Application of a Nonlinear Model Predictive Controller to the Anaerobic Digestion of Readily Biodegradable Wastes

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Abstract: A nonlinear model predictive controller for the anaerobic digestion of readily biodegradable substrates is presented. The controller aims to achieve a planned methane production, following a reference trajectory for the whole operation. Using an existing dynamic model of anaerobic digestion, the controller optimizes the operation conditions by conveniently manipulating a set of process variables such that the methane flow rate follows the reference trajectory. The controller works in a sequential approach, i.e., the plant trajectory is estimated over a prediction horizon with a simplified dynamic model of the process that includes only two biological reactions: *acidogenesis* and *methanogenesis*; then, the model predictions are optimized via a sequential quadratic programming method to match the desired trajectory. Due to the simplicity of the process model, the iterative optimization process is solved in a relatively short time. Both the dynamic model of the process and the optimization algorithm are implemented in MATLAB. The controller is tested in a simulation case study treating a readily biodegradable liquid effluent, where the same process model is used to mimic the measurements of the real plant.

Keywords: NMPC, Anaerobic Digestion, Biogas, Process control.

1. INTRODUCTION

One of the main continuous industrial processes currently available for the treatment of organic waste is anaerobic digestion (AD). It is a biological process catalyzed by a mixed culture of microorganisms that, in the absence of an external electron acceptor, transforms organic matter (solid and/or liquid) into a product called biogas, a gaseous mixture composed mostly of methane and carbon dioxide. Traditionally, this process has been successfully implemented in wastewater treatment plants to treat/reduce excessive biological sludge generated during secondary treatment (an aerobic biological process) of wastewater, and thus recover energy in the form of methane to be consumed in the plant itself. Other wastes such as manures, fruit and vegetable waste, oils and fats and industrial wastes have also been successfully treated by anaerobic digestion and co-digestion (Mata-Álvarez et al., 2014). Each of these wastes is characterized by a different composition and physicochemical conditions, which affect the degree of biodegradability of the waste and ultimately determine the operating strategy to be applied in a continuous digester.

The reaction mechanism of AD is complex; it includes a series of reaction steps in series and parallel, which are grouped into four main steps: 1) hydrolysis, 2) acidogenesis, 3) acetogenesis and 4) methanogenesis (Parker, 2005). The first three reactions are catalyzed by bacteria, and the last one by archaea. The overall kinetics of the reaction mechanism is determined by the hydrolysis and methanogenesis stages (which are the rate-limiting stages of the process), especially hydrolysis in cases where the waste has a higher concentration of organic solids. In contrast, the acidogenesis (formation of C3 - C5 organic chain acids) and acetogenesis (C2 acid) stages are relatively faster, which favors the formation of these C2 - C5 volatile fatty acids (VFA). The accumulation of these VFA can lead to severe acidification of the system, which negatively affects the pH of the digester and, consequently, the activity of biocatalysts. In general, a neutral or slightly alkaline pH (7.0 - 7.5) is considered adequate for the anaerobic digestion process. Finally, the growth kinetics of the different groups of microorganisms often follows a Monod kinetics, which implies a non-linear growth of the microbial population with respect to the concentration of the waste fed to the digester. This last characteristic makes the overall AD process a non-linear process.

In general, the dynamics of the process is slow, i.e., the process hydraulic retention time (HRT) is in the order of 20 - 40 days, and even longer depending on the solids content of the waste and its degree of biodegradability. Because AD is a non-linear process, which is difficult to model and uncertain, the operating strategy at the industrial level is usually conservative in terms of loading, i.e., a security margin is applied to the organic loading rate (OLR) to avoid organic overloading and acidification of the system. Consequently, industrial AD digesters (with sizes in the order of several thousand cubic

meters) are operated far from their maximum methane production potential to ensure the stability of the operation.

