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Contribution of modeling and control for improving nutrient recycling via reuse

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Abstract: This paper presents a systemic viewpoint making use of modeling and control tools to promote the flexibility of a water reuse chain and dynamically adapt the quality of treated waters to plant needs, notably using output feedbacks. The proposed approach was developed within the framework of the European Control4Reuse project dedicated to the development of an integrated approach for improving water and nutrient recycling in agronomy. Within this framework, the notion of flexibility of treatment systems for reuse is developed together with its evaluation using a dedicated simulation platform.

Keywords: Automatic control for reuse, flexibility of treatment systems, modeling and simulation

Introduction

Reuse of treated wastewater, although known as not being a systematic solution to the water stress, is an important lever within circular economy approaches. Until recently, reuse essentially covered the area of water, taking only exceptionally into account the possibility of recycling the nutrients it contains in spite of the progresses that have been done in wastewater treatment plant (WWTP) capabilities and performances.

One important problem is that the actual WWTPs are designed to provide treated wastewater with a quality that complies with normative constraints compatible with their discharge into the environment. By definition, this makes their use for fertigation limited while increasing their functioning costs. Introducing flexibility – the capacity of a wastewater treatment plant to modulate the quality of treated water – allows us to think the WWTP in terms of a waste resource recovery facility (WRRF) – sometimes also called circular-economy based treatment plants - as long as the quality of the delivered water is used for agronomic purposes instead of only considering the quantity of water produced. If we can promote this flexibility, it will become possible to process wastewater on a tailored basis to provide a known quality of the treated water (*cf.* Heran *et al.*, 2022, in French). The treated water then complies with normative constraints during periods where no water is needed for irrigation and, in addition, with plant/crop needs during irrigation periods, the whole under sanitary and environmental constraints (Aichouche, 2021). This flexibility, makes an intensive use of control theory necessary in order to precisely control the whole reuse chain not only to manage the quantity of water provided to plants for irrigation but also its quality optimally adapted to – dynamically – match plant needs. While this flexibility notion is directly related to the treatment step, this strategy directly refers to what we can name the "Water on Demand" concept (WoD) in the field of irrigation science (Harmand *et al.*, 2022).

To promote this strategy, we claim that WRRFs must definitely take over WWTPs (Regmi *et al.*, 2019). From a systemic viewpoint where the system of interest would be the "reuse chain" (say, a WWRF connected with the transport and possibly the storage of water, also considering soil and crop/plant), the input is the raw wastewaters characteristics and flux and the outputs the plant needs. From a control point of view, such a system may be controlled using the available controls (via “actuators”) that are mostly situated at the treatment plant step (aeration power, hydraulic and solid fluxes, etc…) and the available measurements (via “sensors” and monitoring systems in general, preferentially “online”, for instance the humidity in soils) able to monitor plant growth/biomass production. For such an approach to be put in practice, we need to couple input-output models of wastewater treatment plants (or WRRF here), of water transport and storage, of irrigation systems and others describing the soil and the growth of plants. For each of these reuse chains, such models exist in the literature. In addition, transport and storage models can be coupled with those describing WRRF dynamics. However, WRRF and crop models have been developed by experts of very different fields (typically IWA models for treatment plants have been developed by biotechnologists and engineers in process/chemical engineering, and by hydrologists or agronomists for others and in particular for plant growth modeling as proposed in (Brisson *et al*., 2003)). These models are different in nature, with distinct "characteristic times" and different inputs and outputs, usually not compatible with all models: it is thus a very challenging task to couple them.

