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ABSTRACT

Treated wastewater contains vital crop nutrients and offers the possibility for not only irrigation but also fertilization from a renewable source. The feasibility of replacing conventional chemical fertilizers with wastewater reuse is investigated, focusing on the implications of coupling irrigation and fertilization. We consider a multi-objective dynamic optimization problem of crop irrigation and fertigation with treated wastewater, with the objectives of maximizing crop production and minimizing environmental costs. A double modelling method is proposed that relies on both a modern complex crop model – the simulation model – and a low-order dynamical systems model – the control model – to solve efficiently the optimization problem, whilst maintaining a detailed representation of the system of study. Through a case study, we show that it is possible to achieve high levels of crop production. The maximum nutrient concentration of the reclaimed waters $C_{N\,\max}$ is a key parameter of the system performance: when $C_{N\,\max}$ is high enough, it is possible to substitute entirely conventional fertilization for irrigation with wastewater. However, when $C_{N\,\max}$ is small, our results highlight that meeting crop needs would require excessive irrigation, with the added risk of dilution of the nutrients already present in soil. We find that there is a maximum amount of nutrients that can be delivered efficiently to the soil-crop system and identify the conditions when wastewater irrigation is only be capable of providing a portion of the crop needs and should be complimented with other sources of fertilization. The double modeling method and the control model provide a means to estimate the key quantities to determine the best strategy to adopt for wastewater fertilization, as well as to obtain efficient and simple controls, that could be applied in practice.

1. Introduction

Irrigation plays a vital role towards guaranteeing food security, in particular in the arid and semi arid regions of the world, where natural resources of freshwater are increasingly scarce. In response to these issues, the reuse of treated wastewater in agriculture has been considered and studied up to now as a means to benefit from an alternative water resource. Nonetheless, wastewater contains nutrients vital for crop growth and therefore reclaimed waters have the potential to become a renewable source of fertilizers (Ait-Mouheb et al., 2018; Hao et al., 2022). This is particularly interesting as the current industrial production of crop nutrients is a major concern, with life cycle analysis revealing that fertilization represents one of the main contributions to the greenhouse gas emissions of crop production (Azeb et al., 2020). Most notably, the production of N fertilizers via the Haber-Bosch process requires large quantities of natural gas and is responsible for up to 2% of the worlds' energy consumption (Erisman et al., 2008).

Crop water and nutrient needs are fundamentally dynamic, changing throughout plant life, and therefore, to maximize crop growth, it is important to control irrigation and fertilization dynamically, according to crop needs and perturbations due to weather. The optimal use of reclaimed waters for agriculture would therefore require the dynamic adaptation of wastewater treatment, in terms of nutrient quality and quantity. Recently, studies have shown that it is indeed possible to operate a wastewater treatment plant to produce effluent of time-varying quality (Neto et al., 2021). Moreover, a new approach has been proposed to achieve even better recovery of nutrients, and transform treatment plants into wastewater resources recovery facilities (Aichouche, 2021; Miller-Robbie et al., 2013). It is still a challenge to manage treatment systems to retain nutrients while guaranteeing a water free of pathogens and micro-pollutants, but

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technologies are being developed, such as membrane filtration systems, precisely allowing to deliver safe water (Judd, 2010).

The specificity of considering wastewater irrigation for fertilization is that water and nutrient inputs to the soil-crop system become coupled, even if it is considered that the concentration of nutrients in wastewater can be controlled independently of the irrigation flow rate. Indeed, adding nutrients to the soil in this manner requires adding water and therefore providing sufficient nutrition to the crop could require more water than needed. Excessive irrigation would not only waste precious water but would also lead to drainage and loss of nutrients through leaching, which would be detrimental to crop growth. Furthermore, crop water and nutrient requirements are not the same, with inputs required at different periods of the growth cycle and thus, controlling wastewater irrigation only considering crop water requirements, could lead to a missed opportunity to fertilize efficiently.

The focus here is on nitrogen (N) fertilization, especially considering that nitrogen is one of the most important nutrients for crops and currently, its impact and dynamics in the soil-crop system are the most well understood. As crops absorb nitrogen present in soil water, uptake depends on the N concentration in soil water, with the possibility of a deficit if the concentration is too low. An important issue here is that N concentration in the soil water will change with water inputs and losses, with either dilution if the soil water accumulates or increase of concentration if there is a reduction in soil water. Therefore, adding water with a low concentration of nitrogen could result in diluting the nitrogen already present in the soil and as a consequence, such an input would actually reduce N uptake. The challenge of fertilization with wastewater reuse thus resides in managing the impact of irrigation on the available nutrients for the crop, especially considering the low concentrations of N reported in wastewater.

When considering the optimization of a cropping system, a variety of criteria, often representing conflicting interests, need to be optimized. On one hand, maximizing crop production requires high irrigation and fertilization rates but on the other hand, costs of farming practices should be minimized, calling for reduced inputs. In addition, with the increasing scarcity of water resources and the limited quantity of N in wastewater, it is key to irrigate and fertilize efficiently and the total amount of water and N used should be minimized. The environmental impact of agriculture should also be considered, in particular in the case of N fertilization as the leaching of nitrogen to groundwater represents an important source of pollution (de Vries et al., 2021). Thus, there is a need for decision support tools that allow to explore the trade-offs between different objectives, in order to provide information to practitioners.

In this work, irrigation with reclaimed waters is studied with the objective of understanding how to benefit not only from an extra water resource but also from the nutrients present in wastewater for fertilization. The aim is to explore to what extent wastewater irrigation can supplement or replace conventional practices based on the use of chemical fertilizers. We also investigated how this might be done in practice, considering the problems arising from the coupling of irrigation and fertilization. To this end, using crop models and techniques from dynamic optimization, efficient irrigation and fertilization strategies are determined by solving multi-objective optimal control problems. A specific approach, the double modeling method, is developed to deal with the challenge of solving dynamic optimization problems for a complex crop model.

The outline of the article is as follows: section 2 presents the double modeling method; section 3 details the multi-objective dynamic optimization problem considered; section 4 presents a case study of wastewater reuse and finally section 5 gives conclusions.

2. Double Modeling Method

A lot of knowledge has been embedded in state-of-the-art crop models since their early development in the 1980s, and they now take into account all aspects of a cropping system. These models simulate, on a daily basis, crop growth as influenced by interactions between plant, soil, weather and farming practices. They have been validated for a wide range of crops and climates, and therefore are the preferred tools to investigate the optimization of management strategies. However, these are generally computer models with a complex mathematical structure that makes it difficult to directly apply dynamic programming techniques (Schütze and Schmitz, 2010). Moreover, generic optimization algorithms will also have difficulties in finding the global optimum of management strategies at a fine time step.

In the context of dynamic optimization, decision models do not necessarily need to be as detailed as models developed for scientific purposes and the understanding of internal processes. Simple models offer a number of practical advantages, in terms of computational time and guarantee of optimality. With models expressed as dynamical systems, it is possible to leverage mathematical properties to design specific methods for a faster and more efficient resolution of optimization and control problems. Furthermore, soil and crop monitoring remains challenging and costly to implement, often resulting in relatively poor online measurements. The problem studied here is characterized by a few number of decision variables, and with limited input and poor outputs, simple models are often better suited.

As a result, studies on determining efficient irrigation and fertigation strategies have been mainly done according to one of the following approaches: (i) applying a generic numerical optimization procedure to a complex crop model (Brown et al., 2010; Schütze et al., 2011; Cheviron et al., 2016; Linker et al., 2016) or (ii) by using a dedicated dynamic programming approach on a simple crop model (Bright, 1986; Sunantara and Ramírez, 1997; Schütze and Schmitz, 2010; Kalboussi et al., 2019).

We propose here a hybrid approach, the double modelling method, that takes advantage of both types of models to derive efficient control laws for a complex system. Double modelling is a term already used to refer to multiscale modelling, for the representation and understanding of the emergence of macroscopic laws (Lesne, 2006). However, double modelling has been very rarely considered with the primary objective of designing control strategies, apart from a few particular studies (Hassam et al., 2015; Barbier et al., 2016). The present work goes further towards the integration of both models, and we show how the double modelling method can be an iterative process, going back and forth between models to compute controls.

It has been shown, for some time now, that relatively simple models can reproduce complex real world systems, albeit with a limited domain of validity (Haddon et al., 2020; Pérémé et al., 2023; Haddon et al., 2023). Similarly, we have found that it is also possible to replicate a simulation of a detailed complex model with a simplified model. Indeed, we can calibrate the parameters of a simple model to get a good agreement with specific outputs of a complex model, for a given scenario (i.e. a fixed set of parameters of the complex model). This is the key observation underpinning the double modelling method and allows us link both models.

When considering the use of a model for optimization, there is in general an important trade off between model complexity and practical resolution of the optimization problem. Instead, the double modeling method proposes a means to benefit from the specific advantages of two different types of models in order to compute efficiently an optimum, without sacrificing the quality of representation of the system of study. On one hand, a complex model, the simulation model, is used to make detailed simulations as well as evaluate solutions optimization objectives precisely. On the other hand, a simple model, the control model, is used for an efficient resolution of the optimization problem.

An important aspect of the approach presented here is that the control model is not only intended as a computational device but is also meant to provide insights into the optimal control problem. Indeed, designing a control model that is physically meaningful with relevant variables representing key elements of the system, allows to qualitatively analyze the relation between the computed solutions and system components. Therefore, the represented processes are selected based on the optimization objectives and decision variables, in order to model the impact of controls and thus understand the input-output behavior of the system. In addition, with the objective of efficiently solving dynamic optimization problems, the selection of an adequate mathematical structure is essential and justifies the choice of using a system of ordinary differential equations (ODE).

In practice, the first step of the double modelling method is to design a control model tailored to the studied problem. Then the control model parameters are calibrated from a reference simulation of the complex model in order to approximate as best as possible the simulation model for the chosen scenario. Next, the control model is used to compute a control by solving a dynamic optimization problem. With the simulation model, the computed control is then evaluated in a more realistic setting, which also allows to assess the quality of the control model. Indeed, if there is still a good agreement between models with the computed control and for the same set of parameters calibrated with the reference simulation, then this demonstrates the quality of the control model and of its calibration. However, if there is an important difference between models, either the parameter estimation is restarted with a new reference simulation based on the computed control or the control model is modified to better fit the simulation model.