Since the dynamics of the AD process is slow and the process is non-linear, it is very useful to have a dynamic model of the anaerobic digestion process that allows estimating the characteristics of the gas and liquid effluents of a digester operating continuously. In this way, in a few minutes it is possible to obtain the simulated result of several months of operation from start-up to steady state, to study the feasibility by AD of a given organic waste, as well as to estimate the OLR profile that can be applied to the system to maximize methane production and, at the same time, to maintain the stability of the operation against overloads. Currently, the Anaerobic Digestion Model No. 1 (ADM1) is the reference model used for AD simulation (Batstone et al., 2002). The model considers the four main biological reactions: hydrolysis, acidogenesis, acetogenesis and methanogenesis; the physicochemical acid-base equilibria; and the liquid-gas transfer processes for CH_4, CO_2 and H_2 components. In addition, it considers particulate and soluble components for wastes and different groups of microorganisms as particulate components to catalyze the different biological reactions. Based on this model, other versions have been developed that incorporate new substrates and processes not initially included in ADM1, or adapted for co-digestion (Derbal et al, 2009; Arnell et al., 2016). In addition to the ADM1 model, simpler models have also been developed, such as the one developed by Bernard et al. (2001), which models the AD process with only two biological reactions (acidogenesis and methanogenesis) and only two groups of generic microorganisms (acidogenic and methanogenic). In total it results in only four/six differential equations. This model is very useful for the simulation of easily biodegradable liquid wastes that do not contain inhibitors, such as sugar industry wastes, ethanolic effluents, etc. Because of its simplicity and computational speed, the model of Bernard et al. (2001) has been used for the development of controllers based on process models (Nguyen et al., 2015; Steyer et al., 2006).

For anaerobic digestion there is no universal control algorithm. Depending on the waste characteristics and operating conditions to be used, a variety of controllers have been developed, using different combinations of controlled variables, and manipulated variables. In general, according to Jimenez et al. (2015), the most used controlled variables include methane flow rate, pH, liquid effluent COD or combinations of these, and as manipulated variable, mostly the dilution rate. Occasionally, OLR has also been used as a manipulated variable, or alkalinity as a controlled variable. The different types of controllers that have been developed for AD include classical PID controllers, fuzzy logic expert systems or neural networks. In addition, model predictive controllers were also developed for AD (Mauky et al., 2016; Ahmed and Rodríguez, 2020).

In the present work, a nonlinear model predictive controller (NMPC) for anaerobic digestion based on the process model developed by Bernard et al. (2001) is developed to estimate the set of manipulated variables to be applied to a biogas plant so as to achieve a given methane production trajectory. In this case, the biogas plant is also simulated by the model of Bernard et al. (2001). The aim of the paper is to demonstrate by simulation the implementation of an NMPC controller coupled to a simple model of the AD process.

2. NONLINEAR MODEL PREDICTIVE CONTROLLER

The NMPC control scheme is illustrated in Fig. 1. The procedure includes an optimization algorithm (with an objective function subject to a set of constraint equations and boundary conditions) and a simplified non-linear model of the AD process. The non-linear model predictive controller is designed as a tracking controller aiming at calculating a set of manipulated variables (control inputs, u) such that the controlled variable *methane production rate* (process output, y) follows a given reference trajectory y^{ref} on discrete time intervals.
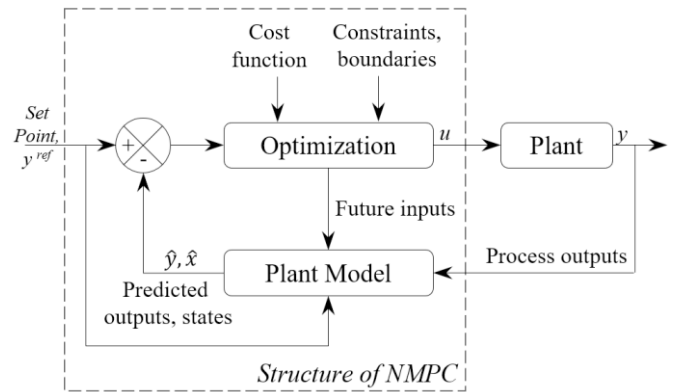

Figure 1. Scheme of the non-linear model predictive controller for anaerobic digestion.

2.1 Plant Model

The dynamic model for AD developed by Bernard et al. (2001) is adopted as the plant model to predict the process outputs ($\hat{y}$) and *states* ($\hat{x}$), as well as to estimate the future control inputs (u). In addition, the same model is used to mimic the real plant (x and y).