Instead of following this approach, we propose to use these different models in another way: instead of trying to couple them all together, we use the plant growth models and WRRF models separately in a two step approach as initially proposed in (Aichouche 2021). In a first step, we apply control theory on plant growth models only. We solve the following optimal control problem: given *i*) a dynamical model of a culture, *ii*) an objective function to be optimized (for instance, maximize the final biomass produced) and *iii*) a set of constraints (for instance, the amount of resources available), the task is to find the dynamic control inputs (quantity and quality of water) to be delivered to the plant (by the WRRF), under given weather conditions. This problem can be solved analytically as long as simple models are available or numerically otherwise, for instance in using the so-called "double modeling approach" (Bouzama *et al*., 2021) or (Haddon *et al*., 2021). In a second step, these optimal inputs are considered as "setpoints" for the WRRF model, in which different levers for actions (actuators) are used within "feedback loops" to follow them as best as possible. To do so, many control approaches may be mobilized and applied in practice (Aichouche, 2021).

Since the weather conditions cannot be known a long time in advance, this scheme can be iterated over a given period of time, for example using "receding horizon control" or "adaptive optimal control" approaches.

The paper is organized as follows. First, models of the WRRF and of the crop growth are recalled. The general scheme is then presented in more detail: results of optimal control strategies using crop models are presented. Finally, the concept of flexibility and simulations results of interesting irrigation scenarios both using simple and advanced control methods are presented before some conclusions and perspectives are drawn.

Material and Methods

From an automatic control viewpoint, the problem which is posed refers to the control of a nonlinear system (the WRRF) in the presence of disturbances (input water flow, water characteristics and weather…). More particularly, it is a problem called "setpoint tracking", such "setpoint" being the result of an optimal control problem solved using crop models.

Generating the setpoint: a double modeling approach applied to describe growth rates of plants/crops

The WoD concept refers to the ability of a decision system to deliver the appropriate quantity and quality of water needed by a plant at a given time *t*. The setpoint is generated by solving an optimal control problem of crop irrigation and fertigation with treated wastewater, with the objectives of maximising crop production and minimizing environmental and farming costs (*cf.* for instance Boumaza *et al.*, 2020) in which however the problem is solved without consideration of nitrogen. Although there are a variety of well validated crop models, most cannot be used for standard control techniques because their mathematical structure is unclear and they are essentially simulation models. Instead, a double modelling method can be used to benefit from both a modern detailed crop model - the simulation model - together with a low-order dynamical systems model - the control model as the one proposed in (Pelak *et al.*, 2017). The procedure followed is schematically represented in the following Figure.

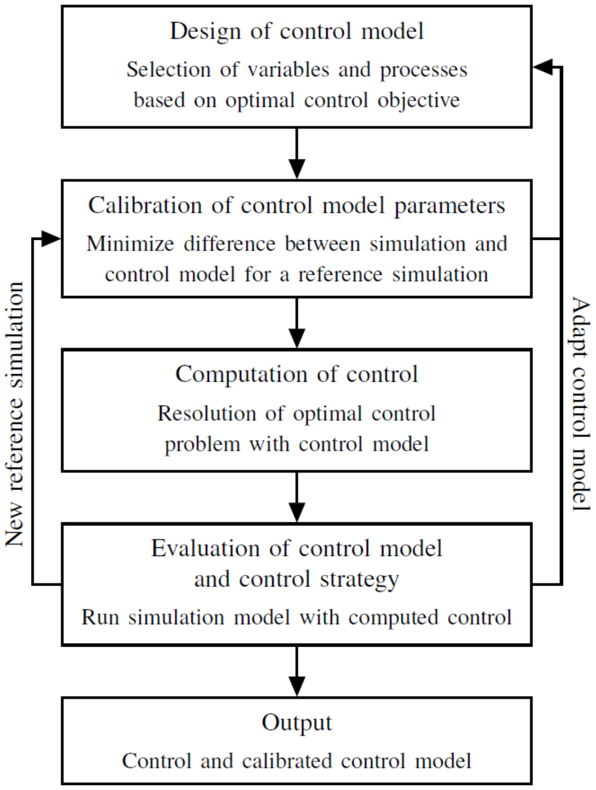


Figure 1: The double modeling method.