As a result, the double modelling method is (i) an iterative approach to find a locally optimal control but also (ii) a method to obtain a model, approximating locally the simulation model and suited for the application of tools from control theory. The main steps of the double modelling method are illustrated in Figure 1.

2.1. Simulation Model

The simulation model considered here is STICS (Brisson et al., 2003, 2009), a generic and robust crop model that is developed and used by an international community of researchers. It is based on a mechanistic approach and centered around the water, nitrogen and carbon balances of the cropping system, with a detailed representation of the soil and crop. This complex computer model has over 600 parameters and options to simulate a variety of farming systems and has been validated for a diversity of crops in different climatic conditions. STICS has been used in a wide range

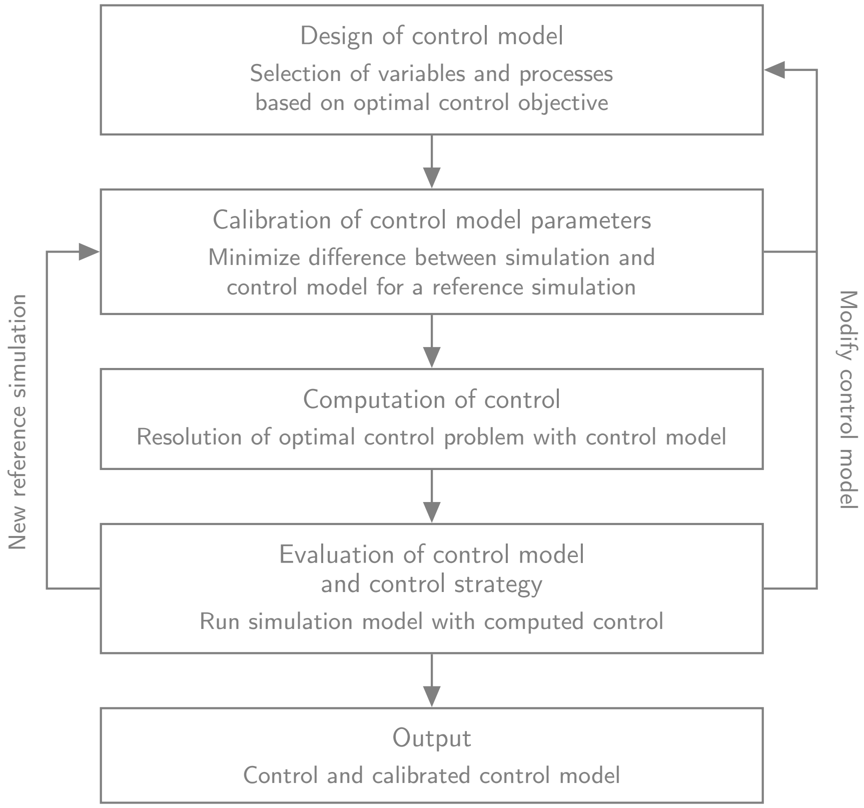

Figure 1: Double modelling Method

of studies, such as the effects on cropping systems of climate change (Leclère et al., 2013) or biotic stresses, and has also been used for recommendations of farming practices such as the application of nitrogen fertilizers (Houlès et al., 2004).

2.2. Design of control model

For the problem studied here, the control model must focus on the water and nitrogen dynamics of the soil-crop system, with variables representing soil moisture and soil N to follow the impact of controls. Concerning the objectives, crop biomass needs to be computed as a measure of production and to estimate the environmental impact of fertigation, N leaching should be taken into account.

The model designed here is adapted from a continuous time dynamical system model developed by Pelak et al. (Pelak et al., 2017), and a similar model was recently validated in wastewater irrigation experiments (Haddon et al., 2023). This model is based on concepts present in the AquaCrop model (Steduto et al., 2009) and features a spatially homogeneous representation of the crop-soil system. The crop is represented by the above-ground dry biomass per unit area B [kg m^{-2}] and the canopy cover C [m^2 m^{-2}], which is the fraction of ground covered by the crop. The soil variables are the vertically averaged soil water content relative to total soil volume S [m^3 m^{-3}] and soil nitrogen mass per unit area N [g m^{-2}].

In the control model, the soil variables are computed from balance equations and for the soil water, the model considers rain R and irrigation I as inputs and accounts for losses due to crop transpiration T, evaporation E and leakage Q,

$$z\dot{S}(t) = R(t) + I(t) - T(t, C, S) - E(t, C, S) - Q(S) \tag{1}$$

The depth of soil z over which the water balance is computed is taken here as the maximum rooting depth.

Transpiration and evaporation follow the dual crop coefficient approach, originated in the FAO methods (Allen et al., 1998), and are both computed from the reference evapotranspiration $ET_0(t)$, which is the major weather input that combines solar radiation, temperature, wind and vapor pressure. The transpiration rate is

$$T(t,S,C) = K_{cb} ET_0(t) K_s(S) C \tag{2}$$

where $K_s(S)$ is the water stress function.

$$K_s(S) = \begin{cases} 0 & \text{if } S < S_w \\ \frac{S-S_w}{S_*-S_w} & \text{if } S_w \leq S < S_* \\ 1 & \text{if } S^* \leq S \end{cases} \tag{3}$$

The evaporation rate is

$$E(t,C,S) = K_{ec} ET_0(t) K_r(S)(1-C) \tag{4}$$

with the evaporation reduction function $K_r(S)$.

$$K_r(S) = \begin{cases} 0 & \text{if } S < S_h \\ \frac{S-S_h}{1-S_h} & \text{if } S_h \leq S \end{cases} \tag{5}$$

The various parameters are listed in table 2.2.

The drainage dynamics are modified from those in (Pelak et al., 2017) to better follow the behavior in STICS and a tipping bucket approach is considered.

$$Q(S) = \begin{cases} 0 & \text{if } S < S_{fc} \\ k_{sat} \frac{S-S_{fc}}{S_{sat}-S_{fc}} & \text{if } S \geq S_{fc} \end{cases} \tag{6}$$

The soil nitrogen balance considers losses due to plant uptake U and leaching L, as well as input from fertilization F_N,

$$\dot{N} = F_N(t) - U(t,C,S,N) - L(S,N). \tag{7}$$

Plant nitrogen uptake is the product of transpiration and a nitrogen uptake limitation function

$$K_N(S,N) = \min\left(\frac{N}{zS}, \eta_c\right), \tag{8}$$

which models crop growth reduction in case of low soil nitrogen concentration. The nitrogen leaching depends on the leakage rate and the nitrogen soil concentration $L(S,N) = a_N \frac{N}{zS} Q(S)$.

The canopy cover follows a logistic growth in (Pelak et al., 2017) however it appears that the formulation used therein leads to dynamics that are very sensitive to water and nitrogen stress, as well as time variations of ET_0 when using values that are computed from daily weather data. Instead, a modified equation is used here: we replace the constant metabolic limitation parameter with water and N stress and introduce a parameter to fix the maximum canopy cover, similarly to what is done in AquaCrop,

$$\dot{C} = r_c(t,S,N)\, C \left(1 - \frac{C}{C_{\max}}\right) - M(t,C). \tag{9}$$

Limitations due to water and N stresses and ET_0 are only present in the growth rate,

$$r_c(t,S,N) = r_G K_N(S,N) K_s(S)\, K_{cb}\, ET_0(t) \tag{10}$$

Leaf senescence at the end of the growth cycle is accounted for with

$$M(t,C) = \begin{cases} 0 & \text{if } t \leq t_{sen} \\ \gamma(t-t_{sen})C^2 & \text{if } t_{sen} < t \end{cases} \tag{11}$$

Table 1
Control model parameters

	Description	Calibration Method
z	Soil depth	From STICS
S_h	Hygroscopic point	From references
S_w	Wilting point	From STICS
S^*	Point of incipient stomatal closure	From STICS
S_{fc}	Field Capacity	From STICS
S_{sat}	Saturation	From references
k_{sat}	Saturated hydraulic conductivity	From references
K_{cb}	Transpiration crop coefficient	Minimization of error with STICS
K_{ec}	Evaporation crop coefficient	From references
η_c	Maximum nitrogen concentration taken up	Minimization of error with STICS
a_N	Leaching fraction of N	Minimization of error with STICS
r_G	Canopy growth rate	Minimization of error with STICS
$C_{\max}$	Maximum canopy cover	From STICS
t_{sen}	Date of onset of leaf senescence	Minimization of error with STICS
γ	Slope of increase of senescence after t_{sen}	From reference
W^*	Normalized daily water productivity	Minimization of error with STICS
ET^*	Evapotranspiration stress level	Minimization of error with STICS

The model follows the formalism of AquaCrop with accumulation of biomass proportional to crop transpiration, which allows the representation of growth limitations in case of water stress.

$$\dot{B} = W^* \frac{K_N(S,N)}{\eta_c} K_s(S)\, K_{cb}\, C\, \min\left(\frac{ET_0(t)}{ET^*}, 1\right) \tag{12}$$

As in (Pelak et al., 2017), growth is also reduced in the case of nitrogen shortage. Finally, an extra limitation due to weather is considered here to represent slower growth in case of lower temperatures or less radiation, and for this reference evapotranspiration is used.

2.3. Calibration of control model parameters

First, the link between the simulation and control model must be clearly established, in order to compare the variables, processes and outputs of both models and thus further help to understand the computed control. This also allows the interpretation of simulations of the two models together and will be particularly helpful to guide the calibration of the control model parameters.

A local sensitivity analysis was carried out by computing the sensitivity of the model variables due to the variation of each parameter alone. Sensitivity of the optimization objectives and constraints also give important information on which parameters must be estimated precisely. This analysis also reveals which variables are impacted by which parameter and can help in the calibration process to understand the parameters that must be adjusted to reduce errors on a variable. From this, the parameters that must be calibrated are selected (table 2.2) and for the less sensitive parameters, values from literature are used, such as from (Pelak et al., 2017). For some parameters, that have an important mechanistic interpretation, it is possible to use directly a corresponding parameter from the simulation model, such as some parameters representing soil properties (see Annex).

