PowerPar). The first determines the radius of the rhizosphere, in turn conditioning diffusion of chemical compounds and biological reactions, whereas root exudation is the main source of low molecular C compounds in the rhizosphere used as substrate during methanogenesis.

Figure 3b ranks parameters according to their relevance for N_2O emission. Also in this case, SOM decomposition appears as the most important process driving emission, with the parameters determining the amount of slow and fast cycling C in soil ranked in the first group, the C/N ratio of incorporated organic matter in the second and a Q10 response parameter in the third. The presence of C/N ratio probably indicates the dependence of production and emission of this gas on mineral N availability in soil, which can be limited by the occurrence of N immobilization due to high C/N ratios of added organic matter. N availability is also related to standard rate of urea hydrolysis (UreaHydrolysisCoeff), found in group 2. Two parameters specific for modulating denitrification response to temperature and substrate concentration (Q10_Denitr and Vmax_Ac_NO2) are in groups 3 and 4, respectively: such process – in rice paddy fields – is indeed the major pathway of N_2O production. Peaks of emission occurring after urea top dressing show high variability among different years (Figure 4c), suggesting that N_2O emission can be influenced by environmental conditions – especially soil temperature – and timing of fertilization, since plant N uptake probably reduces the pool of N available to be converted into N_2O.

Interestingly, within the most relevant parameters (i.e., group 1) in explaining variability of all the outputs there is always Vmax_Ac_O2, a kinetic parameter modulating acetate oxidation. For CO_2 emission this is probably directly linked to the production of CO_2 associated with acetate oxidation, whereas its ranking for N_2O and CH_4 probably points out the importance of acetate – representing in the model a range of organic C compounds deriving from SOM degradation – as a substrate and electron donor in a number of soil processes.



CO_2 emission

CH_4 emission

N_2O emission

Agromanagement

Figure 4. Variability of simulated emission in the hottest (1993) and coldest (2010) years of the period 1991-2010. For each day, the range between the minimum and maximum cumulated emission is reported. a: CO_2 emission; b: CH_4 emission; c: N_2O emission; d: agromanagement operations.

4.4.2. Influence of boundary conditions on model outputs

Outputs of the simulations performed for sensitivity analysis studies were also employed to investigate the dependence of CO_2, CH_4 and N_2O emission on boundary conditions in rice paddy system (Figure 5). Years 1993 and 2010 were analyzed, since they are characterized by the highest and lowest average temperature in the cropping season, respectively. CO_2 emissions (Figure 5a) highlighted a marked response to soil temperature – especially when soil is not submerged – due to the Q10 expression modulating biological processes. The difference between the rate of emission during dry and flooded periods is explained by the interactions among some limiting factors, i.e., (i) the decline of SOM decomposition as soil water content approaches saturation, (ii) the switch of microbial community from aerobic metabolism to fermentation, leading to the incomplete oxidation of organic C and favoring methanogenesis and (iii) the low diffusion of CO_2 in liquid phase. CH_4 emission (Figure 5c) displayed significant difference between dry and flooded periods, as expected: methanogenesis occurs only in anaerobic conditions and the presence of oxygen has a two-fold effect in suppressing CH_4 emission, i.e., the inhibition of methane production and the stimulation of methanotrophic bacteria. Therefore, CH4 emission occurring in absence of flood water is limited to the short periods following field drainage, when part of the CH_4 entrapped in soil can diffuse to atmosphere. On the other hand, temperature dependence of such process during flooding is not straightforward and displays high variability across years. The resulting average pattern highlights a steep increase of emissions in the range of soil temperature between 10 and 18°C. Beyond this range, trends of emission in the studied years diverge and in 2010 two local minima of emission occur at 19 °C and 23 °C; at high soil temperatures (> 23 °C). CH_4 emission in 1993 drops, whereas in 2010 tends to increase. Such contrasting results underline the non-linearity of the response of this process to environmental conditions (Neue et al., 1997), which can only partially explain the variability of the phenomenon. CH_4 emission is indeed the result of complex interactions among different components of the system, e.g., the availability of C substrate and alternate electron acceptors, the presence and activity of root system and the impacts of agricultural management practices (Le Mer and Roger, 2001). N_2O emissions display a considerable dependence on soil temperature, similar to that observed for CO_2. In this case, however, substrate availability (i.e., mineral N) plays a major role in modulating gas emission, which occurs especially after N fertilizations. The relation between mineral N in soil and N_2O emission is shown in Figure 5e: both in flooded and dry conditions, it is possible to find a range where emission linearly increases with N content in soil. During flooding, it is likely that most of the emitted N_2O derives from nitrification, a minor part being produced by nitrification in the rhizosphere, where oxygen is supplied by plant aerenchyma. On the contrary, N_2O after drainage mainly derives from oxidation of NH_4^+ to NO_3^-. Unexpectedly, the highest emission recorded does not correspond to the highest amount of available mineral N: similarly to CH_4, other aspects of the system may interact with processes leading to N_2O release in atmosphere.

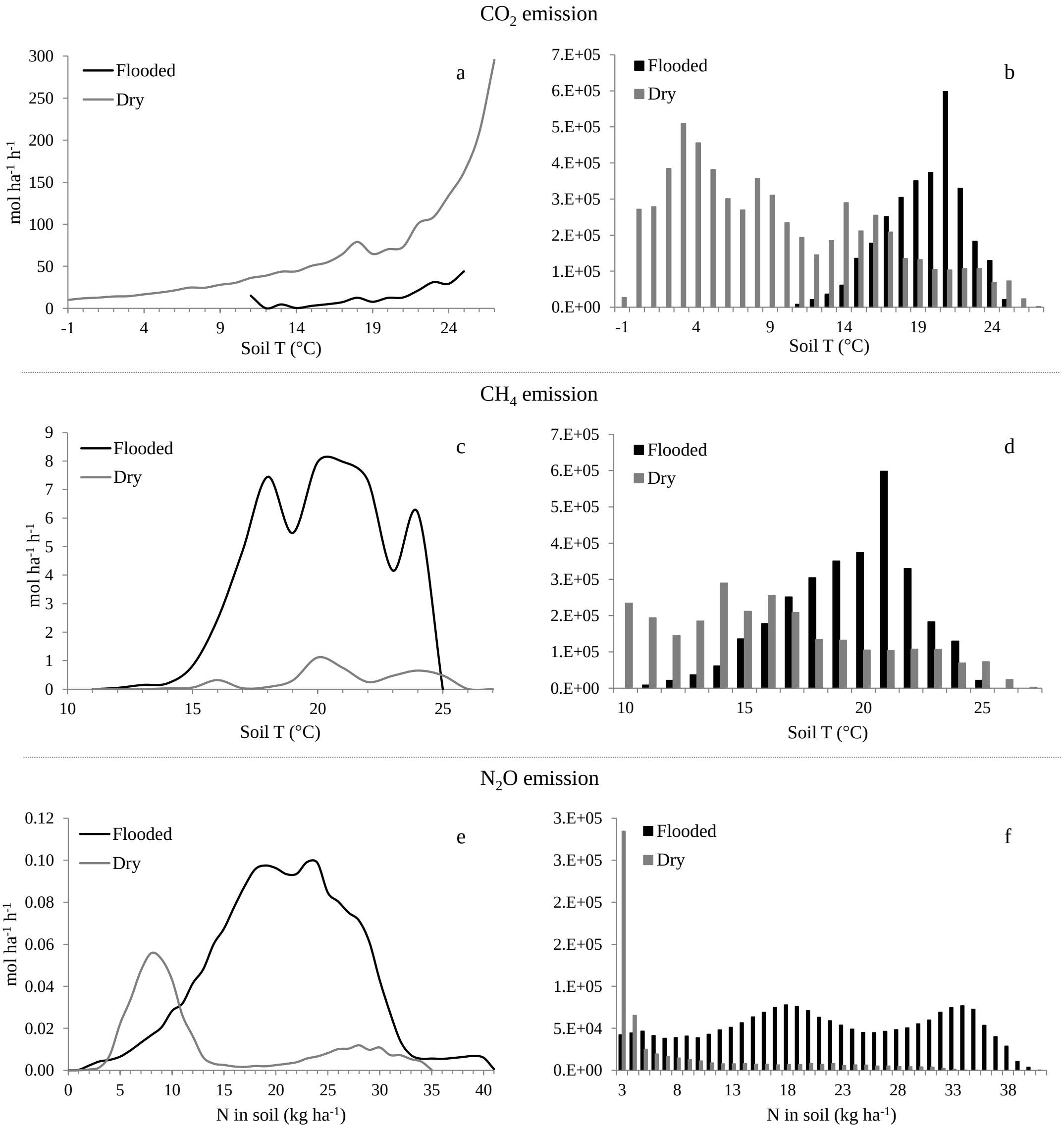


Figure 5. Simulated hourly CO_2 (a), CH_4 (c) and N_2O (e) emission in response to boundary conditions. Solid lines represent the average simulated values in sensitivity analysis experiments performed with 1993 and 2010 meteorological data. Charts in b, d and f report the number of simulated values for each X value.