The control model is designed to capture the essential dynamics relating to the controlled inputs whilst being adapted to the resolution and understanding of the problem. The simulation model (Brisson *et al.*, 2003) is considered for its detailed representation of the cropping system and is used to guarantee the validity of the results. In practice, for a given scenario (*i.e.* a fixed set of parameters of the simulation model), the control model parameters are calibrated to get a good agreement between outputs of both models. Then, the problem for the control model can be solved, for example with a dynamic programming technique. To deal with the multiple objectives, the problem can be recast as a constrained optimal control problem by considering an optimization criterion only on the final crop biomass and setting the other objectives as constraints. These are irrigation costs and the environmental impact of nitrate leaching and thus correspond to imposing an upper bound on the total amount of nitrogen added through irrigation. By solving the problem for different values of the constraint, a range of optimal controls is obtained, the so-called Pareto front, from which it is possible to analyze the trade-offs between the different objectives. Finally, the results can be further evaluated with the simulation model. Within the present work, the problem of maximizing the final biomass produced was solved. An example of setpoint generated using such optimization approaches will be presented in section "Results and discussion"

A flexible platform as a candidate for a WRRF

When amending plants with nitrogen, the form of nitrogen delivered is important from an agronomic viewpoint. In particular, nitrate is more easily accessible than ammonium. But it is also more mobile. The right amending policy will depend on soil characteristics (and notably its acidity), weather forecast, and notably the temperature, agricultural practices: all these parameters will be important to minimize N2O production and nitrogen washout in soil. In addition, it may happen that over some time period no water for irrigation is needed anymore: in such a case the WRRF must deliver a treated water complying with normative constraints, with nitrogen concentrations less than given thresholds. Different scenarios will be studied here: the production of ammonium, the production of nitrate and the total treatment of nitrogen by the WRRF.

A first condition is to consider a system, flexible enough, for each of these scenarios to be feasible. A candidate for such an objective is represented in Figure 2.

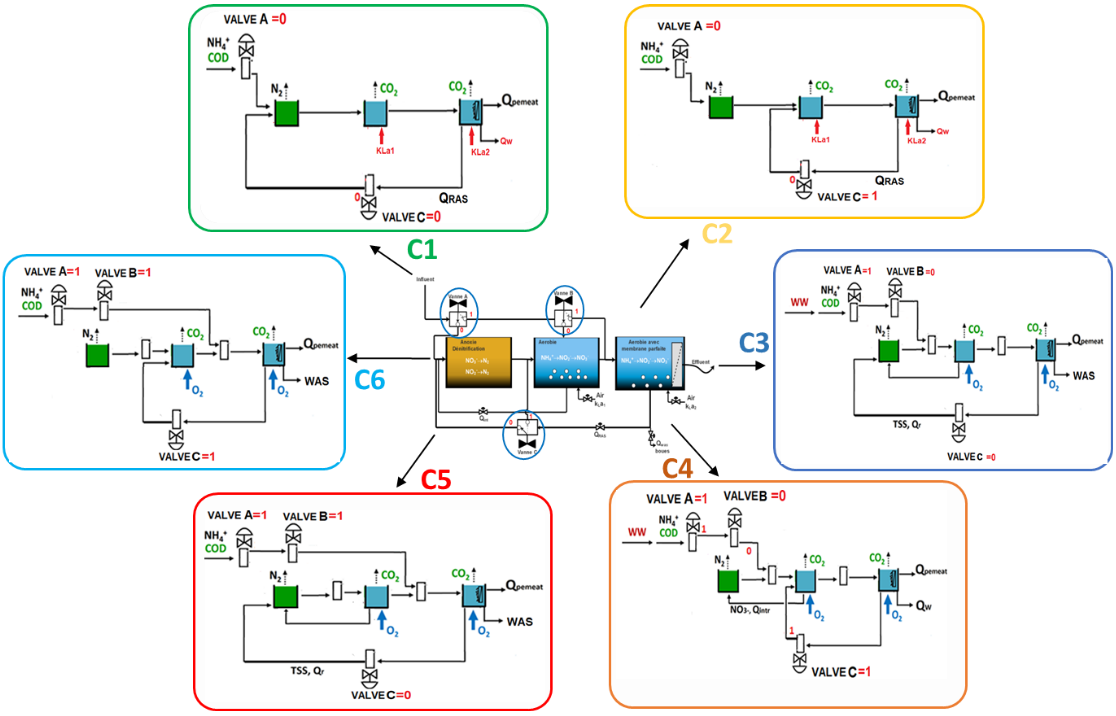
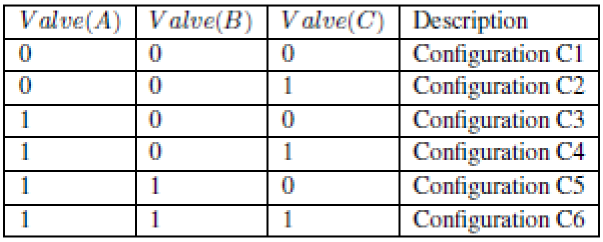