For the other parameters that have been selected, calibration is carried out by minimizing the difference between models with standard optimization algorithms. Several error functions are possible, either the difference for one variable or a (weighted) sum of errors over several variables. The standard root-mean-square error (RMSE) is used when only one variable is considered,

$$RMSE = \sqrt{\frac{1}{N_t}\sum_{i=1}^{N_t}\left(y_i^C - y_i^S\right)^2} \tag{13}$$

Table 2
Control model variables and functions

	Description	Unit
B	Above-ground dry biomass per unit area	kg m^{-2}
C	Canopy cover	m^2 m^{-2}
E	Evaporation	mm d^{-1}
ET_0	Evapotranspiration	mm d^{-1}
F_N	Fertilization rate	kg ha^{-1} d^{-1}
I	Irrigation rate	mm d^{-1}
K_N	N uptake limitation function	g m^{-3}
K_r	Evaporation reduction function	—
K_S	Crop water stress function	—
L	Leaching rate	g m^{-2} d^{-1}
M	Leaf senescence rate	d^{-1}
N	Soil nitrogen mass per unit area	g m^{-2}
Q	Leakage	mm d^{-1}
R	Rain	mm d^{-1}
r_c	Canopy cover growth rate	d^{-1}
S	Vertically averaged soil water content relative to total soil volume	m^3 m^{-3}
T	Crop transpiration	mm d^{-1}
U	Crop nitrogen uptake	g m^{-2} d^{-1}

Table 3
Optimization problem variables and parameters

	Description	Unit
F_N	Fertilization rate	kg ha^{-1} d^{-1}
F_{N0}	Initial fertilization	kg ha^{-1}
$\overline{F}$	Total N added through irrigation	kg ha^{-1}
$\mathcal{F}$	Total fertilization	kg ha^{-1}
I	Irrigation rate	mm d^{-1}
$I_{\max}$	Maximum irrigation rate	mm d^{-1}
$C_{N\max}$	Maximum N concentration of irrigation water	g m^{-3}
η_I	N concentration of irrigation water	g m^{-3}

with N_t the number of time steps over which the error is computed and y_i^S and y_i^C are respectively the values of the variable for the simulation model and control model, at time step i. When considering the errors on several variables, a sum of relative RMSE is used, which is the RMSE normalized with the mean of the simulated model variable:

$$relRMSE = \frac{RMSE}{\frac{1}{N_t}\sum_{i=1}^{N_t} y_i^S} \tag{14}$$

The next task is to select the reference simulation of the complex model that will be used to compare both models. It is important to consider a case that covers a range of operating conditions in order to capture, in the control model, the essential behavior relevant to the optimal control problem. For instance, the water and nitrogen dynamics play an essential role in the problem at hand and therefore the reference simulation should have periods where the crop experiences water and nitrogen stresses to guarantee that these effects are represented in the control model.

The parameter identification is done in several steps, first with the error on a single variable and calibrating only the parameters that impact that variable the most. By iterating in this fashion through all the variables it is possible to get a first estimation of the parameters. However, to get coherent results, it is necessary to conduct a final calibration that considers the error on all control model variables. In addition, to make sure that the control model remains relevant and not just a computational model, attention is paid to the proper fit of processes and internal model indicators such as the water and N stress functions. Furthermore, the partition between the different processes involved are considered and for example the proportions of soil water lost through transpiration, evaporation and leakage should be coherent.

3. Optimal control problem formulation

3.1. Control Variables

The case of a crop irrigated with treated wastewater is considered here supposing that the water flow rate and N concentration of the irrigation water can be controlled. The control variables are the irrigation flow rate I [mm d^{-1}] and nitrogen concentration of irrigation water η_I [g m^{-3}]. Models can be straightforwardly adapted for fertigation by taking the fertilization rate (units of mass per unit surface and per day), as product of irrigation flow rate and N concentration of irrigation water,

$$F_N = I\eta_I. \tag{15}$$

Restrictions are imposed on the controls, with limits $I_{\max}$ to the daily irrigation volume and $C_{N\max}$ to the maximum nitrogen concentration of the irrigation water.

An equivalent formulation is to consider I and F_N as the control variables, with the coupling of controls then imposed through a constraint on the upper bound of fertilization depending on the irrigation flow rate and the maximum N concentration,

$$F_N \leqslant IC_{N\max} \tag{16}$$

This formulation avoids the non-linearity (15) in the dynamics, which are then affine in the control variable, and in practice this leads to a problem that is easier to solve. Moreover, for the dynamic programming approach considered here, the constraint on the set of admissible controls actually reduce the search space, thus leading to a faster resolution.

3.2. Multi-objective dynamic optimization

When considering multi-objective optimization, one approach is to optimize a weighted sum of the considered criteria. By varying the weights, different objectives are preferred and a range of solutions is obtained, the so-called Pareto front, which represents the different compromises to be made. An alternative is to optimize a single criterion and impose upper or lower bound constraints on the other objectives. Then solving the problem for different values of the bounds allows to obtain the relation between the optimized criterion and the constrained objectives, which is essentially the Pareto front. In fact, for finite dimension optimization and under suitable assumptions, there is an equivalence between both formulations and the weights of the former approach can be considered as the Lagrange multipliers associated with the constraints of the latter method (Boyd et al., 2004).

Formulating multi-objective problems as constrained optimization problems is a particularly meaningful approach when certain types of objectives are considered. Indeed, for a criterion representing a cost, this formulation allows to compute a solution for a given cost directly and for example here, it is of interest to impose a budget of N fertilization and optimize the other objectives. Moreover, in the case of an objective function representing an environmental impact, using constraints may be more justified as there are tipping points that must not be exceeded and this can be better represented with an upper bound constraint. For instance, it is vital to avoid compromising the quality of groundwater when it is used for human consumption and therefore the concentration of N in leachate must not exceed the drinking water quality, which gives a clear upper bound to impose.

3.3. Constrained optimization formulation

We consider here the dynamic optimization of wastewater irrigation as the constrained optimal control problem of maximizing crop production under constraints on the cropping system inputs.

Crop yield is the standard measure of crop production and is generally used as the primary objective function to be maximized. In detailed models, such as in STICS for certain crops, yield is computed from crop biomass, through a so-called harvest index, which is a function accounting for the various stresses affecting the harvested biomass of the crop. However, in the model from Pelak et al. (Pelak et al., 2017), yield Y is computed with a constant harvest index h, assuming that the stresses are already accounted for in biomass growth. Then, yield is proportional to the crop biomass

$$Y = hB. \tag{17}$$

This simplification is particularly interesting as maximizing final yield becomes equivalent to maximizing final crop biomass. There is thus no need to compute yield during optimization, thereby eliminating a model variable and improving the efficiency of computations.

Next, efficiency of fertilization is imposed with a constraint on the total amount of nitrogen added by irrigation. Denoting t_0 and t_f the fixed initial and final time and $\overline{F}$ the maximum total mass per unit area of nitrogen allowed, the constraint is

$$\int_{t_0}^{t_f} F_N(t)\, dt \leqslant \overline{F}. \tag{18}$$

With the focus here on the fertilizing benefit of wastewater reuse, the problem of maximizing the final crop biomass with the constraint (18) is solved for a range of values of $\overline{F}$. This allows to represent the optimized crop production as a function of the N budget, which shows the trade-off between fertilization and production.

In order to understand how much water is needed for optimal fertilization, there is no constraint set on the total irrigation volume and the amount of water used is not directly limited. In fact our results will show that the previous constraint (18) already leads to efficient irrigation. Indeed, excessive irrigation can not be optimal as it would result in nitrogen losses through leaching or a decrease of the N concentration due to dilution. Then, increasing the soil water content too much can cause reduced N uptake leading to N stress and slower biomass growth. Therefore, constraining the total N budget limits irrigation as well as N leaching, which is also left unconstrained.

Nonetheless, to check that controls do not lead to groundwater pollution, the N concentration in leachate will be compared to a critical threshold. Following the approach used in (de Vries et al., 2021), the critical nitrate concentration in leachate is set from the WHO drinking water limit of 50 mg NO_3 L^{-1} (Organization et al., 2003), which is also the threshold used in the EU Nitrate directive (Directive, 1991). This can be converted from mg NO_3 L^{-1} to mg N L^{-1}, with the conversion factor $f_{N-NO_3} = 14/62$, to obtain $C_{N crit}$ the critical N concentration in leachate,

$$C_{N crit} = 11.29 \text{ mg N L}^{-1}. \tag{19}$$

Other environmental and health hazards related to the re-use of wastewater are neglected, and it is supposed that they are managed by the wastewater treatment or a multi-barrier approach (World Health Organization, 2006).

For the control model, the crop development process is idealized and for example does not represent the germination process adequately. Moreover, the initial stages of crop life are critical, and they should be optimized with other objectives than those under consideration here. The time interval of optimization is therefore taken from the stages of emergence to maturity, as computed by STICS. The initial conditions for the control model are then taken by converting the values of the corresponding variables of the simulation model.

In summary, the optimal control problem solved is the following.

$$\begin{cases} \text{Maximize} & B(t_f), \\ \text{over all} & (I, F_N) : [t_0, t_f] \to [0, I_{\max}] \times [0, I_{\max} C_{N\max}], \\ \text{such that} & S(\cdot), N(\cdot), C(\cdot) \text{ and } B(\cdot) \text{ satisfy } (1), (7), (9), (12), \\ & F_N(t) \leqslant I(t) C_{N\max} \quad \forall\, t \in [t_0, t_f], \\ & \int_{t_0}^{t_f} F_N(t)\, dt \leqslant \overline{F}. \end{cases} \tag{$\mathrm{P}_{\overline{F}}$}$$

3.4. Numerical resolution

We solve numerically problem ($\mathrm{P}_{\overline{F}}$) with the dynamic programming algorithm implemented in the toolbox BocopHJB (Bonnans et al., 2017). This method computes the value function of the problem, which is the optimal value of the objective as a function of initial conditions and time. Then, from the value function, an optimal control can be computed for any initial condition.

This is particularly interesting in the context of the multi-objective optimization approach used here, which is based on solving problem ($\mathrm{P}_{\overline{F}}$) for a range of the constraint bound $\overline{F} \in [F_1, F_2]$. Indeed, in practice, constraint (18) is implemented by first adding a state variable I_F, representing the accumulated fertilization at time $t \in [t_0, t_f]$,

$$\frac{d}{dt} I_F(t) = F_N(t). \tag{20}$$

Then (18) corresponds to a constraint on the final value of I_F. This can be done for $\overline{F} \in [F_1, F_2]$ by imposing

$$I_F(t_0) = F_2 - \overline{F} \qquad \text{and} \qquad I_F(t_f) \leqslant F_2 \tag{21}$$

In other words, the upper bound of constraint (18) can be changed by varying the initial condition of I_F. Thus, with the numerical method used here, after an initial investment to compute the value function, the range of solutions associated with different values of the constraint bound can be computed rapidly, thereby obtaining the Pareto front.