4.4. Concluding remarks

The software library (UNIMI.CRONO) presented in this paper is aimed at collecting models for the simulation of C and N dynamics in agricultural soils. It is designed to maximize usability and extension, as well as the integration in complex modelling solutions. These features – representing the state-of-the-art of modular model development – overcome some of the limitations affecting current soil models and will likely contribute to update UNIMI.CRONO with the latest outcomes in soil science. The development a modelling solution for rice cropping system allowed to test model sensitivity to input parameters in a range of conditions consistent with those characterizing the study area. Sensitivity analysis was carried out considering GHGs emissions as the main synthetic variables to evaluate system's performance. This analysis pointed out the high interrelation of underlying processes leading to the emission of CO_2, CH_4 and N_2O, with soil organic matter, agricultural management and soil-plant interactions playing a major role. In such a complex scenario, simulation modelling appears as the best option to synthetize, interpret and quantify at process level phenomena which determine the emergent properties of a system. Nevertheless, rigorous validation of CRONO_C and the modelling solution have to be performed before they can be employed for operational purposes.

4.5. Appendix A

Description of the parameters under sensitivity analysis.

Parameter	Description
CarbonEffluxRateAtApex	Carbon efflux rate at root apex
HumusC	Amount of slow cycling organic carbon in soil
HumusCN	C/N ratio of humus
HumusDecompositionCoeff	Decomposition coefficient of the humus pool
IsohumicCoefficientPoolsSOM	Isohumic coefficient of the soil organic matter pools
LitterC	Amount of organic carbon derived from incorporation of crop residues
LitterCN	C/N raio of incorporated organic matter
LitterDecompositionCoefficient	Decomposition coefficient of the incorporated organic matter pool
MaxN2OConcInhibCH4genesis	Maximum nitrous oxide concentration for inhibition on methanogenesis
MaxNOConcInhibCH4genesis	Maximum nitric oxide concentration for inhibition on methanogenesis
MicrobialCarbonUseEfficiency	Carbon use efficiency of microbial community
MinN2OConcInhibCH4genesis	Minimum nitrous oxide concentration for inhibition on methanogenesis
MinNOConcInhibCH4genesis	Minimum nitric oxide concentration for inhibition on methanogenesis
N2O_MaxNitrificationFraction	Nitrous oxide maximum nitrification fraction
NH4_MaxImmobilizationFraction	Maximum immobilization of ammonium, as a fraction of ammonium pool
NO_MaxNitrificationFraction	Nitric oxide maximum nitrification fraction
NO3_MaxImmobilizationFraction	Maximum immobilization of nitrate, as a fraction of ammonium pool
PowerParameter	Power parameter for the estimation of local efflux of C as a function of distance from root apex
Q10ForAerobicMineralization	Relative increase in aerobic mineralization rate following a temperature rise of 10 °C
Q10ForAnaerobicMineralization	Relative increase in anaerobic mineralization rate following a temperature rise of 10 °C
Q10ForDenitrification	Relative increase in denitrification rate following a temperature rise of 10 °C
Q10ForMethaneOxidation	Relative increase in methane oxidation rate following a temperature rise of 10 °C
Q10ForMethaneProduction	Relative increase in methane production rate following a temperature rise of 10 °C
Q10ForNitrification	Relative increase in nitrification reduction rate following a temperature rise of 10 °C
Q10ForRespiration	Relative increase in respiration rate following a temperature rise of 10 °C
Q10ForUreaHydrolysis	Relative increase in urea hyrolysis rate following a temperature rise of 10 °C
RelativeInflux	Influx of C relative to external concentration
RhizosphereThickness	Radius of the area around roots influenced by root activity
RLDExtinctionCoeff	Root Length Density Extinction Coefficient by depth
Root_shootConductance	Conductance at the root-shoot interface
RootLengthPerMassOfRoot	Average ratio between root length and root mass
RootPorosity	Porosity of root
RootSurfaceGasExchange	Fraction of the root surface active in gas exchange
Shoot_headspaceConductance	Conductance at the shoot-headspace interface
ShootPorosity	Porosity of shoot
ShootRadius	Shoot radius
UreaHydrolysisCoefficient	Urea hydrolysis standard rate
Vmax_Acetate_N2O	Potential rate of conversion of electron acceptor
Vmax_Acetate_NO	Potential rate of conversion of electron acceptor
Vmax_Acetate_NO2	Potential rate of conversion of electron acceptor
Vmax_Acetate_NO3	Potential rate of conversion of electron acceptor
Vmax_Acetate_O2	Potential rate of conversion of electron acceptor
Vmax_CH4_O2	Potential rate of conversion of electron acceptor
Vmax_CH4genesisFromAcetate	Potential rate of conversion of electron acceptor
Vmax_CH4genesisFromH2	Potential rate of conversion of electron acceptor
Vmax_H2_N2O	Potential rate of conversion of electron acceptor
Vmax_H2_NO	Potential rate of conversion of electron acceptor
Vmax_H2_NO2	Potential rate of conversion of electron acceptor
Vmax_H2_NO3	Potential rate of conversion of electron acceptor
Vmax_H2_O2	Potential rate of conversion of electron acceptor
Vmax_NH4_O2	Potential rate of conversion of electron acceptor

A MODELLING SOLUTION TO SIMULATE RICE CROPPING SYSTEM: INTEGRATING AGRICULTURAL MANAGEMENT, CROP PRODUCTION AND ENVIRONMENTAL IMPACTS

Tommaso Stella, Simone Bregaglio, Nicolò Frasso, Marcello E. Chiodini, Carlo Gilardelli, Roberto Confalonieri

5.1. Abstract

Cropping system simulation models enable to perform an integrated assessment of the processes underlying crop production and the environmental impact of agricultural activities. They thus allow to set up experimental designs to test the nonlinear impacts of alternate farmer practices– irrigation water use, straw and nutrient management – to optimize the management and the performance of cropping systems. Here we present a modelling solution to simulate a comprehensive set of biophysical processes involved with the paddy rice cropping system, considering the crop development and growth, the soil water dynamics, the effects of fertilizers on nitrogen leaching and the emission of greenhouse gases as driven by farmer management strategies. The evaluation of the solution in reproducing field data related to rice biomass accumulation (R^2 = 0.99), and CH_4 (R^2 = 0.88) and CO_2 (R^2 = 0.79) emissions revealed good accuracy and adherence to the real system. The solution was then used to evaluate the impacts of alternate nitrogen fertilization managements on rice yield, CH_4 and N_2O emissions and nitrogen leaching, in a 3 × 2 factorial experiment with two factors, i.e. the amount of nitrogen applied (3 levels, low, medium and high) and the number of top dressing fertilizations (2 levels, two or three applications). The software implementation promotes reuse and extension of the solution, which can be adapted to simulate other cropping systems.

Keywords: Agricultural management, BioMA, environmental impacts, greenhouse gas emission, rice cropping system.

Software availability: The modelling solution (.NET 4.5 project) and the graphical user interface are distributed free of charge for noncommercial purposes on request to interested users (cassandra.lab@unimi.it).

5.2. Introduction

Contemporary agriculture is facing a number of challenges arisen from the needs of enhancing productivity to guarantee food security and to achieve the goal of sustainability (Tilman et al., 2002), threatened by the influence of agriculture on carbon, water and nutrient cycles as well as on atmospheric and soil chemistry. Rice (*Oryza sativa* L.) agriculture is in the spotlight due to its primary role for nutrition of over half of the world's population (Juliano, 1993) and the environmental challenges associated with flooded rice systems, such as the use of large amount of water for irrigation and the emission of greenhouse gases (Johnson-Beebout, 2009). The unique water management contributes to make rice paddies one of the most important source of anthropogenic methane (CH_4; Yan et al., 2009) and nitrous oxide (N_2O; Akiyama et al., 2005).

In the last decades, simulation models were developed to provide accurate predictions of crop production whilst addressing the issue of resource management in farming systems (Keating et al., 2003). Despite available dynamic models have the potential to address different domains in the agroecosystem, their integration in a complete simulation environment is rarely being realized, with most of available tools focusing either on crop or on soil processes. In the first case, a number of crop growth models were proposed, e.g., DSSAT (Jones et al., 2003) and Wageningen models (van Ittersum et al., 2003), allowing the simulation of a limited set of soil processes, especially water and nutrient fluxes, to support farmer management (e.g., CropSyst; Stöckle et al., 2003). On the other hand, biogeochemical models implement a detailed description of soil physics and biology (Blagodatsky and Smith, 2012), providing sound approaches to simulate the environmental impacts as mediated by soil. Given the key influence of the crop (Wassmann and Aulakh, 2000) and the farmer management (Ju et al., 2009) in modulating these impacts, the lack of coordination between crop and biogeochemical models often limits the applicability of available models to real conditions (e.g., Gu et al., 2009). Pioneer attempts to integrate crop and biogeochemical models were made by Zhang et al. (2002), who coupled the DNDC model (Li et al., 1992) with algorithms to reproduce crop growth and development. The resulting software application has been adapted to simulate a range of production systems worldwide (Giltrap et al., 2010), including rice (Fumoto et al., 2008).