This simplified AD model assumes that the process can be reduced to two main stages: *acidogenesis*, where substrate S_1 is degraded by acidogens (X_1) and transformed into volatile fatty acids (S_2) and CO_2; *methanogenesis*, where volatile fatty acids (VFA) are degraded into CH_4 and CO_2 by methanogenic archaea (X_2). Mathematically, the model is defined as an ODE system, including the following states: microbial degraders X_1 and X_2, organic substrates S_1 and S_2, alkalinity (Z) and inorganic carbon (C).

$$\frac{dX_1}{dt} = \mu_1 X_1 - \alpha D X_1$$

$$\frac{dX_2}{dt} = \mu_2 X_2 - \alpha D X_2$$

$$\frac{dS_1}{dt} = D(S_{1in} - S_1) - k_1 \mu_1 X_1$$

$$\frac{dS_2}{dt} = D(S_{2in} - S_2) + k_2 \mu_1 X_1 - k_3 \mu_2 X_2$$

$$\frac{dZ}{dt} = D(Z_{in} - Z)$$

$$\frac{dC}{dt} = D(C_{in} - C) - q_C + k_4\mu_1 X_1 + k_5\mu_2 X_2$$

where:

$$q_C = k_{La}(C + S_2 - Z - K_H P_c)$$

$$P_c = \frac{\varphi - \sqrt{\varphi^2 - 4K_H P_T(C + S_2 - Z)}}{2K_H}$$

$$\varphi = C + S_2 - Z + K_H P_T + \frac{k_6}{k_{La}}\mu_2 X_2$$

$$q_M = k_6\mu_2 X_2$$

$$pH = -\log_{10}(K_b \frac{C - Z + S_2}{Z - S_2})$$

$$\mu_1 = \frac{\mu_{1\,max}S_1}{K_{S1} + S_1}$$

$$\mu_2 = \frac{\mu_{2\,max}S_2}{K_{S2} + S_2 + (S_2^2/K_{I2})}$$

C and C_{in} are the total inorganic carbon concentration (mmol/L); D is the dilution rate (d^{-1}); k_1 is the yield for substrate degradation; k_2, yield for volatile fatty acids (VFA) production (mmol/g); k_3, yield for VFA consumption (mmol/g); k_4 and k_5, yields for CO_2 production (mmol/g); k_6, yield for CH_4 production (mmol/g); K_b, equilibrium constant (mol/L); K_H, Henry's constant (mmol/L/atm); k_{La}, liquid-gas transfer constant (d^{-1}); K_{I2}, inhibition constant (mmol/L); K_{S1}, half-saturation constant (g/L); K_{S2}, half-saturation constant (mmol/L); P_C, CO_2 partial pressure (atm); P_T, total pressure (atm); q_C, carbon dioxide flow rate (mmol/L/d); q_M, methane flow rate (mmol/L/d); S_1 and S_{1in}, organic substrate concentration (gCOD/L); S_2 and S_{2in}, VFA concentration (mmol/L); X_1, concentration of acidogens (g/L); X_2, concentration of methanogens (g/L); Z and Z_{in}, total alkalinity (mmol/L); α is the fraction of bacteria in the liquid phase; μ_1, specific growth rate of acidogens (d^{-1}); $\mu_{1\,max}$, maximum acidogens growth rate (d^{-1}); μ_2, specific growth rate of methanogens (d^{-1}); $\mu_{2\,max}$ maximum methanogens growth rate (d^{-1}). Table 1 shows the values of the model parameters.

Table 1. Values of AD model parameters (Bernard et al., 2001).