4. Case Study of Fertilization with Wastewater Reuse

4.1. Description of case study

We now present a case study of the optimization of fertilization through wastewater reuse. The unpredictability of weather has an important impact on agricultural yields and is a serious problem that must be addressed by decision support tools. However, here the focus is understanding the feasibility of fertilization with wastewater and thus the rain and evapotranspiration time-series are considered known in advance to factor out the stochastic nature of weather.

We focus on a modern corn cultivar grown on a loam type soil. We consider field and weather data from 2013 and taken for the city of Gaillac, near Toulouse in the southwest of France (43° 54' 05" N, 1° 53' 57" E). Sowing is on 22 April (day 112 of the year) but the time interval of optimization $[t_0, t_f]$ is taken from the stage of emergence as computed by STICS, which is here 8 May (day 128), until harvest at maturity as computed by STICS, here 4 September (day 247).

The weather series used comprises 270 mm of rain and 646 mm of reference evapotranspiration over the entire growth cycle, with most of the precipitations occurring with heavy rains during the first half of the growing season, keeping the soil water content near field capacity. For the first months, irrigation can lead to N leaching and there are thus limited opportunities to add nitrogen through fertigation. On the other hand, the summer months are drier with little precipitations threatening yield, especially considering the important water needs of corn. This scenario therefore presents difficulties for irrigation and fertilization management in the case of wastewater reuse as water and nitrogen inputs are required at different periods.

4.1.1. Design of experiment

For purposes of comparison with standard practices, use of a typical fertilizer is also considered. It is supposed to be carried out at sowing in a single application of ammonium nitrate, and we denote the corresponding mass of nitrogen per unit area added as F_{N0}. For this type of fertilizer, STICS computes immediate losses during application, which are mainly due to volatilization and microbial immobilization of the ammonium. On the other hand, assuming that the nitrogen in irrigation water is in nitrate form, such losses during fertigation can be neglected and are not accounted for in STICS. Note also that as this initial fertilization is not directly simulated in the control model as it occurs before the initial time of the optimization problem t_0. Instead, F_{N0} is accounted for through the initial condition of soil mineral nitrogen, which is set from the value computed by STICS at time t_0. With the dynamic programming approach used here, the value function is computed for a range of initial conditions and there is thus no need to solve the problem for each initial fertilization.

Several reference simulations associated with different controls were considered for the calibration of the control model, including controls computed by solving the optimal control problem ($\mathrm{P}_{\overline{F}}$) after a first estimation of parameters had been obtained. However, the best results were achieved from a scenario leading to water and N stresses, that limit crop growth, to ensure that stress and their impacts are correctly calibrated in the control model. The main reference simulation used considers an initial fertilization of $F_{N0} = 80$ kg ha^{-1} along with 2 irrigation events (26 July and 14 August) of 30 mm each but without any nitrogen.

For the standard experiment, the optimal control problem ($\mathrm{P}_{\overline{F}}$) is solved with $I_{\max} = 10$ mm and $C_{N\max} = 0.05$ g L^{-1}, for 3 different initial fertilizations $F_{N0} \in \{0, 40, 80\}$ kg ha^{-1} and for 11 different upper bounds on the total N added through irrigation $\overline{F}$ ranging for 0 to 200 kg ha^{-1}. To explore the impact of control bounds and for instance the effect of a higher maximum daily irrigation, we also consider $I_{\max} = 30$ mm. In addition, the possibility to fertilize

Table 4
Experiment summary

	$I_{\max}$ [mm] Maximum daily irrigation	$C_{N\max}$ [g L^{-1}] Maximum N concentration of irrigation	F_{N0} [kg ha^{-1}] Initial fertilization	$\overline{F}$ [kg ha^{-1}] Total N added through irrigation
Reference	30	0	80	0
Standard	10	0.05	$\{0, 40, 80\}$	$[0, 200]$
Low $C_{N\max}$	10	0.03	$\{0, 80\}$	$[0, 200]$
High $I_{\max}$	30	0.05	$\{0, 80\}$	$[0, 200]$
Low $C_{N\max}$, high $I_{\max}$	30	0.03	$\{0, 80\}$	$[0, 200]$

Reference simulation has 2 irrigations (26 July and 14 August) of 30 mm each but without any N.

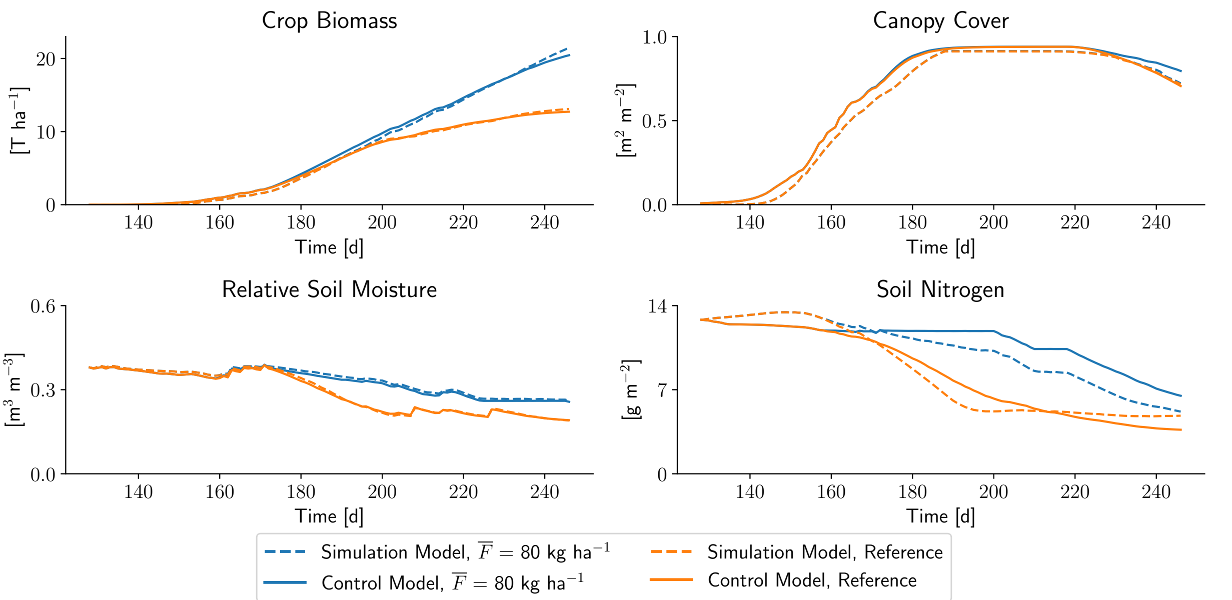

Figure 2: Control model and simulation model for the reference scenario and the optimal control of the standard experiment for $\overline{F}$ = 80 kg ha^{-1}, both consider an initial fertilization of F_{N0} = 80 kg ha^{-1}.

efficiently with wastewater low in nitrogen is studied by imposing $C_{N\max} = 0.03$ g L^{-1}. Therefore, problem ($P_{\overline{F}}$) is also solved for different combinations of these control bounds, which are summarized in Table 4.1.1.

4.2. Calibration and evaluation of control model

At first, parameter estimation was attempted using the model as originally published in (Pelak et al., 2017), but difficulties were encountered for the calibration of certain variables and dynamics. Accordingly, the control model was modified, as previously described (Section 2.2), and changes concerned mainly the canopy cover and leakage dynamics. This required several iterations of the double modelling process, which consisted in modifying and calibrating the control model followed by an evaluation with the simulation model. Thus, a set of parameters was found allowing to reproduce precisely the reference STICS simulation (Figure 2).

The controls obtained for the standard experiment (Table 4.1.1) can be used to generate an important number of different STICS simulations that can be used to validate the control model. Soil water is consistently very well predicted

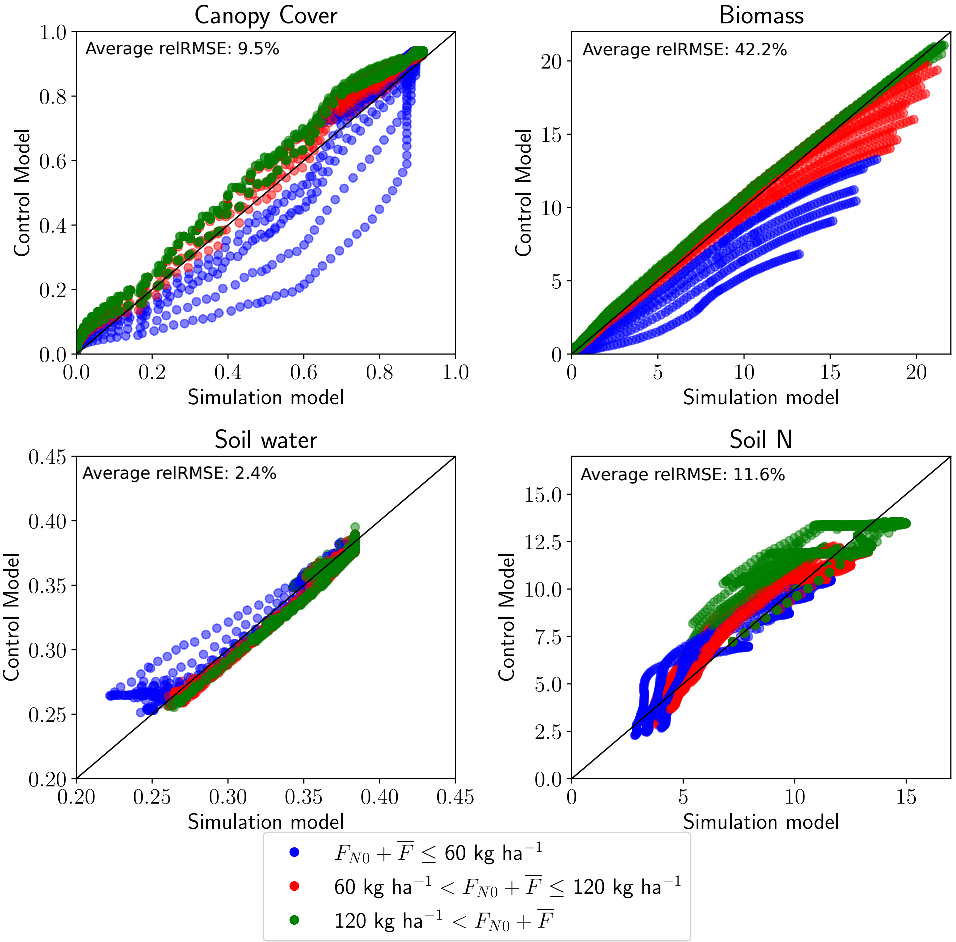

Figure 3: Values of control model variables plotted against values of simulation model for all simulations of the standard experiment. Colors indicate the total fertilization $\mathcal{F}$ which is the sum of initial input F_{N0} and input through irrigation $\overline{F}$.