The software architecture adopted in agricultural models has contributed to constrain the integration, reuse and extension of available simulation tools (Holzworth et al., 2010). Nowadays, the adoption of component oriented programming in the development of agro-environmental models led to advanced modelling frameworks such as APSIM (Holzworth et al., 2014) and BioMA (Donatelli et al., 2012). The latter encourages the modular development of biophysical models, isolated within extensible software components providing approaches for the simulation of processes characterizing specific domains (e.g., crop, soil, farmer management). Modelling approaches belonging to one or more components can be linked to compose modelling solutions (MSs) with a fine granularity, thus maximizing the possibilities of their improvement through hybridization (Donatelli et al., 2014) and adaptation to new needs (e.g., Stella et al., 2015). This paper presents the implementation of a MS to assess the performance of paddy rice cropping system in terms of productivity and environmental impacts. To achieve this aim, the MS simulates the mutual interactions among crop growth and development, biogeochemistry, soil water and temperature dynamics, as modulated by meteorology and farmer management choices. In this study, a preliminary evaluation of the agreement between measured and simulated data using field data was performed, and the opportunity of employing the MS to study the effects of alternate management strategies on crop yield, nitrogen leaching, CH_4 and N_2O emissions was explored.

5.3. Materials and methods

5.3.1. Biophysical models implemented to simulate paddy rice cropping system

The MS is composed by models belonging to different domains of the agro-ecosystem. Domains description is encapsulated within discrete units, i.e., the software components; each component collects libraries of model approaches for the simulation of processes characterizing one specific domain. The models included in the MS were selected according to their suitability to simulate rice paddy environment and to their input data requirements. This criterion allowed to select the process model requiring less input or intermediate variables estimated by other models in the MS.

The component UNIMI.SoilW provides the MS with models for the simulation of water infiltration, redistribution in soil and root water uptake: potential infiltration rate is calculated according to Smith and Parlange (1978), as a function of hydraulic conductivity, net capillary drive and cumulative infiltration. Redistribution of water in the soil profile is simulated via a modified tipping bucket approach, with water movements reduced by soil hydraulic conductivity, allowing water content to be higher than field capacity (Nietsch et al., 2011). These models allowed to reproduce the water fluxes in flooded paddy rice soils. The EPIC (Williams et al., 1989) approach for root water uptake was selected, requiring root depth, soil water content and crop potential transpiration as input variables. UNIMI.SoilT models are used to estimate surface and soil temperature at different depths: surface temperature is a function of daily air temperature (Parton, 1984) when the field is not flooded, whereas soil profile temperature is influenced by bulk density, damping depth, average annual air temperature and soil profile temperature of the previous day (Nietsch et al., 2011). An empirical approach derives flood water temperature from air temperature, leaf area index, water height and water temperature of the previous day; during flooding periods, temperature of soil surface temperature is set equal to flood water temperature.

Models for carbon and nitrogen transformations in soil are provided by the component UNIMI.CRONO: selected models calculate (i) the decomposition of soil organic matter pools according to first order kinetics and the associated nitrification, ammonification and humufication processes (Wu and McGechan, 1998), (ii) the microbial-mediated reactions involving alternative electron acceptors, allowing to simulate both aerobic and anaerobic processes leading to the emission of greenhouse gases (Xu et al., 2007), (iii) the diffusive transport of chemical compound in soil (Schjønning et al., 2003), diffusion through plant aerechyma (van Bodegom et al., 2001) and ebullition of dissolved gases (Tang et al., 2010) and (iv) the soil-plant interactions mediated by roots i.e., crop nitrogen uptake (Abrahamsen and Hansen, 2000) and root carbon exudation (Personeni et al., 2007). The dynamic simulation of root length density in the soil profile is performed according to Ritchie (1988). Simulation of crop growth and development is performed by the WOFOST-GT2 model (Stella et al., 2014) implemented in the UNIMI.CropML component. In order to account for limitation to growth due to water and nitrogen supply scarcity, routines from

UNIMI.CropML_WL and UNIMI.CropML_NL components were linked to the crop model. In particular, a water stress factor reduces assimilation as a function of the ratio between potential and actual evapotranspiration, whereas the ratio between critical and actual nitrogen concentration in plant tissues conveys the degree of crop nitrogen stress. Critical nitrogen concentration determines crop nitrogen demand, and its estimation relies on the nitrogen dilution principle proposed by Greenwood et al. (1990).

Farmer management events (i.e., sowing, harvest, fertilizations and irrigations) are triggered by models belonging to CRA.Agromanagement component (Donatelli et al., 2006): they quantify the impact of the event via a set of parameters which can be listened by each software component, in turn determining a change in the state variables of the related domain. Finally, the component CRA.Clima provides the modelling solution with models for the estimation of hourly air temperature (Campbell, 1985), reference evapotranpiration and solar radiation (Hargreaves and Samani, 1985).

5.3.2. Software architecture

Figure 1 shows the Unified Modelling Language (UML) diagram of the MS, which is implemented as a Microsoft C# class library managing the interactions between the I/O data produced by models belonging to the different software components. The entry point of the MS is the *RunnerAPI* class, containing instances of *Adapter* classes (Gamma et al., 1994) and managing their call. *Adapter* classes, in turn, encapsulate the logic to perform dynamic simulation, by calling specific models selected among those provided by software components. The components implemented in the MS communicate different times in each integration time step, via the methods provided by *ISimulationComponent* interface. Even if models have different internal time steps (spanning from a minute to a day), a daily communication time step between *Adapters* is chosen. Information produced during the simulation is stored in dedicated classes i.e., *DataTypes*, containing the instances of the data structures of the components implemented in the MS; *DataTypes* are shared by all the *Adapter* classes of the MS, making possible the communication of models belonging to different domains, meant as the possibility of exchanging variables among software components. The *Adapter* class of the component CRA.AgroManagement is able to publish specific events, i.e. agricultural management operations, which are listened by other *Adapters* via the *HandleEvents* method of the *ISimulationComponent* interface. This leads, for example, to the publication of an irrigation event by the *AdapterAgromanagement* class, with a date and an amount of applied water as parameters. All the *Adapters* in the MS can listen to this event, but only the *Adapter* of the UNIMI.SoilW component produces an impact on the cropping system by modifying the soil water content. However, since *DataTypes* classes are shared, models invoked by other *Adapters* may be influenced by the change in the states of the system, e.g., by reducing the water stress simulated by the crop model.

Figure 1 also shows the dependencies among the software components in the MS: components simulating soil and crop domains depend on CRA.ModelLayer, providing the interfaces implemented by the *domain classes* describing the domain (*IDomainClass*) and by the *strategy classes* calculating the variations of the states of the system (*IStrategy*). The components collecting the strategies have explicit dependencies on the components containing the domain classes: this means that the description of the biophysical domain does not depend upon the modelling approaches selected, but the opposite. The simulation of the nitrogen limitation to crop growth depends on models for water limitations, in turn being driven by models for potential conditions (i.e., with solar radiation and air temperature determining crop production), reflecting the hierarchy in growth factors widely adopted in crop modelling (van Ittersum et al., 2003). Each component implementing models to react to agricultural management depends to CRA.Agromanagement. The MS project, finally, instantiates classes belonging to all the other components, thus establishing dependencies to each of them.