Parameter	Value	Parameter	Value
k_1	42.14	C (t = 0)	65
k_2	116.5	C_{in} (t = 0)	60
k_3	268	D (t = 0)	0.34
k_4	50.6	S_1 (t = 0)	1.8
k_5	343.6	S_{1in} (t = 0)	9.5
k_6	453	S_2 (t = 0)	3.0
K_b	6.5E-7	S_{2in} (t = 0)	93.6
K_H	16	X_1 (t = 0)	0.8
k_{La}	19.8	X_2 (t = 0)	0.8
K_{I2}	256	Z (t = 0)	60
K_{S1}	7.1	Z_{in} (t = 0)	62.5
K_{S2}	9.28	α	0.5
$\mu_{1\,max}$	1.2	P_T	1
$\mu_{2\,max}$	0.74		

2.2 Optimization

The optimization objective of the predictive controller in Fig. 1 aims at minimizing the cost function J, expressed as:

$$\min_{\mathbf{u}} J = w_0 \sum_{t=1}^{t=h_p} \|y - y^{ref}\|^2 + \sum_{j=1}^{j=nm} w_j \Delta u_j^2$$

with $\quad \Delta u_j^2 = \sum_{t=1}^{t=h_c}\|u(t) - u(t-1)\|^2$

subject to

$$\dot{\mathbf{x}} = f(t, \mathbf{x}, \mathbf{u}) \ , \quad \mathbf{x} = \begin{bmatrix} X_1 \\ X_2 \\ S_1 \\ S_2 \\ Z \\ C \end{bmatrix} \ , \quad y = g(\mathbf{x}) \ , \quad \mathbf{u} = \begin{bmatrix} D \\ S_{1in} \\ S_{2in} \\ Z_{in} \\ C_{in} \end{bmatrix}$$

$$\mathbf{LB} \le \mathbf{u} \le \mathbf{UB} \ , \quad \mathbf{A} \cdot \mathbf{u} \le \mathbf{b} \ , \quad \mathbf{b} = \begin{bmatrix} D + \Delta D_{max} \\ S_{1in} + \Delta S_{1in\_max} \\ S_{2in} + \Delta S_{2in\_max} \\ Z_{in} + \Delta Z_{in\_max} \\ C_{in} + \Delta C_{in\_max} \end{bmatrix}$$

where y is the control variable *methane flow rate* (q_M); y^{ref} is the reference trajectory (setpoint) for methane production rate; h_p is the predictive horizon; h_c is the control horizon; nm is the number of manipulated variables ($\mathbf{u}$); $\mathbf{LB}$ and $\mathbf{UB}$ defines the lower and upper boundaries for $\mathbf{u}$. $\mathbf{A}$ is the matrix for inequality constraints applied to the manipulated variables, and $\mathbf{b}$ includes the maximum move rate values for $\mathbf{u}$. Finally, w_0 and w_j stands for a set of factors weighting the different terms of the cost function J.

Table 2. Parameters values of the optimization process

Parameter	LB	UB	Δu_{max}	Value
D	0	0.70	0.25	
S_{1in}	0	20	5.0	
S_{2in}	0	150	25	
Z_{in}	0	120	25	
C_{in}	0	120	25	
dt (in days)				0.1
h_p				10*dt
h_c				5*dt
w_0				95
w_j				1

2.3 NMPC implementation

The NMPC controller is implemented in MATLAB®, where the strategy adopted in this study is the so-called sequential approach; that is, the solution of the ODE system is computed independently from the NLP, in a two-stage process: 1) system simulation of AD process and 2) optimization. Firstly, the ODE system of the anaerobic digestion model is solved using the MATLAB solver *ode45* to obtain the model predictions for NMPC optimization. Secondly, the NMPC optimization is conducted using the *fmincon* MATLAB function that solves the sequential quadratic problem (SQP). In addition, the gradient and Hessian of the objective cost function are not provided; instead, *fmincon* solver performs a numerical

estimation of both gradient and Hessian. Finally, the simulations are run on a computer equipped with an Intel Core i5 430M Processor (2.26 GHz) and 4 GB RAM and 64-bit Windows 10 operating system.

3. RESULTS AND DISCUSSION

The simulation of an AD experiment treating wine distillate waste (Bernard et al. 2001) is carried out with the NMPC controller, where this effluent is very readily biodegradable by anaerobic digestion. An organic loading rate (OLR) between 3.2 - 4.2 gCOD/L/d and HRT of 3 - 4 days is applied, and a total operation of 10 days is simulated. An initial *setpoint* for methane production is set at 50 mmol/L/d at time zero and follows a reference trajectory with stepwise increases of 5 mmol/L/d every 2.5 days up to 65 mmol/L/d in the days 7.5 - 10.0. The sampling rate (dt) is 0.1 d. The predictive controller is applied using a prediction horizon h_p of 1 day (10 steps dt), and a control horizon h_c of 0.5 days (5 steps dt). In total, the NMPC controller performs 100 sequences of prediction and optimization from t = 0 d to t = 10 d, with 1-day prediction horizon, a horizon moving forward every dt.