with an average relRMSE of 2.4% and with the water stress indicators of both models showing very similar behavior. Control model performance for soil nitrogen is also satisfying for all controls, with an average relRMSE of 11.6% and with the overall trend of N consumption by the crop well reproduced. Minor differences can be observed due to the simpler representation of N dynamics and for example, the absence of N mineralization in the control model explains why the slight increase of soil N during the first month as computed by the simulation model is not seen in control model (Figure 2). Water leakage and N leaching are very well predicted, in particular the time at which these occur (Figure 5). On certain occasions, despite the leakage flux being very similar between both models, the N leaching flux can differ and this can be explained by a nonuniform distribution of nitrogen in the soil column in STICS. Indeed, in the simulation model, it is considered that the leached N is from the bottom soil layers, whereas in the control model, N in leachate is computed from the average N concentration over the active soil depth. Nonetheless, the simplified representation of a homogeneous soil column in the control model produces good results and in particular with the control problem in mind, the impact of irrigation and fertilization on the soil variables and dynamics is captured well by the control model.

Control model performance for the crop variables is also good overall, although it varies with fertilization (Figure 4). The canopy cover is in general well predicted with an average relRMSE of 9.5%, but problems can be noted when total fertilization is beneath 60 kg ha$^-1$ (Figure 3). These occur during the first phase of canopy development, with the control model appearing to underestimate growth, but once the maximum canopy cover has been reached, both models coincide. The accuracy of the control model for the biomass strongly depends on fertilization, with an average

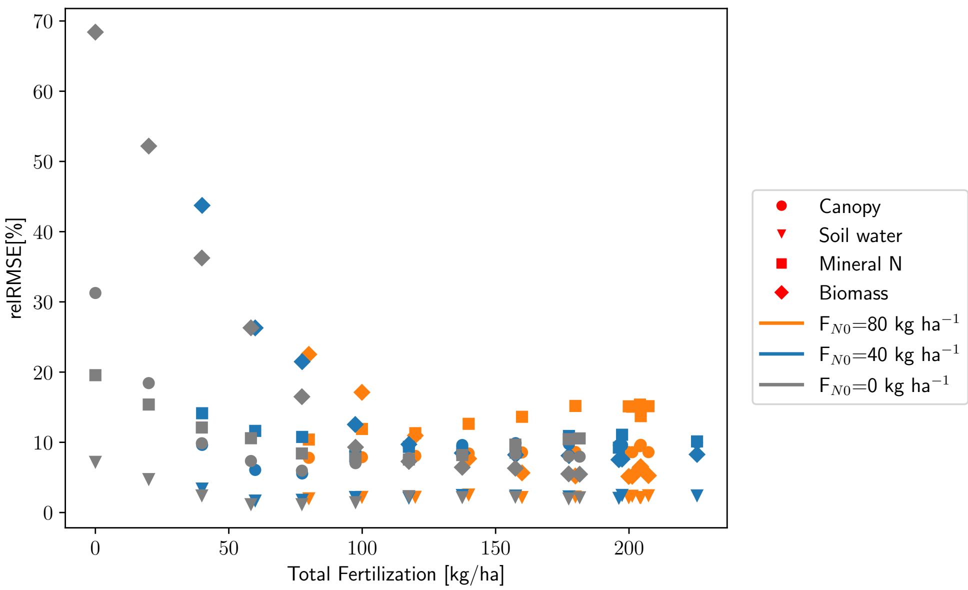

Figure 4: Relative error (relRMSE) between control model and simulation model for the reference and standard experiment, as a function of the total fertilization $\mathcal{F} = F_{N0} + \int_{t_0}^{t_f} F_N(t)\, dt$.

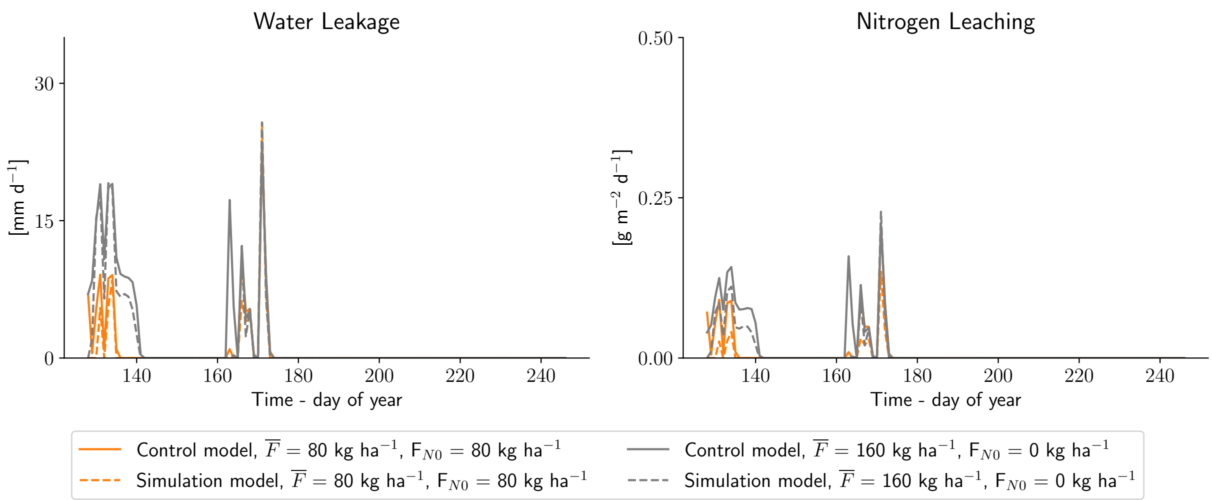

Figure 5: Water leakage and N leached for 2 different initial fertilizations F_{N0} but with the same total fertilization, for the standard experiment.

relRMSE of 42.2% when the total input of nitrogen is less than or equal to 60 kg ha^{-1} but for more than 120 kg ha^{-1} this error drops to only 6.6%. Considering in addition that biomass is in general underestimated by the control model, these problems seem to be due to excessive growth limitations when N deficit occurs. Particular attention was given to the calibration of stresses with a reference simulation that comprised both nitrogen and water deficit but the reduction of water dynamics was not only more important but also lead in itself to a limitation of N uptake, which depends on the transpiration flux. This indicates that the considered parameters of N stress are not the best for low N inputs, considering in addition that the reference simulation was based on an initial fertilization of 80 kg ha^{-1}. Furthermore, the representation of N limitation on biomass growth in the control model could be more developed as it is only dependent on soil N status, whereas in STICS N stress also depends on the N concentration of the crop. However, to reproduce

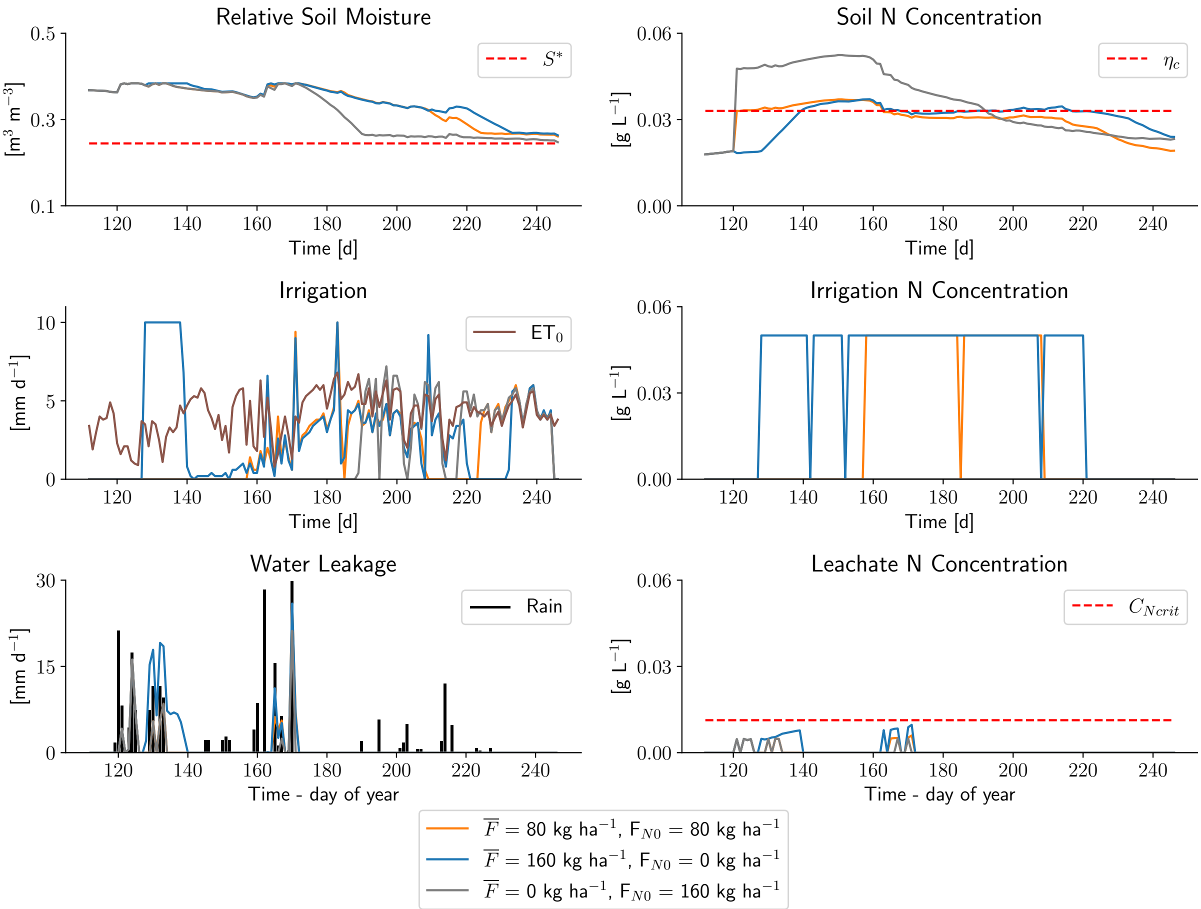

Figure 6: Relative soil moisture, soil N concentration, controls, water leakage and leachate N concentration for 3 different controls corresponding to a total fertilization of 160 kg ha^{-1} for the standard experiment. Values are from the simulation model and with the soil variables are also shown the control model parameters involved in the stress functions: S_* the critical soil moisture and η_c the critical N concentration in soil water. The entire growth cycle from sowing to harvest is shown, to display the impact of the initial fertilization (day 120), whereas optimization begins only at emergence (day 128).

this would require adding a variable and several parameters, increasing the complexity of calibration and affecting the control model efficiency. These results allow to assess the domain of validity of the control model and its calibration and indicates that the control model should be either adapted or re-calibrated to study the issue of crop management in case of N deficit.