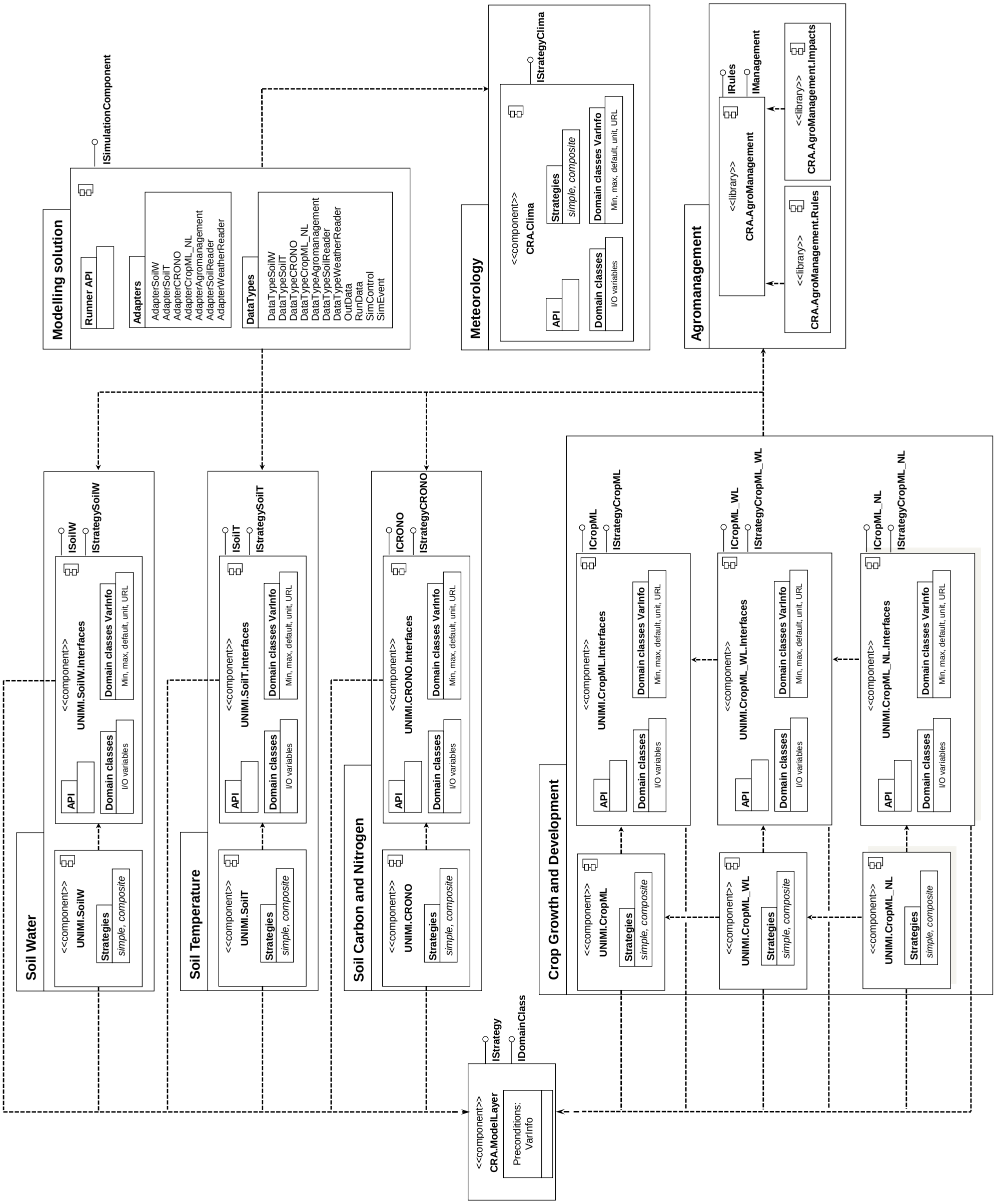


Figure 1. Unified Modelling Language (UML) diagram of the software components which make up the modelling solution. The software units simulating soil and crop have a dependency (arrow dotted line) to CRA.Core.ModelLayer and CRA.AgroManagement. The modelling solution has dependencies to soil and crop components, CRA.Clima and CRA.AgroManagement. The interfaces (circle and solid line) implemented by each component are reported.

A Graphical User Interface (GUI) was developed to allow users to configure and run simulations, visualize and save outputs (Figure 2). The GUI automatically reads from text files the input needed to run the simulation, i.e., meteorological data, soil properties and agricultural management; if measured data are provided, the GUI links them to the related simulated data series. From the GUI, users can select the simulation site (meant as the complete set of input data), start and end dates of the simulation (multi-year simulations are allowed), and configure the main crop and soil parameters. Soil is by default divided into three overlapping layers. Information needed to run the simulation is stored within *DataTypes* classes of the GUI, and passed at begin of simulation to the proper *DataTypes* of the modelling solution, which is invoked via the *RunnerAPI* class. At the end of the simulation the output data are copied to GUI *Datatypes*: the user can select the variables to visualize, spanning from the crop (e.g., phenology, yield, nitrogen uptake) to soil (e.g., soil water and nitrogen content, temperature in the profile) and emission of greenhouse gases (CO_2 and CH_4). The user is also allowed to customize the time period of plotted data and export simulation outputs as text files.

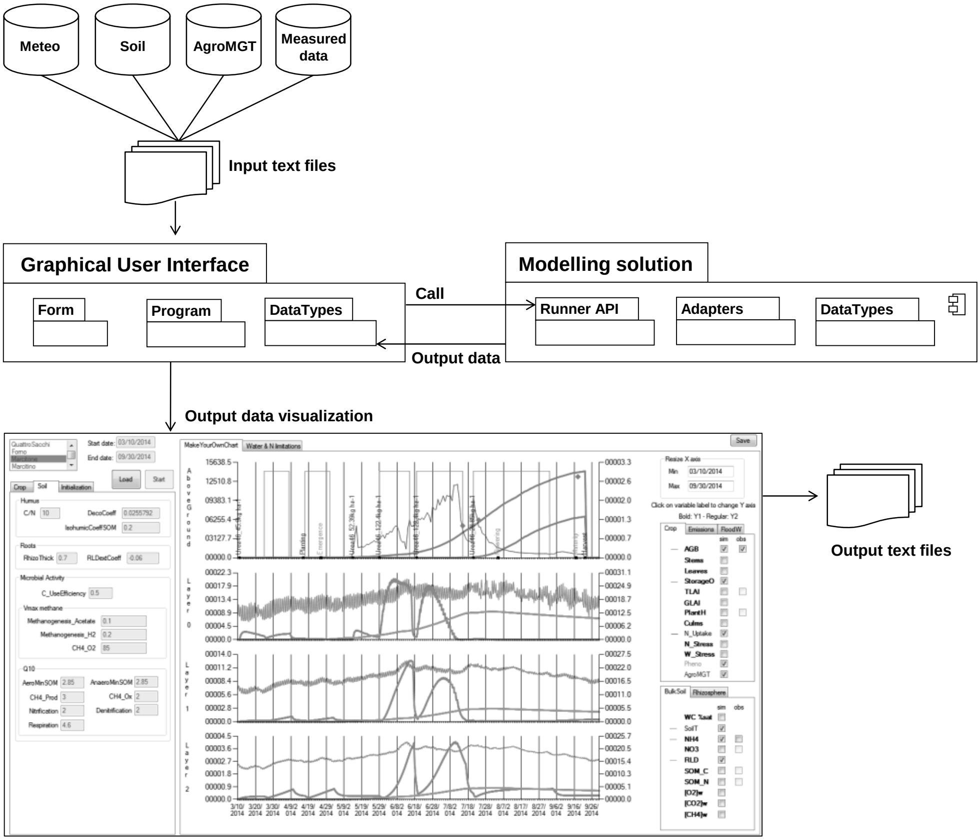


Figure 2. Functioning of the graphical user interface (GUI). Input needed to run a simulation are stored within specific text files. User may modify the simulation period and/or parameters' values via the GUI. Data types classes of the GUI and the modelling solution (MS) communicate in order to provide (i) the MS with data needed to run the simulation and (ii) the GUI with output data. Once the simulation is finished, the GUI allows to choose the visualized output within a specified period and to save all output data.

5.3.3. Field scale evaluation of the modelling solution

A paddy rice field was monitored in 2014 in Northern Italy (Gaggiano, 45°24'N 9°2'E) in order to collect preliminary data to evaluate MS ability to simulate the dynamics of crop, soil and greenhouse gases during the cropping season. The soil in Gaggiano is sandy loam (sand 55.3%, silt 41.1%, clay 3.6%), characterized by pH = 6, organic carbon content = 14 g kg^{-1}, C/N ratio = 10 and bulk density = 1.23 kg dm^{-3}. The field was row seeded on dry seedbed with 140 kg ha^{-1} seeds cv. Sole on 16th April, leading after emergence to a plant density of about 100 plants m^{-2}. Before sowing, 46 kg ha^{-1} of urea (N concentration = 46%) were incorporated in soil (11th March), and the field was kept flooded to favour the emergence of weeds, controlled with a chemical treatment. After emergence, four top dressing fertilizations were applied with 115 kg ha^{-1} of ammonium sulphate on 14th April, 122 kg ha^{-1} of urea on 29th May and on 19th June, and 70 kg ha^{-1} of urea on 21st July; each fertilization event was performed after drainage, with continuous flooding during most of the growing season. Plant samples were collected three times during the crop cycle (15th July, 24th July and 18th September) to measure aboveground dry biomass and tillering index (i.e., 3 tillers per plant at heading) whereas total leaf area index was measured twice (28th July and 25th August). Crop flowering was recorded in the first week of August, and harvest was performed at 20% grain humidity on 22nd September. From the end of July an eddy covariance station was equipped with a sonic anemometer (Young) for high frequency wind measurements; CO_2 and H_2O were monitored with the Li-Cor 7500 open path, and CH_4 was measured with the fast methane analyzer LGR RMT200. At the same time, the temperatures of surface soil and above-canopy temperatures at 2 m, and the irrigation water levels (average 0.03 m) were monitored. Meteorological data as input to the MS were measured by the nearest station belonging to the regional network of ARPA, located at Motta Visconti (about 20 km from the monitored field).