Figure 2: A flexible platform for the reuse of water for agronomic purposes (Aichouche, 2021).

The flexibility of the platform is obtained through the possibility of changing the position of three valves allowing to orientate the different fluxes of the wastewater to be treated through three oxic and anoxic tanks. Depending on the position of these valves, 6 configurations of interest, numbered C1-6, may be obtained and reported in Table 1.

Table1: Valve position for the 6 configurations of interest



$Valve(A)$	$Valve(B)$	$Valve(C)$	Description
0	0	0	Configuration C1
0	0	1	Configuration C2
1	0	0	Configuration C3
1	0	1	Configuration C4
1	1	0	Configuration C5
1	1	1	Configuration C6

The sanitary risks are supposed to be controlled by the presence of an appropriate membrane before the treated water is rejected/sent to the soil/plant stage. To produce mainly NH4 (favouring neither nitrification nor denitrification), the C5 position is appropriate, whereas to produce a nitrate-rich effluent (favouring nitrification), one would rather use the C3 configuration. For a complete treatment (favouring both nitrification and denitrification), the configuration C1 should be preferred.

Modeling of the flexible platform

To simulate the system, the available models proposed by the IWA were used (Henze *et al*., 2000). In such a configuration, it is important to be able to modulate nitrogen content in the effluent, including the forms of nitrogen (ammonium, nitrate while avoiding nitrite formation). Indeed, controlling the form of nitrogen may be of interest from an agronomic viewpoint: nitrate is the most easiest accessible form for plants/crops but is more subject to leaching than ammonium. Thus, at a given time, depending on weather forecast, it may thus be interesting to produce one nitrogen form or another. The ASM1, which does not models two step nitrification, was thus modified to allow for the nitrification process to be simulated appropriately (obtaining the so-called ASM1-2ND model as proposed by (Ostace *et al*., 2011)) while the stoichiometry and the consistency of kinetics of the whole was corrected according to (Hauduc, 2011).

Results and Discussion

Notice that in (Aichouche, 2021), two specific cases were investigated in details: strategy #1 was developed to control the output concentration in nitrate while the strategy #2 was able to control the ratio of the ammonium and nitrate concentrations. Industrial control structures, *i.e.* strategies in which the different possible configurations of the system were considered as disturbances, were proposed and evaluated (Aichouche, 2021; Neto *et al*., 2021).

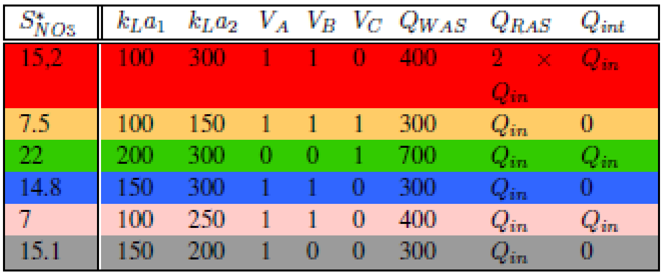
Hereafter, we first present results obtained in open-loop as a proof of concept to test the flexibility of the proposed flexible platform and then results obtained with the strategy #1 mentioned hereabove.