Figures 2, 3, and 4 show the results for the control variable, $y = q_M$, the process variables, $x = \{X_1, X_2, S_1, S_2, Z, C\}$, and the manipulated variables, $u = \{D, S_{1in}, S_{2in}, Z_{in}, C_{in}\}$. The methane production flow q_M (Fig. 2), follows a trajectory practically superimposed to the reference trajectory established as setpoint for the entire operation, y^{ref}. To achieve the required methane flow rate, the manipulated variables change their values throughout the operation (Fig. 3). Among these, the dilution rate (D) and the concentrations of the organic substrates (S_1 and S_2) are the ones that are adjusted the most over time. This is an expected result, since, if a higher methane flow rate is to be produced, the flow rate of the feeding should increase as well as the organic content of the feeding. On the contrary, alkalinity (Z) and inorganic carbon (C) variables do not contribute to higher methane production. Therefore, their values in the feeding remained practically unchanged throughout the operation. Their contribution is focused on another aspect of the AD process: the stability of the operation. A digester should have a certain level of alkalinity and bicarbonate content (the buffering agent in the broth) to maintain the pH in a suitable range to (i) guarantee the activity of the biocatalyst and (ii) avoid some inhibition, acidification, and overloading processes. In this example, it has been assumed that the alkalinity and inorganic carbon content provided by the feed is sufficient to maintain the pH close to neutral (pH data not shown). In those cases where pH is considered a control variable, these two manipulated variables (Z and C) would play a more relevant role during the optimization.

It is also worth noting that in general practice only the dilution rate (D) is manipulated in digesters treating a single residue. The composition of the organic content cannot be customized in its constituents. Only some inorganic additives could be used to improve nutrients or alkaline content. On the other hand, when several residues are treated under anaerobic co-digestion, it would be possible to consider customizing the proportions at which those substrates are blended. This is in

fact the target application we had in mind while developing this preliminary simulation benchmark.
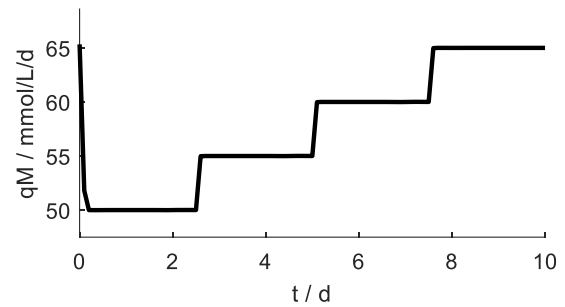

Figure 2. Dynamic response of the control variable q_M by applying the NMPC controller.
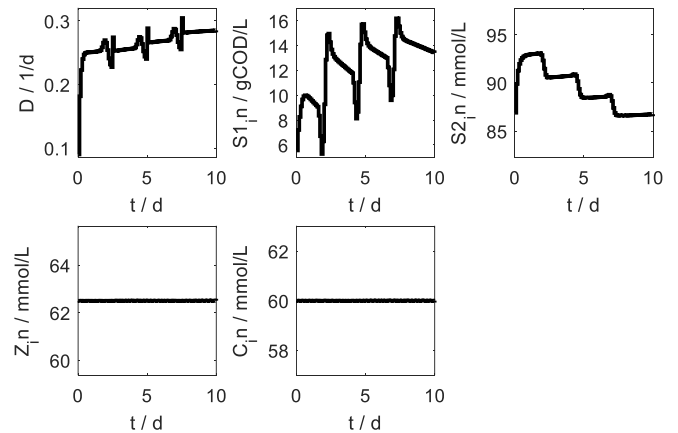