Overall, these results show that, with a single set of parameters, the control model is capable of reproducing simulations from STICS for a range of different controls. Furthermore, from Figure 3, we can see that the control model respects the order relation for biomass, in the sense that if, for the control model, a given control leads to less biomass than another control, then this is also the case in the simulation model. This is particularly important when considering an optimization problem, and we can therefore suppose that the control model is an appropriate local approximation of the simulation model that can be used for the problem studied here.

4.3. Exploration of optimized wastewater reuse

4.3.1. Properties of the optimized controls

To first analyze the computed controls, Figure 6 compares results for 3 different initial doses of N but with the same total fertilization of 160 kg ha^{-1}. Soil variables are shown, with soil N concentration computed as $\eta = \frac{N}{zS}$ from the values of the simulation model for the total soil nitrogen N and the relative soil water content S, both up to maximum rooting depth z. Similarly, N concentration in the leachate is computed from the leaching N flux and the water leakage flux, both from the simulation model.

Looking at the soil N concentration allows a better understanding of the optimized fertilization strategy computed here since, in the control model, N stress (8) occurs when the soil N concentration is below the critical threshold η_C. This explains why the computed controls seek to avoid N stress by maintaining soil N concentration greater or equal to η_C. To understand how this can be achieved, it is interesting to write the dynamics of the soil N concentration η for the control model. Focusing on periods between rain events and when there is no leakage, i.e. $S \leqslant S_{fc}$, the dynamics of the soil N concentration are

$$zS\frac{d\eta}{dt} = I\eta_I - TK_N(\eta) + (T + E - I)\eta. \tag{22}$$

The last term represents the impact of either the dilution of N in the case of water inputs or the increase of concentration due to water losses. This shows that the strategy of increasing irrigation to deliver more N will need to compensate for the effect of dilution and is therefore not sustainable, especially considering it would also eventually lead to leaching.

To increase or maintain η, the N concentration of the irrigation water must be such that

$$\eta_I \geqslant \frac{T}{I}\min(\eta, \eta_C) + \frac{I - T - E}{I}\eta. \tag{23}$$

Therefore, having a concentration of N in irrigation equal to η_C might not be enough to maintain soil N concentration at this critical level. This also shows that it is difficult to reach a soil N concentration greater than $C_{N\,\max}$, and thus it is not feasible to build up important nitrogen reserves in the soil due to the low concentrations of nitrogen in wastewater. For example, here $C_{N\,\max} = 0.05$ g L^{-1} is only slightly greater than $\eta_C = 0.033$ g L^{-1}. This explains why the N concentration in irrigation water is always maximum or null for the computed controls. In fact, the amount of N delivered to the soil-crop system is varied by changing the irrigation flux and not the N concentration in irrigation water.

For the present case study, during the first months, soil water content is close to field capacity and there are few opportunities for irrigation without the risk of leaching. For the second part of the growth cycle, once the crops canopy has developed, evaporation becomes negligible. Then irrigation serves to compensate for losses mainly due to transpiration and therefore to avoid N stress, the concentration of N in irrigation needs to be greater than η_C.

Concerning irrigation, the computed controls also serve to avoid water stress and this is achieved by maintaining soil water content above a threshold, represented by the control model parameter S^*. Notice that the irrigation follows closely the daily variations of reference evapotranspiration, in particular at the end of the growth cycle, when the soil water content is kept just above S^*. In general, water is never added in excess as this would dilute soil nitrogen and thus, the irrigation policy obtained here is also efficient, computing the necessary amount of water needed to compensate for evapotranspiration losses and with extra irrigation only to add nitrogen.

The case of irrigation without nitrogen ($\overline{F} = 0$ with $F_{N0} = 160$ kg ha^{-1}) constitutes the baseline irrigation that is needed to avoid water stress and for example, there is no irrigation at the beginning of the growth cycle because soil water is kept high with rains. Note also that this irrigation policy avoids diluting the soil nitrogen already present and this explains why soil moisture is kept just above S^* at the end of the season and not any higher. It is possible to observe that compared to this baseline, the control for $F_{N0} = 80$ kg ha^{-1} with $\overline{F} = 80$ kg ha^{-1} maintains the soil water content at a higher level during the second part of the growth cycle, but actually both controls are close during the period from day 180 on-wards. In fact, the control for $\overline{F} = 80$ kg ha^{-1} requires only 10.8 % more irrigation than for $\overline{F} = 0$ kg ha^{-1} and this extra water is needed to deliver nitrogen in the first part of the season, around day 160, when the first nitrogen deficit appears.

For the case without an initial N dose ($F_{N0} = 0$ kg ha^{-1} with $\overline{F} = 160$ kg ha^{-1}), there is an important irrigation at the very beginning in order to deliver a large quantity of N and bring the soil N concentration up to η_C. This essentially corresponds to an initial fertilization but this method of delivering a large dose of N shortly after sowing results in an important water leakage as the soil water content is already high at the beginning of the growth cycle. Nonetheless, the concentration of nitrogen in leachate remains under the critical level C_{Ncrit}, as for the other cases shown in Figure 6.

4.3.2. Performance and trade-off analysis

Computing controls by solving problem ($\mathrm{P}_{\overline{F}}$) for a range of upper bounds $\overline{F}$ allows to represent the final crop biomass and total N leached as a function of total fertilization $\mathcal{F} = F_{N0} + \int_{t_0}^{t_f} F_N(t)\,dt$ and of the total irrigation

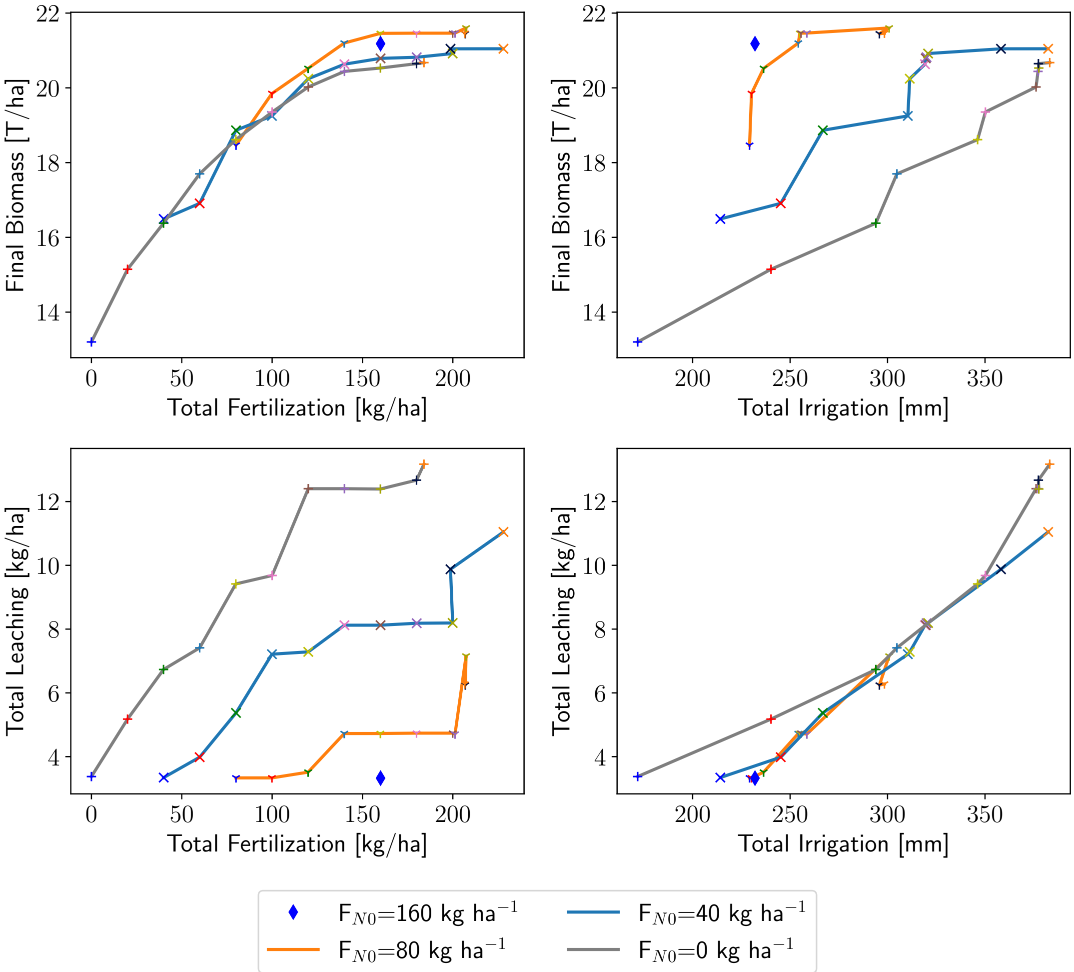

Figure 7: Final crop biomass and total leaching as a function of total fertilization $\mathcal{F} = F_{N0} + \int_{t_0}^{t_f} F_N(t)\ dt$ and irrigation. Values from the simulation model are shown for 3 different initial fertilizations F_{N0} for the standard experiment. Each color of markers correspond to a value of $\overline{F}$, the upper bound on the total N added through irrigation, and for example, red markers are values associated with $\overline{F}$ = 20 kg ha^{-1}. For comparison, results are shown (blue diamond) for the case of an initial fertilization of 160 kg ha^{-1} and irrigation without nitrogen, i.e. the solution for $\overline{F} = 0$.

volume required by the computed controls. These represent the Pareto fronts obtained and illustrate the trade-offs between production, fertilization, irrigation and N leaching (Figure 7).