Information on agricultural management and measured data were employed to calibrate the MS via the GUI, i.e., tuning some parameters via trial error technique to visually reduce the gap between measured and observed data. In particular, leaf area index and aboveground biomass were used as reference data to calibrate the crop model parameters, whereas soil analysis allowed to initialize soil organic matter; The incorporation of crop residues with plowing was implemented as a pool of fast cycling organic matter in the uppermost soil layer. Emission data of CH_4 were split into calibration and validation dataset: the former was used as a reference to calibrate model parameters driving the fast cycling organic matter pool and the root–shoot conductance, which is a key factor in gas transport through plant aerenchyma known to be highly variable across varieties (van Bodegom et al., 2001). CO_2 emission data were employed as a synthetic variable to evaluate MS performance in simulating processes involving carbon cycle in the cropping system, i.e., crop photosynthesis and respiration, and the dynamics of organic matter in soil. The complete set of parameters and values specified via GUI is reported in Appendix A; remaining parameters were kept at default value.

5.3.4. Applicability of the modelling solution as experimental tool

After calibration, the MS was applied to analyse the impact of alternate N fertilization strategies on the environmental and productivity components of the system in the same site and cropping season. A factorial experiment was designed to test the capability of the MS to differentiate system responses according to timing and rate of nitrogen applications. Yield (kg ha^{-1}) was chosen as the synthetic variable to describe the productivity, whereas N leaching losses (kg N ha^{-1}) and CH_4 emission (kg C ha^{-1}) were used to quantify the environmental impacts of the cropping system. N losses were evaluated as total N leaching and N_2O emission (kg N ha^{-1}); cumulated CH_4 emission was recorded to investigate the potential extent of CH_4 mitigation achievable through the modulation of N fertilization.

Two factors were arranged, i.e. the amount of nitrogen applied (3 levels, low, medium and high) and the number of top dressing fertilizations (2 levels, two or three applications). N fertilization strategies were designed according to local agronomic practices (Zavattaro et al., 2008): one fourth of the paddy surface receives only inorganic products (mainly urea), with about 70 kg N ha^{-1} spread at sowing and 80 kg N ha^{-1} as top dressing. Top dressing is generally split into two applications, respectively at tillering stage and at panicle differentiation. Irrigation water is generally managed as continuous flooding with three short droughts, i.e., after emergence to promote rooting and before the application of top dress fertilizers. From this information a standard agricultural management for 2014 was defined as follows:

- at sowing (16th April) 70 kg N ha^{-1} as urea were applied and flooding (water height = 0.03 m) was set;
- from 7th to 16th May the field was drained to simulate rooting drought;
- crop was top dressed with 40 kg N ha^{-1} respectively 9th June and 21st July, corresponding to simulated mid-tillering and panicle differentiation stages. Before each fertilization, the field was kept dry for five days;
- flooding was interrupted on 2nd September, when the crop was approaching physiological maturity.

Starting from this management (i.e., normal nitrogen, 150 kg N ha^{-1}; NN hereafter) a high nitrogen (HN) and a low nitrogen (LN) managements were defined. These were obtained as NN ± 50% N, thus leading to the application of 225 kg N ha^{-1} for HN and 75 kg N ha^{-1} for LN. The resulting total amount of applied N in the three treatments is in line with the minimum, average and maximum amounts reported by Zavattaro et al. (2008) for Northwest Italian paddy rice system. An alternate fertilizer splitting was tested for each level of applied N, by adding a top dressing fertilization at the end of rooting drought and keeping the total amount of fertilizer unchanged: all the treatments are reported in Table 1.

A two way, multivariate ANOVA was performed to quantify the main effects of the levels of applied N and top dressing fertilization strategy on yield, CH_4 and N_2O emissions and N leaching. Normality of distributions was assessed with Shapiro-Wilk test and the absence of outliers was confirmed by Grubbs test. The post hoc Newman-Keuls method was performed to rank significantly different sample means.

Table 1. Experimental design of the alternate fertilization strategies simulated.

		N amount (kg ha^{-1})				
Nitrogen level	top dressing events	sowing	rooting drought	mid-tillering	panicle initiation	total
NN	2	70	0	40	40	150
HN	2	105	0	60	60	225
LN	2	35	0	20	20	75
NN	3	35	35	40	40	150
HN	3	52.5	52.5	60	60	225
LN	3	17.5	17.5	20	20	75

5.4. Results and discussion

5.4.1. Model outputs: an overview

Figure 3 highlights the main output variables estimated by the MS and displayed by the GUI, i.e., those related to gas emissions, crop growth and development, and to soil water and nitrogen dynamics. All these variables have interconnected patterns and are strongly influenced by the farmer management, especially in terms of fertilization and irrigation. Urea is progressively hydrolyzed after its application, leading to an increased availability of ammonium in soil (Figure 3e) and a peak in crop nitrogen uptake (Figure 3b), according to plants requirements. In flooded conditions soil water content is maintained at saturation (Figures 3e and 3f), and conversion of ammonium into nitrate – i.e., nitrification – is limited by oxygen availability, mainly supplied by diffusion from atmosphere through plant aerenchyma. When the field is dried, remaining ammonium is rapidly nitrified, exposing a consistent amount of nitrogen to the risk of leaching at the following flooding event. The last top-dressing fertilization induces a peak in crop nitrogen uptake (Figure 3b) with almost any variation in soil nitrogen concentration, indicating a moderate stress before urea application and the high efficiency of the last event, performed at panicle initiation. Simulation of crop growth is in line with measured data (Figure 3c): the MS estimates a biomass at harvest around 14 t ha^{-1}, and a total leaf area index (LAI) of 3.5 m^{2} m^{-2}. The green LAI reaches a peak just before flowering, and it rapidly decreases while the crop approaches physiological maturity. In this phase photosynthesis contribution to grain filling is progressively reduced, and yield formation is partially sustained by remobilization of carbon reserves from stem parenchyma, modeled according to Stella et al. (2016), taking into account both crop nitrogen status and water stress in modulating this process. From crop emergence until flowering partitioning of photosynthates to roots sustains the increase of root length density (RLD) in the soil profile (Figure 3d); the highest values of this variable (i.e., about 10 cm cm^{-3}) are recorded in the uppermost soil layer. Simulated gaseous emissions (Figure 3a) are particularly dependent on crop growth and agricultural management. Negative values of CO_2 emissions indicate a net carbon absorption by the cropping system, occurring whenever photosynthesis rate is higher than crop respiration and degradation of organic matter in soil. The highest carbon absorption is then achieved around flowering when photosynthetic active tissues (green LAI) reach a peak and environmental conditions – air temperature and solar radiation – are optimal for photosynthesis. Considering a daily dynamic, hourly CO_2 emission values are associated with photosynthesis, resulting in net absorption during day (with a peak in the afternoon), and a net emission in the night. Net CO_2 emission increases during the year as a function of the average soil temperature, which is a key driver in soil organic matter degradation; comparing flooded and dry periods, the latter causes higher emissions, due to both the higher mineralization rates occurring when water does not saturate soil (and respiration processes are favored compared to fermentation) and the higher diffusion potential of CO_2 in the gaseous phase. Nevertheless, the establishment of flooding conditions boosts anaerobic metabolism in soil, resulting in the production and emission of CH_4, which has about 15-30 times greater infrared absorbing capability than CO_2 on mass basis (Rhode, 1990), impacting on the radiative forcing added to atmosphere. Methane emission progressively increases during the cropping season, its production and mobility being influenced by soil temperature; moreover, as the crop develops, more methane is emitted through plant aerenchyma, according to the model proposed by van Bodegom et al. (2001), since root length density, number of tillers and LAI increase during the cropping season. The peaks of CH_4 emission occurring generally in the warmest hours of the day are mainly explained by ebullition of gas bubbles (Nouchi et al., 1994). Low soil temperature and inhibition of N compounds on methanogenesis (van Bodegom and Scholten, 2001) may explain lower emission simulated before planting and during early crop development.