Figure 3. Dynamic response of the manipulated variables $u = \{D, S_{1in}, S_{2in}, Z_{in}, C_{in}\}$ by applying the NMPC.
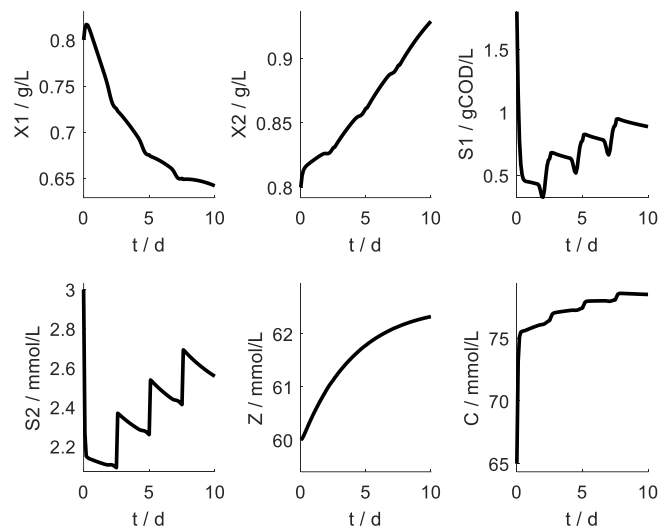

Figure 4. Dynamic response of the process variables, states = $\{X_1, X_2, S_1, S_2, Z, C\}$ by applying the NMPC.

Finally, Fig. 4 shows how the *states* change over time, due to the action of the manipulated variables. The concentrations of

acidogenic bacteria (X_1) and methanogenic archaea (X_2) change their relative concentration as the methane production setpoint increases. Kinetically speaking, the acidogenic stage is faster than the methanogenic stage; consequently, the system will tend to increase the methanogenic microbial community with respect to the acidogenic community to better balance the net flows of VFA generation and uptake, without causing the accumulation of intermediate products. An interesting case is the profile of S_1 and S_2 substances in the reactor. It is evident that the higher the concentration of S_1 in the feed stream, the higher the concentration of this component inside the reactor, as it happens in this study. However, in the case of S_2, despite having decreased its contribution in the feed throughout the operation, the concentration of S_2 in the digester increases. This is because S_2 is a reaction product secreted by the acidogenic bacteria when metabolizing the substance S_1. In this case, as more S_1 is available in the reactor, there is an increase in S_2 levels when higher concentrations of S_1 are degraded. Finally, the alkalinity Z and inorganic C values in the reactor increase slightly because of the acidogenic and methanogenic reactions that produce both carbon dioxide, an inorganic component that dissolved in water provides alkalinity to the system.

3.1 Performance of NMPC

Some statistical data on the performance of the NMPC controller can be seen in Figure 5. For a total operating time of 10 days, with a prediction horizon of 1 day, a control horizon of 0.5 days, and a sampling interval of 0.1 days, the predictive controller takes about 20 - 25 min to solve the 100 prediction/optimization sequences (k).

The choice of the control horizon (h_c) and the prediction horizon (h_p) is linked to the process dynamics. The HRT will depend on the characteristics of the waste (solids content, organic matter content, biodegradability, …) and the type of reactor used. In this study, an anaerobic upflow-fixed-bed reactor with recirculation treating an easily biodegradable liquid waste allows short HRT of 2 to 4 days. Finally, the choice of h_p and h_c should compromise both the execution of the control algorithm in a reasonable time and the feasibility of plant measurements (particularly those process variables that are determined through off-line measurements).

Due to the simplicity of the dynamic anaerobic digestion model used, the optimizer can evaluate the model hundreds of times over the prediction horizon to minimize the cost function J. The values of the cost function J (fcost in Fig. 5) are generally kept very low and close to zero, and only in those periods coinciding with the abrupt step changes of the manipulated variables, the values of the cost function are very far from zero. To minimize the cost function in each sequence k, the SQP algorithm executes between 20 - 40 iterations, in which it evaluates the model function between 600 - 1000 times approximately, to finally solve the optimization problem in an average time of about 15 s for each k sequence of horizon prediction.