The first observation that can be made is that final biomass increases with total fertilization up to a certain limit, after which crop production levels off and remains constant at a maximum achievable value (Figure 7, top left). Indeed, biomass increases steadily for total fertilization $\mathcal{F} < 160$ kg ha^{-1} and beyond this value, there are no real gains that can be made by adding more nitrogen.

It also appears that crop production varies only slightly with initial fertilization and in particular biomass response is very similar for intermediate fertilization rates (Figure 7, top left). Notable differences can be seen mainly in the maximum achievable biomass and the biggest difference observed is when $\mathcal{F} = 160$ kg ha^{-1}, with an initial dose $F_{N0} = 80$ kg ha^{-1} resulting in 4.5% more biomass than no initial fertilization. Interestingly, crop production is very close whether all the nitrogen is added in a single dose or throughout the growth cycle. These results indicate that, as far as crop production is concerned, it is possible to substitute conventional practices of adding fertilizers in a few but large doses with a distribution of smaller quantities throughout the growth cycle.

For a high upper bound $\overline{F}$, the optimization does not find controls that use the entire N budget and this implies that there is a maximum amount of N that can be delivered to the soil-crop system through irrigation. A particularity of fertigation with low concentrations of nutrients is that important quantities of water are needed to apply nitrogen and therefore when the fertilization rate is high, the irrigation volume is already important (Figure 7, top right). Then, adding extra N will lead to either leaching or dilution of the N already present in the soil, and thus it can be impossible to deliver more N to the crop beyond a certain point. For similar reasons, with the highest fertilization rates achieved, there is a sharp increase in both irrigation and N leached which result in nearly no biomass gains, indicating that the extra N added is not useful to the crop.

The controls computed for $\overline{F} = 0$ always lead to the smallest total irrigation for a given initial fertilization F_{N0} (Figure 7, top right). In addition, these irrigation policies result in the same baseline quantity of N leached, which occurs due to heavy rains early in the growth cycle and can not be avoided. Interestingly, for the case $F_{N0} = \overline{F} = 0$, leading to an important N deficit, the optimization finds a compromise by trading off a little water stress for a reduced N stress by letting soil water drop under S^* in order to avoid diluting soil N and thus maintains the N concentration in soil water.

For all computed controls, the resulting total N leached and total irrigation follow a similar behavior and both these quantities are closely related, with a correlation that appears independent of F_{N0} (Figure 7, bottom left). Similarly to biomass production, N leached and irrigation first increase with fertilization and then reach a plateau. On one hand, the increase in nitrogen lost in drainage indicates that there is a compromise between adding N and losing part of it to leaching. However, for 2 successive fertilization budgets (i.e. $\overline{F}$ and $\overline{F} + 20$), the increase in N leached is small compared to the extra fertilization and thus most of the nitrogen is delivered to the crop. On the other hand, the increase in irrigation is not to relieve water stress, because the base irrigation volume computed with $\overline{F} = 0$ is already sufficient to avoid a water deficit. Instead, the higher irrigation volumes are a consequence of the fact that water and N stresses can occur at different times, and thus it can be necessary to irrigate to add N when soil water content is already sufficient. Nonetheless, the amount of extra water needed depends on the initial fertilization and for $F_{N0} = 80$ kg ha^{-1} by adding only an extra 25 mm it is possible to deliver enough N for maximal biomass production. However, for $F_{N0} = 0$ kg ha^{-1}, an increase of 205 mm is needed. More generally, irrigation volumes and N leaching depend on the initial fertilization, leading to important differences in performance of the computed controls that can constitute reasons to select a strategy over another.

4.3.3. *Impact of control bounds*

As previously explained, the maximum N concentration in the irrigation water $C_{N\max}$ can limit the controls' ability to maintain the soil N at a given level, for instance above the N stress threshold η_C. This motivates the study of the case when $C_{N\max} < \eta_C$, to explore the possibility to fertilize efficiently with wastewater low in nitrogen. In parallel, the impact of a higher maximum daily irrigation $I_{\max}$ is also analyzed, since it is the other lever that can allow delivering more N to the soil. Figure 8 compares the Pareto fronts for different combinations of the control bounds and Figure 9 illustrates model variables and computed controls for 3 different combinations with the same total fertilization.

For the case without an initial fertilization and a low $C_{N\max} = 0.03$ g L^{-1}, it is possible to reach high levels of biomass, but this comes at an important cost of a much higher total irrigation and N leached (Figure 8). For $\mathcal{F} = 160$ and $F_{N0} = 0$, crop production is 4.6% less than with $C_{N\max} = 0.05$ g L^{-1}. However, compared to the baseline irrigation required just to avoid water stress, the water volume needed is more than double and the total N leached is 8 times higher. The concentration of nitrogen in leachate is also greater, regularly approaching the critical level C_{Ncrit} and this limit is exceeded for $I_{\max} = 30$ mm and $C_{N\max} = 0.03$ g L^{-1} (Figure 9). With an initial fertilization it is possible to produces as much biomass than with $C_{N\max} = 0.05$ g L^{-1} without excessive irrigation and leaching. For $F_{N0} = 80$ kg ha^{-1} and $\overline{F} = 80$, there is less than 1% difference in crop production and although extra water is needed, here only 45 mm more than the baseline irrigation are required and the increase in leaching is also limited, with only an additional 3.9 kg ha^{-1} of N lost.

Notice in Figure 9, that at the beginning of the growth cycle, for no initial fertilization ($F_{N0} = 0$) the controls are capable of increasing soil N concentration up to η_C but at the cost of important leaching. In the second part of the growth cycle, for both $F_{N0} = 0$ and 80 kg ha^{-1}, when $C_{N\max} < \eta_C$, the controls are not capable of maintaining the soil N concentration at the stress threshold, and instead the soil N concentration η steadily decreases. This confirms that it is not possible to sustain throughout the whole growth cycle a soil N concentration higher than $C_{N\max}$. Therefore,

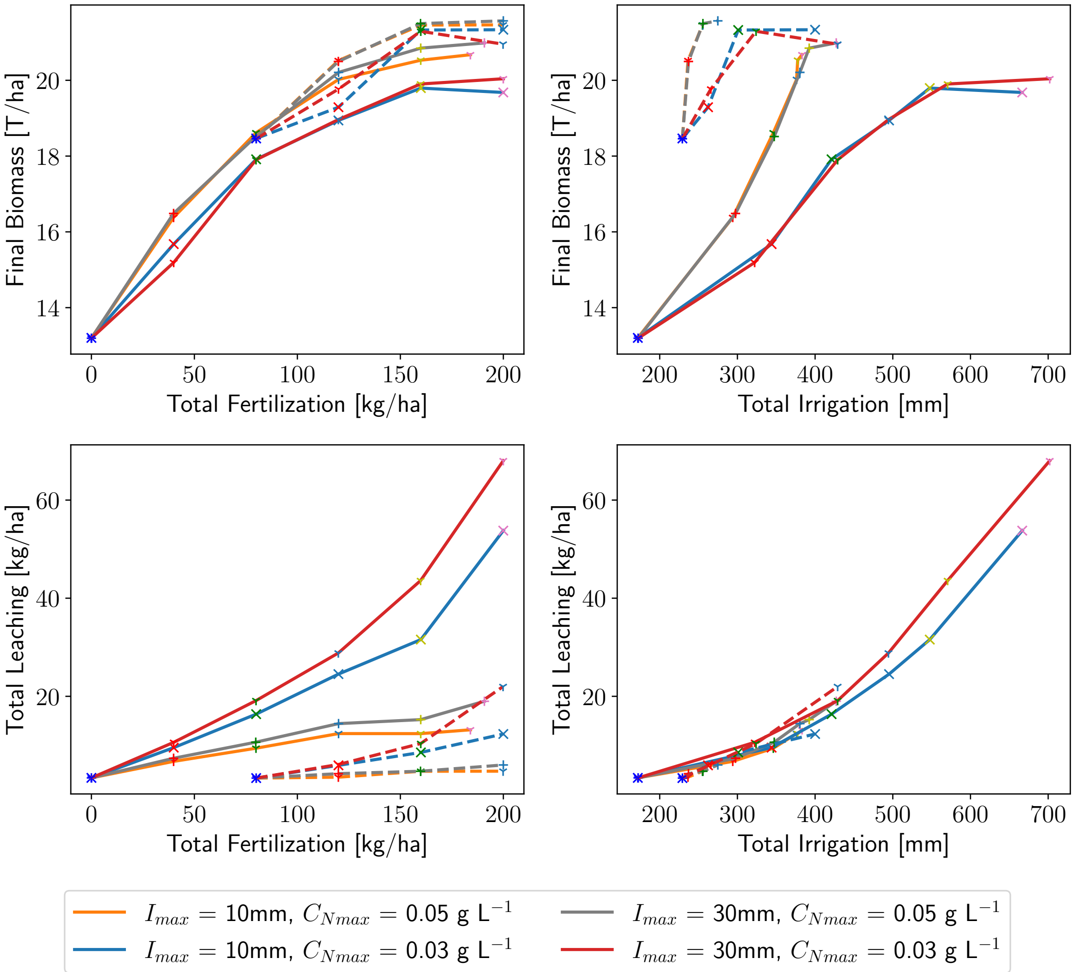

Figure 8: Impact of control bounds on final crop biomass and total leaching, as a function of total fertilization $\mathcal{F} = F_{N0} + \int_{t_0}^{t_f} F_N(t)\, dt$ and irrigation. Values from the simulation model are shown for $F_{N0} = 0$ (solid lines) and for $F_{N0} = 80$ kg ha^{-1} (dashed lines) for different values of the control bounds ($I_{\max}$ and $C_{N\max}$). Each color of markers correspond to a different value of $\overline{F}$, the upper bound on the total N added through irrigation.

with a N concentration in irrigation water much lower than η_C, it is not possible to deliver N to the crop efficiently and fertilization must be complemented with another source of nitrogen.

Increasing the maximum daily water volume from 10 to 30 mm does not change substantially the maximum biomass produced (Figure 8). When irrigation is only required to maintain soil water above the stress threshold, such as at the end of the growth cycle or when $\overline{F} = 0$, irrigation is the same as with $I_{\max} = 10$ mm and follows closely the variations of reference evapotranspiration (Figure 9). However, in general, $I_{\max} = 30$ mm leads to less frequent irrigation with higher daily volumes, in particular when it is necessary to deliver N to the crop. This results in more leakage for the highest fertilization rates, although the total irrigation volumes are the same for a given maximum N concentration of irrigation water. Comparing Figures 6 and 9, notice that for $I_{\max} = 10$ leaching occurs only during the heavy rains but for $I_{\max} = 30$ mm, nitrogen is also lost later in the season due to sustained irrigation.