Proof of concept: open vs closed-loop control

The first control, presented here as a proof of concept of the flexibility of the treatment plant under interest, is an "open-loop control strategy" allowing the user to choose the most appropriate configuration of the pilot plant with respect to the setpoint to be tracked. With respect to a "closed-loop control strategy", an open-loop control is the simplest strategy we can design: it simply relies on the predictions of the model and does not take into account the information provided by measurements. In simple words, consider a model $\dot{x} = f(x, u, w, p), x(0) = x_0, y = g(x)$. Assume everything is known (control inputs, disturbances, initial conditions and parameters model) and further assume our objective is that y goes as close as possible to a setpoint $\overline{y}$. Only using – possibly intensive – simulations of the available model, we can simply try to find the control inputs u such that y indeed joins the target $\overline{y}$ as fast as possible. The most important advantage of this approach is obviously that it may be proposed even in the case the system is not equipped with sensors: in a first step, we build a database in simulating the model with as many conditions as possible. The obtained database allows any user to link output characteristics as a function of input values, including the available actuators for each of the possible configurations C1-C6. In a second step, comparing the required characteristics of the output (nitrogen level and its form) with those saved in the database, one can then establish which configuration and which set of functioning parameters are most suitable to obtain an output concentration y that is the closest to that one saved in the database (which is itself the closest to the desired $\overline{y}$). Then we simply have to apply these configurations and inputs to the system to obtain, theoretically, the required output.

Assume the objective is to successively obtain the nitrate concentrations reported in the first column of Table 2:

Table2: Required succession of nitrate concentrations and the best corresponding configurations found in the database



S^*_{NO3}	k_La_1	k_La_2	V_A	V_B	V_C	Q_{WAS}	Q_{RAS}	Q_{int}
15,2	100	300	1	1	0	400	$2 \times Q_{in}$	Q_{in}
7.5	100	150	1	1	1	300	Q_{in}	0
22	200	300	0	0	1	700	Q_{in}	Q_{in}
14.8	150	300	1	1	0	300	Q_{in}	0
7	100	250	1	1	0	400	Q_{in}	Q_{in}
15.1	150	200	1	0	0	300	Q_{in}	0

Taking into account the input and configuration parameters given in Table 2, we can then apply the change of input and configuration characteristics and obtain the output reported in Figure 3.

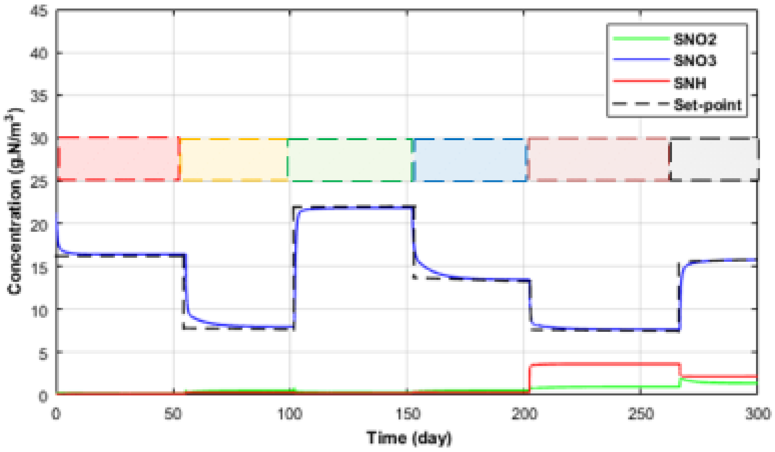


Figure 3: An open loop control strategy: switching each 50 days between the different configuration and input control values allows the control of the output concentrations of NH4 and NO3 in open loop (Aichouche, 2021).