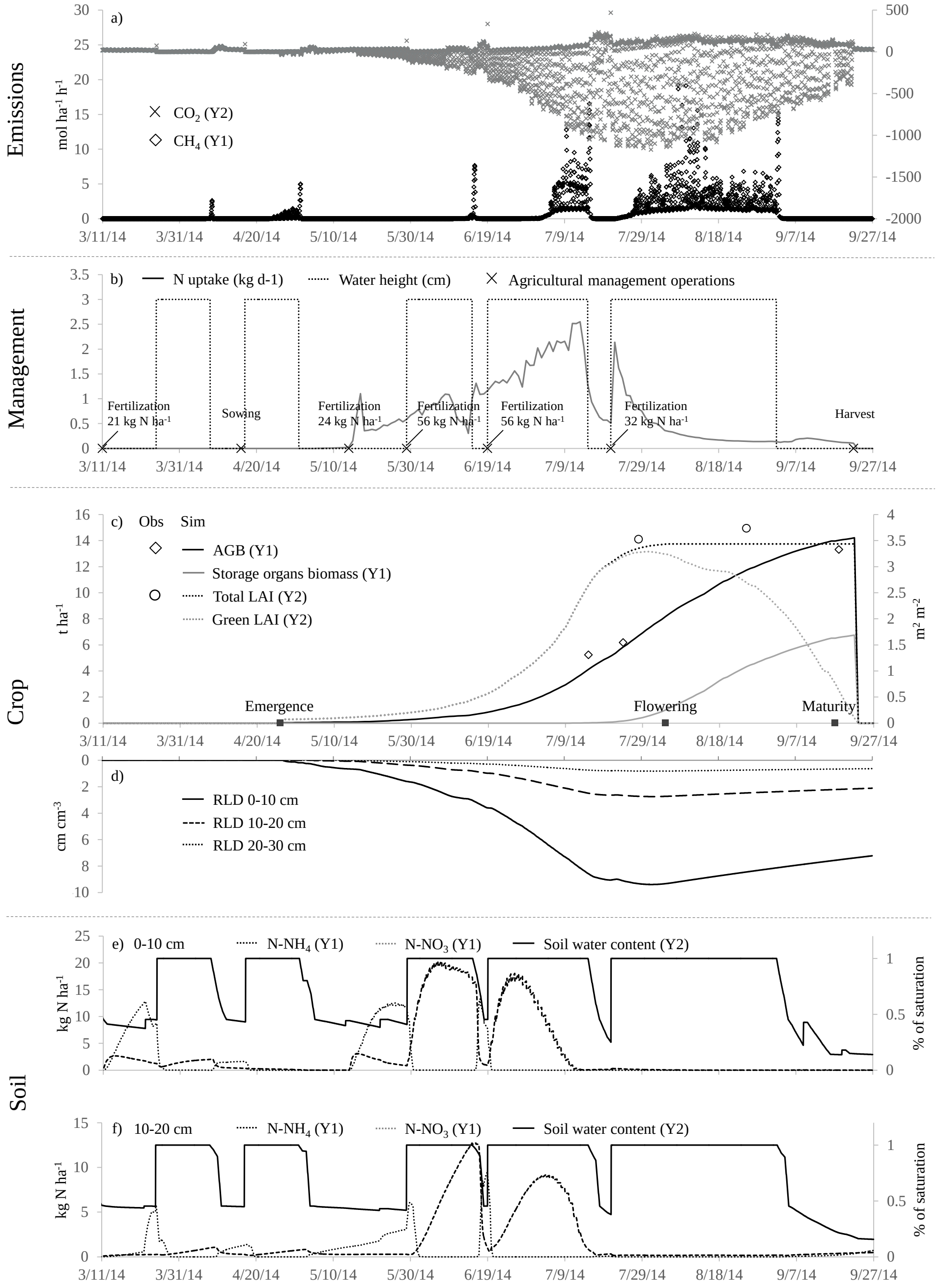


Figure 3. Sample outputs of the modelling solution during the cropping season. a: carbon emissions; b: agricultural management and crop nitrogen uptake; c: crop variables, aboveground; d: crop variables, belowground; e and f: nitrogen and water content in the soil profile.

5.4.2. Evaluation of modelling solutions performance

Measured data related to crop growth were employed to calibrate the crop model implemented in the MS: due to data scarcity, evaluation metrics for aboveground biomass were nearly optimal, achieving R^2 = 0.997 and modelling efficiency (EF; Nash and Sutcliffe, 1970) equal to 0.95. CH_4 emission data in the last period of flooding during the cropping season (i.e., from 7th July to 1st September) were used to give an overall evaluation of the MS to simulate methane production and consumption in soil and its transport to atmosphere. During the dry period after flooding, indeed, the MS did not simulate any CH_4 emission coherently with observed data. The evaluation of the agreement of simulated and measured data was carried out on hourly and daily basis. Daily evaluation was performed as cumulative emission: depending on data availability, 2 to 16 hourly measurements contributed to the daily cumulated emission. Simulated and measured CH_4 emissions are shown in Figure 4b: simulation highlights a clear diurnal pattern due to the variation of soil temperature which, especially in the uppermost soil layer, stimulates the emission of gas bubbles during the warmest hours of the day, consistently with Neue et al. (1997). Such pattern is not so evident in measured data, contributing to the unsatisfactory performance of the MS when evaluated against hourly emission data. In this situation, both calibration and evaluation datasets display negative values of EF and R^2 close to zero. Nevertheless, even if the MS produces estimates of emission with hourly time step, such estimation can be undermined by different sources of uncertainty, involving both model estimates of hourly variables and measured data. Comparing emissions on daily basis, indeed – even if the complete set of 24 hours was never available – produced satisfactorily results both with both calibration (R^2 = 0.85, EF = 0.59) and evaluation data (R^2 = 0.92, EF = 0.88). Coefficient of residual mass (CRM) highlighted slight over- and underestimation of simulated emission with calibration (CRM = -0.1) and evaluation (CRM = 0.02) datasets, respectively. When considering cumulative emission, the relative error (y) of simulated data tends to decrease as the number of hourly data (x) contributing to daily emission increase (linear regression: $y = -0.0197\ x + 0.461$; R^2 = 0.25). This may suggest that hourly under- and overestimations produced by the MS tend to counterbalance on daily basis, and that performance of the model when compared to 24-hours emission could be better to those recorded with available data. Simulated CO_2

emission pattern (Figure 4a) highlighted a marked diurnal variation, mainly due to the crop photosynthetic activity. This was confirmed by measured data, used as an overall evaluation of the ability of the MS to reproduce carbon fluxes in the cropping system. Such diurnal trend allowed to achieve positive values of EF (0.14) and satisfactorily R^2 (0.71) between measured and simulated CO_2 fluxes even considering hourly data. On daily basis evaluation metrics achieved better results, EF reaching 0.44 and R^2 equal to 0.79. As well as for CH_4, relative error of simulated data tends to decrease while increasing number of hourly measures available in a day (y = -0.06 x + 1.51). Nevertheless, CRM (–0.36) highlighted either an overestimation of photosynthesis rates or an underestimation of CO_2 losses following crop and soil respirations. Available data related to crop growth and soil characteristics, however, was not sufficient to support any of these hypotheses.

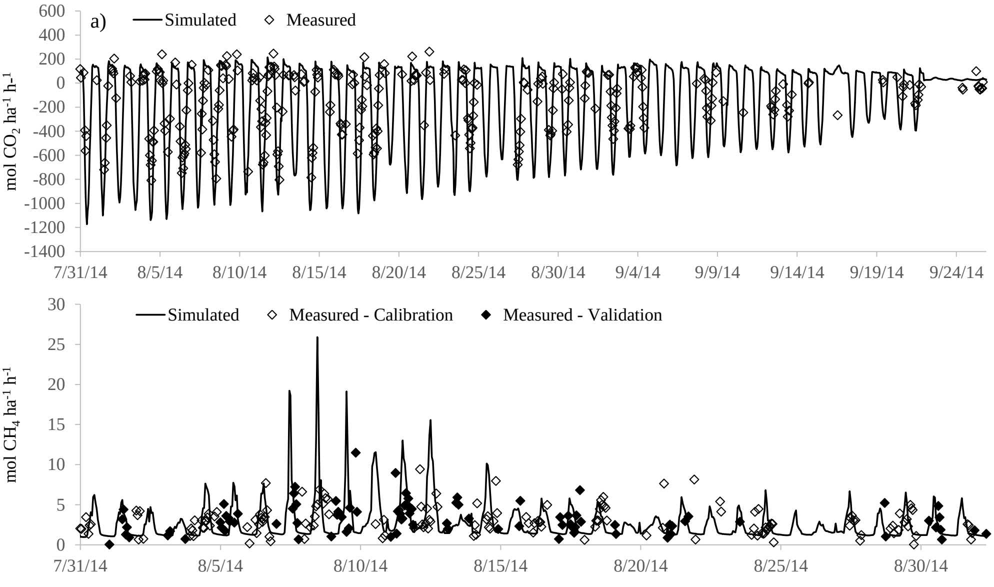


Figure 4. Comparison between simulated and measured emission of CO_2 and CH_4. a: CO_2 emission from 07/31/14 until harvest, negative values indicate a net C sequestration by the cropping system; b: CH_4 emission from 07/31/14 until the end of flooding (09/01/14), data are split between calibration and validation datasets.