5. Conclusions

The case study presented in this work gives a number of insights on the opportunity for fertilization from reclaimed waters. First, it shows that it is possible to obtain high levels of crop production with wastewater reuse, similar to those

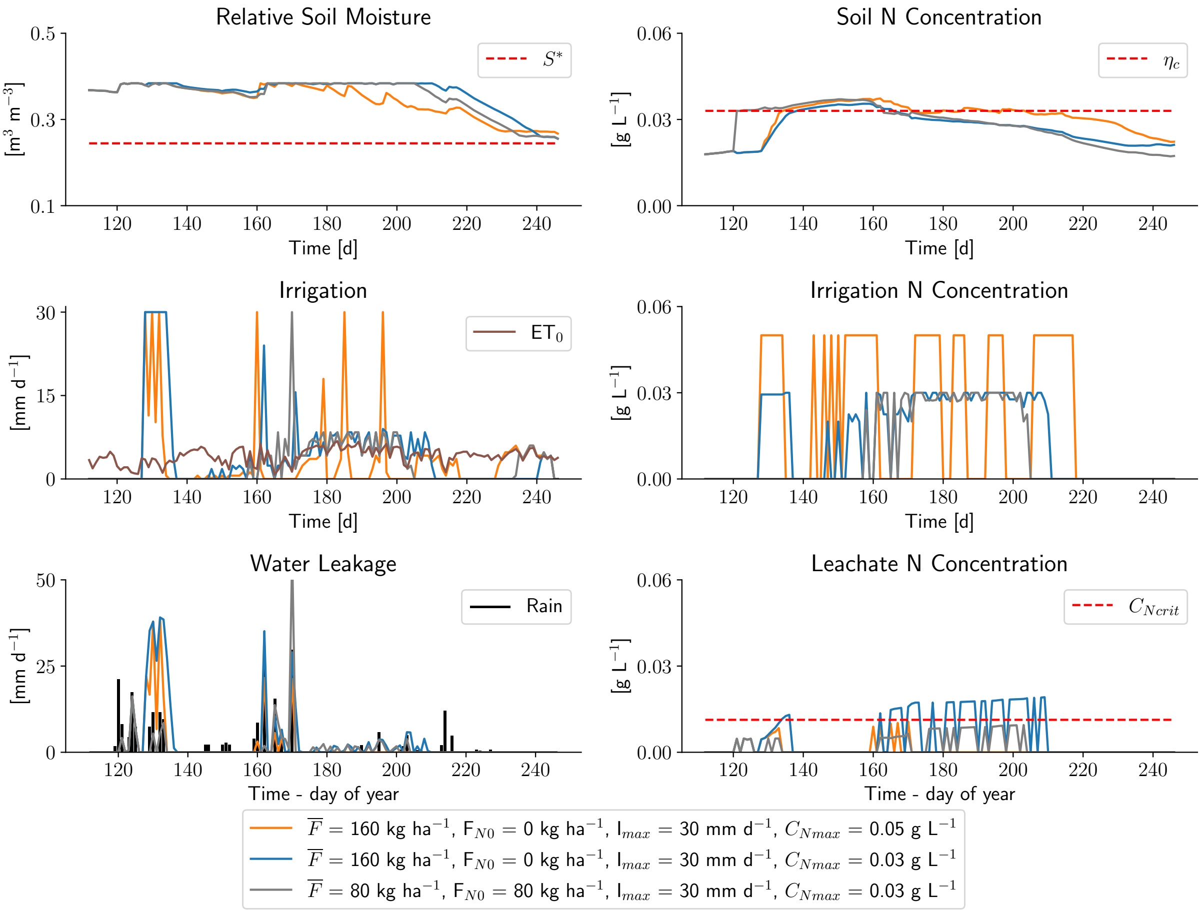

Figure 9: Relative soil moisture, soil N concentration, controls, water leakage and leachate N concentration for a maximum irrigation flow rate $I_{\max}$ = 30 mm d^{-1} and a total fertilization of 160 kg ha^{-1}, for different values of $C_{N\max}$, the maximum N concentration in irrigation water. The soil N concentration is computed from the simulation model variables as $\frac{N}{SZ}$ with S the relative soil water content and N the total soil nitrogen, both up to maximum rooting depth Z. Variables from the simulation model are shown alongside the control model parameters involved in the stress functions: S_* the critical soil moisture and η_c the critical N concentration in soil water. The entire growth cycle from sowing to harvest is shown, to display the impact of the initial fertilization (day 120), whereas optimization begins only at emergence (day 128).

achieved with conventional fertilization. On one hand, we have seen that if the maximum N concentration in the irrigation water $C_{N\max}$ is high enough, then it is possible to substitute entirely conventional fertilization for irrigation with reclaimed waters. On the other hand, if $C_{N\max}$ is small, wastewater irrigation might only be capable of providing a portion of the crop N needs but if it is complimented with conventional fertilization, a high crop biomass can be achieved. In any case, it appears a viable option to deliver nutrients to crops, which should be considered as it is a means to reduce costs and environmental impacts of chemical fertilizers and could even be a possibility in regions where rain-fed agriculture is dominant.

Next, this work illustrates that using wastewater with low concentrations of nutrients raises a number of issues. It has been shown that if $C_{N\max}$ is small, delivering enough N to meet the crop needs from wastewater alone requires excessive irrigation, which is not a realistic solution. In particular, it is difficult to deliver large quantities of nutrients in a short amount of time, without causing important leaching. Another problem seen here is that irrigation with low N can lead to the dilution of the nutrients already present in soil, thereby limiting the maximum concentration of N in the soil that can be reached. As a result, there is a maximum amount of N that can be delivered efficiently to the soil-crop system through irrigation which depends on the value of $C_{N\max}$. The plan of action that should be undertaken therefore also depends on initial N in soil and the case of low initial reserves would require another source of fertilizers at first if $C_{N\,\max}$ is too small.

Determining the best strategy to adopt for wastewater fertilization in a particular situation thus resides in a few key quantities. The double modeling method and the control model offer the possibility to estimate these, such as we have shown here by determining the minimum concentration of N in irrigation waters needed for fertilization with wastewater alone. Indeed, the relation between $C_{N\,\max}$ and the N stress parameter of the control model η_C has been identified as key, and it has been shown that it is possible to meet the crops N needs with only wastewater irrigation when $C_{N\,\max} > \eta_C$. Therefore, the control model parameter η_C provides a concise means to evaluate whether there is enough N in wastewater for fertilization. This is an important benefit of the approach developed here because STICS, like most other crop models, does not have such a parameter as it computes N stress from the crop N content and estimating the required N concentration in wastewater from STICS parameters alone is not straightforward. The methods used here can thus constitute the basis of a decision support tool, in particular with the multi-objective optimization providing a range of solutions to explore the trade-off between different strategies.

This work has also explored the elements that lead to efficient wastewater irrigation. We have seen that the optimal control maintains the system above stress thresholds, represented by control model parameters S^* and η_C. Then, from this, we could propose a feedback control constructed from the control model parameters, with irrigation triggered when the soil water or nitrogen content reaches the corresponding threshold. This further demonstrates the usefulness of the double modeling method and the control model, which is capable of synthesizing the complex mechanisms of crop water and N stresses to obtain parameters representing the critical soil moisture and N levels that must be maintained to avoid stresses. Again, this would not be straightforward with the simulation model only, as it represents the soil as a column of multiple layers of different characteristics and computes different stress indices for the various crop processes affected by water or N deficit. More generally, the double modelling method opens perspectives for the application of automatic control theory to complex modern crop models and future work could tackle problems due to weather uncertainty with receding horizon or adaptive controls.

Acknowledgment

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Annex: Calibration of the control model

STICS represents the soil in detail, dividing the soil profile in 1 cm layers, therefore the soil variables of the control model need to be compared with aggregates of the values from STICS. For the soil water, as it is a relative quantity, the average over the considered active soil depth can be used. The soil N is expressed in units of mass per unit area, therefore the variable of the control model must be compared with the sum of the values from STICS up to the active depth. The active soil depth parameter of the control model thus plays an important role and should be taken as the rooting depth, which varies over the growth cycle of the crop. However, to avoid adding a variable and rooting dynamics, the active soil depth is fixed here and represents the maximum rooting depth. As STICS simulates root growth, the maximum rooting depth calculated by STICS can be used directly to set the soil depth of the control model and this approach has the added benefit of avoiding the calibration of this very sensitive parameter.

The concept of Leaf Area Index (LAI) is used in STICS, but it has been shown that an optical analogy (Beer's law) can be used to convert LAI to canopy cover (Brisson et al., 2009),

$$C = 1 - e^{e_x LAI} \tag{24}$$

with the extinction coefficient e_x. For plant biomass, the two models can be compared directly as they both output the above-ground dry biomass per unit area.

Particularly relevant to the control problem, the parameters corresponding to soil water levels can be adjusted using values from STICS, guaranteeing that the hydraulic properties of the soil are preserved in the control model. Therefore, the wilting point and field capacity are obtained from the average of the parameter values from STICS, and as suggested in (Pelak et al., 2017), S^* can be taken as $(S_w + S_{fc})/2$. In addition, the maximum canopy cover parameter is obtained from the maximum LAI computed by STICS and converted with formula (24).

The water dynamics play a central role in the soil crop system and are therefore calibrated first by minimizing the difference between models only in soil water content, to estimate the transpiration crop coefficient K_{cb}. Likewise, the nitrogen dynamics are adjusted independently by considering the error on the soil N variable to estimate η_C and then the leaching rates of both models are compared to calibrate a_N. Here comparing the N stress indicators of both models is particularly useful to check the calibration of η_C. Then the canopy cover is fitted by adjusting r_G and t_{sen}. The dynamics of S, N and C are highly coupled and thus, these first calibrations must be completed by considering the sum of errors on these 3 variables. In most cases, it is only necessary to re-adjust at this stage K_{cb}, η_C and r_G, as these are the parameters involved in the most important and sensitive processes.

Finally, since the crop biomass is not involved in the dynamics of the other variables, it can be adjusted at the end to calibrate W^* and ET^*.

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