Obviously, as long inputs and setpoints are known and constant and their combination is available in the database (that is: there exists a configuration and input characteristics such as the required outputs were obtained in simulation), the obtained results are very good. However, if this example indeed provides a proof for the concept of flexibility of the proposed platform, this approach exhibits important drawbacks. In particular, as recalled hereabove, it can only be applied if both the input characteristics of the water to be used (the disturbances) and model parameters are perfectly known in advance, and if the system is at steady state. In other words, such an approach would be perfect if the system to be controlled is perfectly described by the model, which is in practice never the case: input disturbances are usually varying with time and model parameters are never perfectly known nor necessarily constant. Thus, this approach is not robust at all with respect to these variables and cannot be used in practice: it is why closed-loop approaches should be preferred.

Closed-loop control strategy #1: a simple industrial control scheme for nitrate control

It is the rule rather than the exception that inputs are unknown. In such a case, closed-loop control (the fact to get online sensors providing information about the actual state of the system) is necessary. Once the setpoint has been generated using for instance the procedure described hereabove, the automatic control can be run and adapted using for instance a PID-like industrial control scheme which only makes use of the available actuators and measurements without directly using the available model of the process. A candidate for such a control strategy is the cascade controller represented in Figure 4a and 4b.

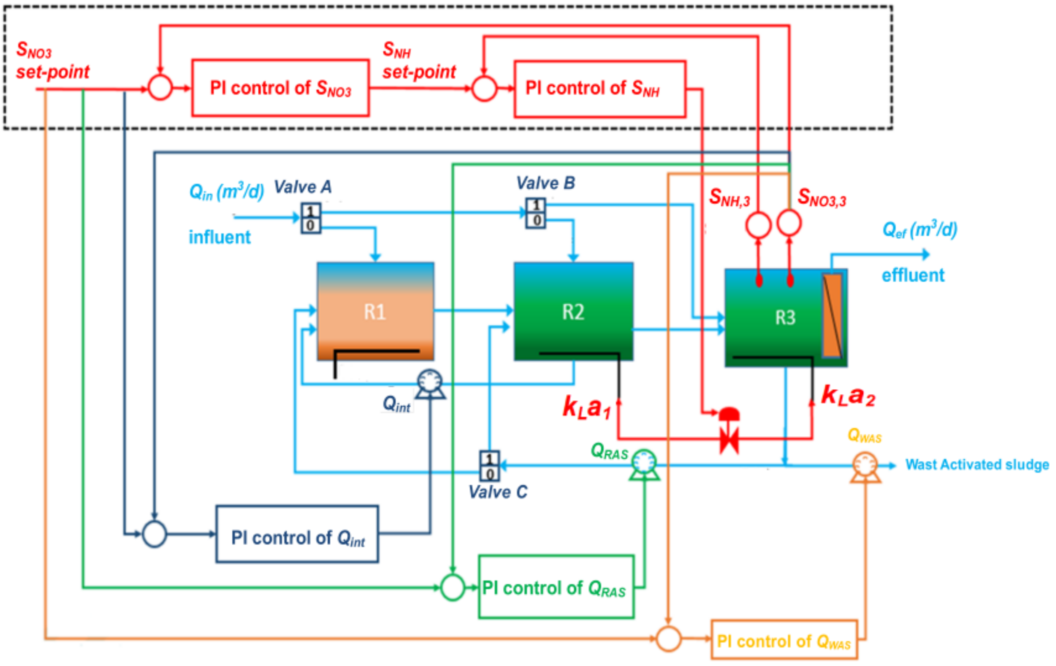


Figure 4a: Available actuators and measurements for the industrial control strategy