5.4.3. Alternate fertilization strategies: crop productivity and environmental impacts

Results of ANOVA quantifying the influence of the levels of applied N and top dressing fertilization strategy on yield, CH_4 and N_2O emissions and N leaching are shown in Table 2; Figure 5 displays average values and standard deviations of such variables simulated for each level of the studied factors. A synthetic overview of the rice cropping system (Gaggiano, 2014) performance in terms of productivity and environmental impacts for each combination factor × level is shown in Figure 6. When considering yield as the dependent variable, low amount of applied N significantly affects cropping system performance (Figure 5a): in this situation, rice production is halved than with medium and high levels of applied N fertilizers. The absence of significant differences between medium and high levels of N suggests that the average amount of fertilizer spread in Northern Italian rice system is near optimal for crop productivity, and that increasing fertilization rates would have involved N luxury consumption by the crop. Processes related to luxury consumption not accounted for in the current version of the MS (such as crop resistance to lodging and diseases) may affect crop productivity and yield. No significant differences were detected between two and three top dressing fertilizations (Figure 5e); nevertheless, a slightly higher yield was simulated with three events both at low and medium N levels (Figures 6a and 6b), due to an increased N uptake. On the contrary, at high N levels the intensified uptake following three top dressings favored structural growth over the accumulation of carbohydrate reserves in stems during vegetative phase, and reduced remobilization of such reserves for grain filling and yield (Figure 6c). Cumulated emissions of CH_4 do not significantly vary across low, medium and high fertilization levels (Figure 5b); however, the slight increase of simulated emission following an increase of applied N may be explained by the higher growth rates of crop, which reaches higher values of LAI, RLD and root biomass. Regardless the fertilization level, CH_4 emission is reduced by three top dressings (Figure 5f), since the presence of nitrate promotes denitrification, which is energetically more favorable compared to methanogenesis and some N compounds produced during denitrification have a direct inhibitory effect on methanogenesis (Klüber and Conrad, 1998). In any case, the extent of the modulation of CH_4 emission appears limited across the treatments: it is likely that factors other than N fertilization, e.g., water management (Li et al., 2005), have a major effect on CH_4 production and transport through the cropping system. N leaching resulted strongly dependent both on the amount of applied N and the splitting of fertilization (Figures 5c and 5g): the higher the applied N, the more N is leached, but this drawback can be partially counterbalanced by splitting fertilization with an additional top dressing. According to simulation results, most of N leaching occurs at the end of rooting drought, especially when fertilizer is top dressed only twice. This is due to the combined simulation of crop N uptake in early growth, soil microbial processes and water dynamics: up to the second fully expanded leaf the main source of nutrients comes from seed reserves (Stansel, 1975, Hoshikawa, 1993), and no N uptake is simulated; after this period, however, N uptake is limited by the development of root system and the low crop biomass, which makes N concentration in plant tissues rapidly reaching the maximum allowed. In such situation, part of the N incorporated at sowing remains in soil during rooting drought, when it is rapidly oxidized to nitrate, which is subject to leaching at the following flooding. N fertilization level produces significant differences ($F = 13.799$; $p < 0.1$) in N_2O cumulated emissions (Figure 5d): N_2O simulated emission is in line with literature values (Akiyama et al., 2005) and increases with fertilization rates, due to their effect in promoting nitrification and denitrification processes. Low N amount in three top dressings lead to a lower emission compared to two, whereas the opposite emerged with high N fertilization (Figures 6a and 6c). N_2O emission always highlights spikes following N fertilizations, but different processes may explain such non-linearity in MS response: with low fertilization level, two top dressings induce higher N concentrations in soil compared to three, thus promoting higher denitrification rates; on the other hand, this effect is counterbalanced at high fertilization rates by the increased leaching with two top dressings compared to three.

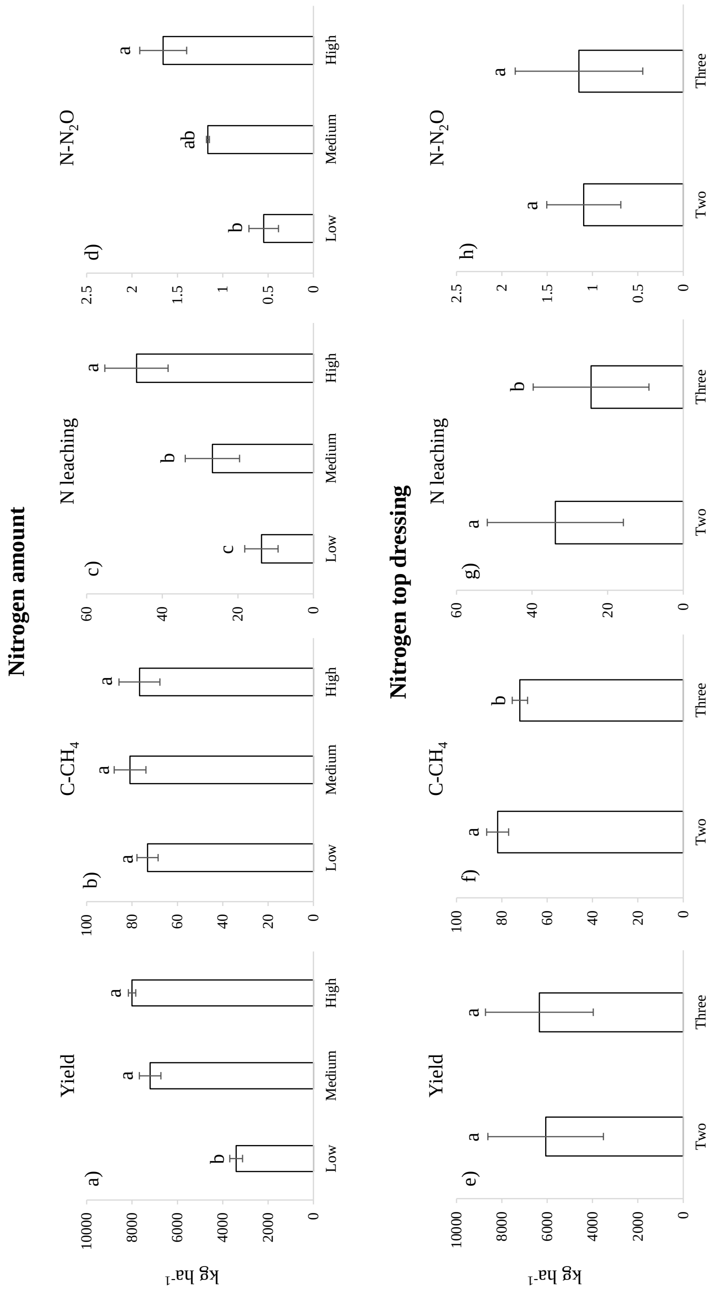


Figure 5. Average values of yield, cumulated C-CH_4 and N-N_2O emissions and N leaching as a function of level of applied N (a-d) and number of top dressing fertilizations (e-h); all units are kg ha^{-1}. Error bars represent the standard deviation of simulated values. Average values are ranked according to Newman-Keuls post hoc test.

Table 2. ANOVA results: main effects of N amount and N top dressing (independent variables) on yield, CH_4 emission, N leaching and N_2O emission.

Variable	N amount (DF =2)		N top dressing (DF=1)	
	F	Pr > F	F	Pr > F
Yield	110.413	0.009	1.075	0.409
C-CH4	6.241	0.138	29.635	0.032
N leaching	135.837	0.007	32.574	0.029
N-N2O	13.799	0.068	0.094	0.788

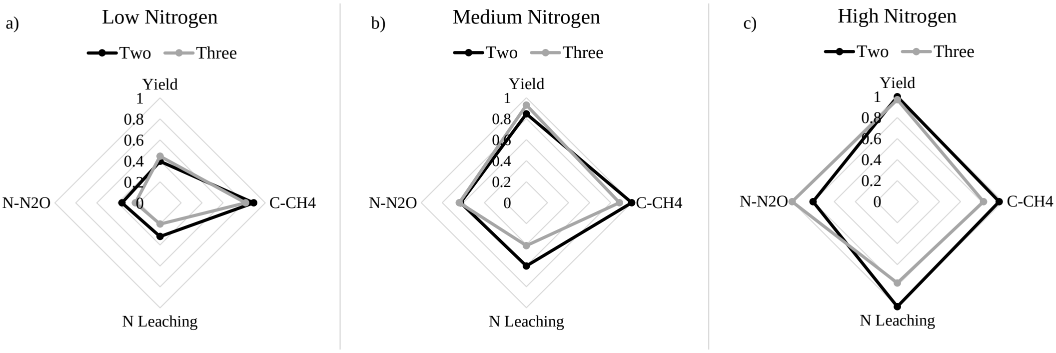


Figure 6. Synopsis of rice cropping system performance in explored conditions. a: low nitrogen; b: medium nitrogen; c: high nitrogen management. Each variable is represented as a fraction of the maximum value of the variable itself recorded in all experiments. "Two" and "Three" refer to the number of top dressing fertilizations performed.

5.5. Concluding remarks

The development of the MS took advantage from existing software components explicitly designed according to the guidelines of BioMA framework to be easily used, composed and extended. The modular development of the MS favours the substitution of implemented models with alternate approaches, simplifying maintenance and further developments. The integration of available models for the simulation of plant diseases (Bregaglio and Donatelli, 2015) and pre-harvest grain quality (Cappelli et al., 2014) appears as the next goal in the development of the MS, which aims at describing multiple aspects of the rice cropping system and their mutual interactions. The suitability of the MS to simulate rice growth dynamics and the emission of CH_4 and CO_2 encourage its adoption as a supporting tool, even if more comprehensive datasets are needed to perform an in-depth assessment of the agreement between observations and simulations. As a research tool, indeed, the MS demonstrated to be effective to perform *in-silico* experiments to test the impact of alternate agronomic strategies on cropping system productivity and environmental impacts. In this context, future works will involve an extensive exploration of the genotype × environment × management interactions in determining rice yield and environmental drawbacks of agricultural activity.