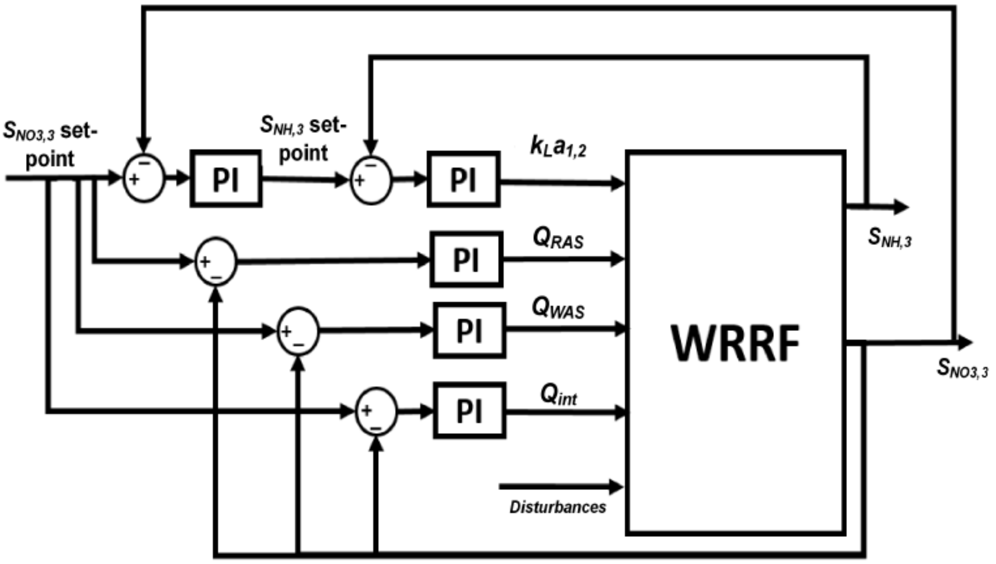


Figure 4b: Cascade control strategy #1 for the regulation of output nitrate concentration

An example of the output substrate concentrations obtained with such a strategy is given in Figures 5 using two distinct configurations (C1 and C3 assuming a total constant input nitrogen concentration of 50 mg/l over the whole period of time).

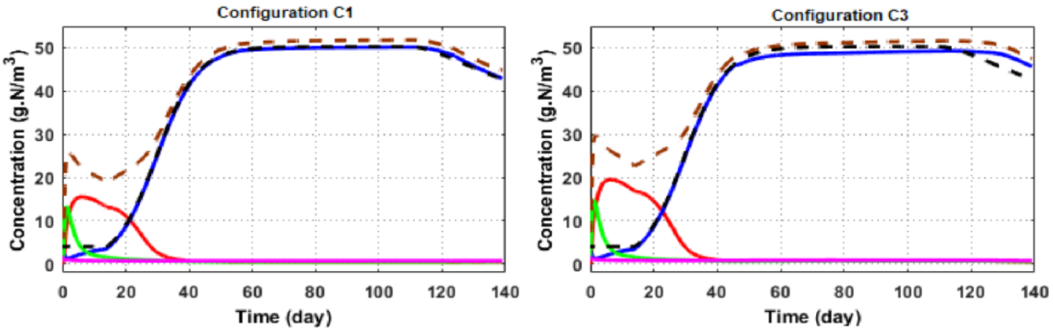


Figure 5: Closed-loop control of nitrogen needs for irrigation with C1 and C3 configurations - NO3 (blue), NH4 (green), NO2 (red) organic nitrogen (pink) concentrations, irrigation set-point (black dashed line) and total nitrogen in the effluent (brown dashed line).

Results show that the setpoint can satisfactorily be tracked as long as there is enough nitrogen in the wastewater to be treated, illustrating the notion of flexibility. As several configurations exhibit comparable results, one may need for different indices to be computed such as the quantity of nitrogen recovered for plants, or the total energy requirements which should be minimized and find the best compromise between profits and costs (data not shown).

Model predictive control

Alternative, more advanced, control strategies can be employed to deal explicitly with operational restrictions and the uncertainty over the influent disturbances. Model predictive control (MPC), specifically, is one such method which has become popular in many industrial applications (Forbes *et al.*, 2015). The approach consists of recursively (in time) determining the control actions for each plant actuator that optimize a given objective function, based on real-time measurements and a dynamical model of the plant. We propose an Output MPC architecture as in Figure 6.