5.6. Appendix A

Parameters values defined via GUI.

Domain	Process/Sub-domain	Parameter (GUI name)	Value	Units
Crop	Phenology	TSUM_em	25	°C-d
		TSUM1	1150	°C-d
		TSUM2	550	°C-d
		Tbase	10	°C
		Topt	24	°C
		Tmax	34	°C
		MaxHeight	60	cm
	Photosynthesis	Tbase	13	°C
		Topt	24	°C
		Tmax	32	°C
		AMAX	23	kg ha-1 h-1
	Partitioning and LAI	SLA em	23	m2 kg-1
		SLA till	17	m2 kg-1
		SPAN	33	day
		RipL0	0.6	kg kg-1
	N uptake and response	GreenwoodBase	2.1	unitless
		GreenwoodExp	0.36	unitless
		EarlyCriticalN	2.5	%
	Aerechyma gas transport	NtillersMaturity	3	tillers plant-1
		PlantDensity	101	plants m-2
		Root-shootConductance	1.00E-05	m3 gas m-2 tiller min-1
Soil	Humus	C/N	10	unitless
		DecoCoeff	0.0256	year-1
		IsohumicCoeffSOM	0.2	unitless
	Roots	RhizoThick	0.7	mm
		RLDextCoeff	-0.06	unitless
	Microbial activity	C_UseEfficiency	0.5	unitless
		Methanogenesis_Acetate	0.1	mol acceptor m-3 water h-1
		Methanogenesis_H2	0.2	mol acceptor m-3 water h-1
		CH4_O2	85	mol acceptor m-3 water h-1
	Q10	AeroMinSOM	2.85	unitless
		AnaeroMinSOM	2.85	unitless
		CH4_Prod	3	unitless
		CH4_Ox	2	unitless
		Nitrification	2	unitless
		Denitrification	2	unitless
		Respiration	4.6	unitless
Initialization	Layer 0	Humus C	18000	kg ha-1 h-1
	Pool Layer 0	Carbon content	1500	kg ha-1
		C/N	30	unitless
		DecompCoeff	0.01	day-1
	Layer 1	Humus C	18000	kg ha-1 h-1
	Layer 2	Humus C	16000	kg ha-1 h-1

GENERAL DISCUSSION AND PERSPECTIVES

6.1. Specific objectives

Specific objectives of this doctorate were:

- The extension of the software component collecting approaches to simulate crop growth and development (UNIMI.CropML) to increase the adherence of crop models to the rice system.
- The definition of a new component (UNIMI.CRONO) collecting models for carbon and nitrogen dynamics in soil, with special focus on the biological and physical processes leading to GHGs emission.
- The development of a modelling solution targeting the simulation of rice cropping system, suitable to assess system’s performance in terms of productivity and environmental impacts in different climatic and management scenarios.

The first objective involved different tasks, documented throughout this thesis. The first step was focused on the development of an improved version of the generic WOFOST model (presented in Chapter 2), to reduce model complexity while enhancing the capability of its integration with advanced tools, such as those for sensitivity analysis and automatic calibration. New functions were developed to describe the dependence of key variables and parameters to air temperature and crop phenology, and canopy representation was improved. This activity was crucial for the progress of the work, providing a crop model which resulted coherent with the requirements of the modelling solution, such as the need of a model based on gross photosynthesis to account for CO_2 losses associated with respiration of above- and belowground organs. Moreover, the reduction of model parameters and the identification via sensitivity analysis of the most important ones allowed to expose few, relevant and biologically meaningful crop parameters in the graphical user interface of the solution, thus simplifying the configuration of simulation environment. The adherence of the model to the actual rice crop was further improved with the definition of a model to simulate carbohydrate redistribution during grain filling (see Chapter 3), a process with a deep influence on rice yields modulated by nitrogen and water availability to the crop. The inclusion of this module in the crop model allows to explain a higher ratio of yield variability among years and increases the suitability of the crop model as a tool for optimizing fertilizer distribution and irrigation. Before this doctorate, the component UNIMI.CropML did not provide any algorithm to simulate the constraints to crop growth related to nitrogen availability and uptake. This gap was filled with the extension of the component documented in Chapter 5, which led to the definition of UNIMI.CropML_NL, collecting approaches to estimate crop nitrogen demand and the degree of nitrogen stress or luxury consumption sensed by the crop. This was a key aspect while integrating crop and soil models within the modelling solution, in order to account for their mutual interactions: soil nitrogen status directly affects growth dynamics of the crop, which in turn modulate soil biological processes via the exudation of organic compounds and release of oxygen in the rhizosphere.

The second objective was achieved with the collection, within a dedicated component (i.e., UNIMI.CRONO), of existing models describing organic matter decomposition, biological mediated reactions in aerobic and anaerobic conditions, transport of molecules in the gaseous and liquid phase, soil-plant interactions at root level and responses to agricultural management practices. This activity is documented in Chapter 4, as well as the sensitivity analysis of the models implemented. Sensitivity analysis was carried out to investigate the effects of the variation of input and parameters on GHGs emission under the conditions characterizing rice paddy fields, and allowed to gain insight into the complex interactions among biological and physical components of the system. UNIMI.CRONO constitutes, in framework of the doctorate, the fundamental piece for the simulation of belowground processes; at the same time it provides the modelling community with a software component which can be easily extended and integrated with the emerging outcomes in soil science.

The path leading to the achievement of the third objective was basically a process of composition (described in Chapter 5): existing software units were combined with those developed during the doctorate, linking models for crop growth and development, biogeochemistry, soil water and temperature dynamics, as modulated by meteorology and farmer management choices. The aim was to provide a tool for the integrated assessment of rice cropping system performance, accounting for crop productivity and some externalities (e.g., nitrate leaching, GHGs emission) deriving from agricultural activity in different climatic and management scenarios. The strength of the approach adopted, compared to current realizations, lays in the modularity of the developed system, fostering maintenance and further development. For example, whenever an implemented sub model turns out to be inaccurate or unsuitable for the simulation of a specific process, it can be easily replaced with alternate models. Similarly, if new functionality is needed, the modelling solution can be extended in a straightforward way by adding new models to existing components and plugging them into the solution.

6 .2. Development achieved

The realization of this work required the adoption of the state of the art of software technology applied to agricultural system modelling in order to manage the complexity characterizing the agro-ecosystem. Component-oriented programming was the unavoidable choice to isolate knowledge in discrete, extensible and interchangeable software units; models were implemented with fine granularity, reflecting the most common level of detail at which research outcomes are typically produced (i.e., process level). This allowed to organize the whole work around a solid, trusted base of existing models and tools, concretely exploring the possibilities of reuse and extension made available by recent advances in the field of environmental modelling. The work itself is in turn characterized by reusability and extendibility, two features claimed as major objectives by the international modelling community. This is not a minor issue, since model development has long been limited by technological bottlenecks precluding model reuse: on the contrary, the design of the current work potentially fosters further development with the addition/substitution of implemented approaches, to reduce the untapped potential of cropping system models. Compared to other realizations in agricultural system modelling, the modelling solution proposed highlights a higher degree of interconnection among simulated domains; such connections can be extended as well as the software components collecting models for soil, water, crop and agronomic practices. The modular nature of both the components and the solution decidedly simplifies code maintenance, and will likely trigger model development via the hybridization of existing models in ways not explored during this doctorate. Even if building modelling solutions is considered per se science, the contribution of the present work is not limited to this aspect: some inconsistencies of the WOFOST model in the representation of the underlying system were solved, as well as constraints limiting its operational use. Moreover, the new model for carbohydrate redistribution during rice grain filling is a step towards reducing the gap between scientific knowledge and its realization in simulation models, contributing to improve crop models' reliability under a variety of conditions.

6 .2. Future perspectives

The current state of development of both the software components and the modelling solution to simulate rice cropping system certainly has not reached its final stage. This, however, does not represent a weakness of the present work: extendibility was built into the original design of the project, in order to promote long term evolution of the solution and the models implemented. Exploiting this feature will allow in future to broaden the application domain of this work. In this context, the integration of available models for the simulation of plant diseases and pre-harvest grain quality appears as the next goal in the development of the solution, which is aimed at describing multiple aspects of the rice cropping system and their mutual interactions.

Regarding operational purposes, this work has so far only scratched the surface. Future activities will involve the design of agricultural management strategies optimized to achieve satisfactory yields with the least water and fertilizer input and/or environmental impacts. Moreover, large area simulations will allow the extensive exploration of the genotype × environment × management interactions in determining rice yield and environmental drawbacks of agricultural activity at global scale under current and future scenarios.

PUBLICATIONS DURING THE DOCTORAL WORK

Submitted

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