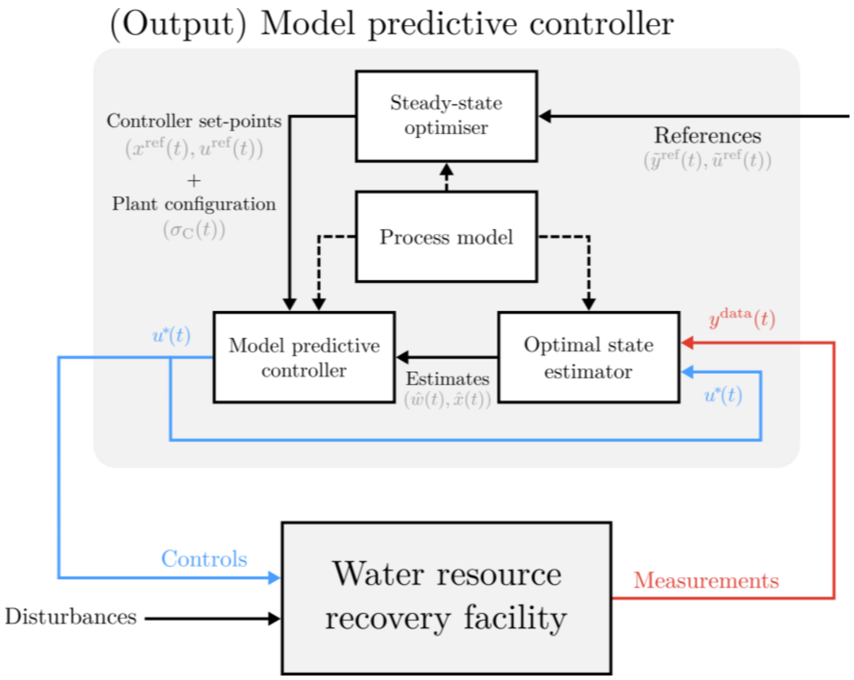


Figure 6: Output-MPC: Control architecture. The operation of the controller is based on the signals representing the state ($x(t)$), outputs ($y(t)$), disturbances ($w(t)$, and controls ($u(t)$) of the process. The function $\sigma_C(t)$ represents the switching mechanism to select a plant configuration (C1-C6).

In our model-based framework, at each time-step, the current state and disturbances to the process are obtained by an optimal state estimator. Based on this information, the predictive controller then determines an optimal sequence of actions over a future horizon to systematically drive the plant towards the desired set-points, while subjected to operational and dynamical constraints. In this strategy, the set-points to the controller are obtained by a steady-state optimizer as operating points that satisfy a reference in terms of the plant's outputs: In our case, reference trajectories of effluent nitrogen generated by the optimal operation of the crop irrigation systems. In particular, the steady-state optimizer should also be responsible for determining in real-time the most cost-effective plant configuration (C1-C6, Figure 2) that can be stabilized around each desired output profile.

In practice, a physical implementation of the proposed control strategy requires a dynamical model which is not only descriptive, but also tractable for the numerical routines used to solve each optimization problem. A common choice is to design quadratic objective functions and consider linear approximations of a first-principles model of the process: Such design choice results in convex optimization problems, which have stable and efficient numerical solutions (Boyd and Lieven, 2004). The performance of this controller in operating a benchmark activated sludge plant for producing reuse water of tailored quality has been investigated in (Neto *et al*., 2022).

Conclusions

The concepts of water on demand and flexibility of treatment systems must be developed and implemented to allow, in dynamic contexts, to adapt water quality to uses. Such concepts not only apply to agronomic needs but also to many others. Both in rural, peri-urban and urban areas, it is necessary to think globally, and dynamically to rethink the way we manage wastewater that definitely should be seen as resources:

- Flexible systems may be properly controlled to track setpoints generated by the appropriate coupling with crop and/or agronomic models both in terms of water quantity and quality to optimize criteria as productivity or nutrient washout;
- Dynamic control and adaptive systems may be used to address robustness issues with respect to systems that are only partially known and subject to disturbances;
- When used for agronomic purposes, appropriate sensors have to be installed when needed and their data processed in order to deliver the appropriate knowledge of actual state of soil and crops to be feedback for closing control loops.

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