With these data we can conclude that, at least for a real AD system in which the reduced anaerobic digestion model simulates well the degradation of the organic waste, we can

expect a fast response of the controller with enough time to modify the manipulated variables in time.

One of the most important limitations of the simple AD model used in this study is that it is only valid for readily biodegradable liquid wastes. To simulate the degradation of complex solid wastes, a more sophisticated model, for example, the ADM1 reference model (Batstone et al. 2002) could be used, which includes the disintegration and hydrolysis stages and considers the inhibition processes that can occur due to the presence of certain compounds. In that case, the optimization procedure will be much slower. In any case, since the dynamics of the anaerobic digestion process are slow (hydraulic residence times of 20 - 40 days) and the changes that occur in the operation are performed with a frequency of days to weeks, we can be confident that the optimizer response could be obtained in time, even if it is computationally more time-consuming.

Finally, in the situation when some process variables required for the model prediction cannot be measured in the real plant, the NMPC controller architecture should incorporate an observer (e.g, a Kalman filter or receding horizon observer). This issue is not discussed in this preliminary study.
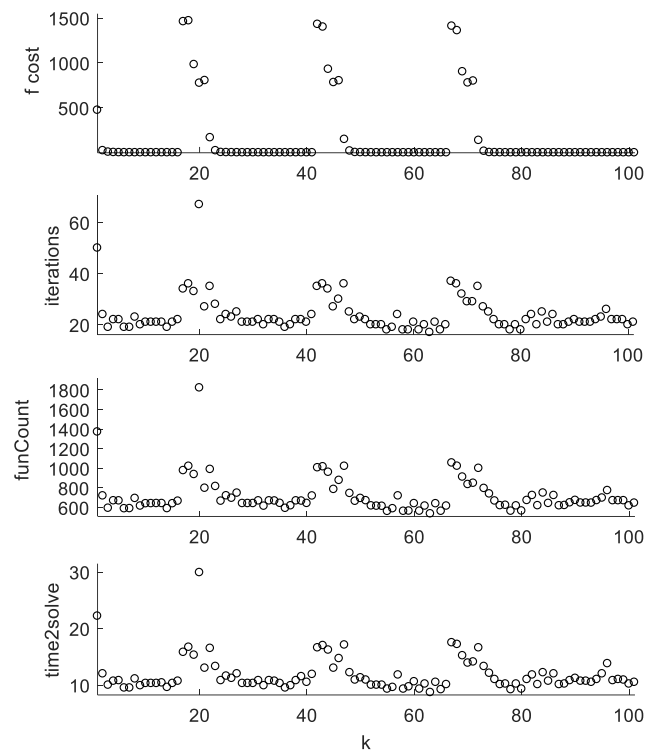

Figure 5. Metrics assessing the performance of the optimization algorithm: cost function J (fcost), number of iterations of SQP algorithm, number of functions evaluations (funCounts), and time elapsed to solve the sequence for the horizon prediction k (time2solve).

3.2 Future perspective. NMPC for co-digestion

Due to the simplicity of the AD model by Bernard et al. (2001), the application of the NMPC controller is limited to biodegradable liquid residues that do not contain recalcitrant

compounds. In on-going developments, an existing dynamic model of the process based on ADM1, implemented in MATLAB® and adapted for anaerobic co-digestion (García-Gen et al., 2015), will be used as plant emulator. A simple dynamic model will be kept as predictor in the NMPC controller, which will require parameter identification and sensitivity analysis in order to determine the critical parameters impacting the controller robusrtness at most.

The simple predictor could be either based on AM2 (Bernard et al., 2001), or derived through a simplification of the reaction pathway considered in the detailed model of (García-Gen et al., 2015), suppressing the acidogenic stage, and keeping hydrolysis, acetogenesis and the two methane production reactions (acetoclastic methanogenesis and hydrogenotrophic methanogenesis). This would allow reducing some state variables and at the same time guarantee a good estimation of gas and liquid effluents while maintaining the flexibility to treat more complex solid wastes under co-digestion. Eventually, the application of the NMPC controller to co-digestion could become a powerful tool to verify the feasibility of a given waste mixture as the feed for a biogas facility.

4. CONCLUSION

A NMPC controller for anaerobic digestion of readily biodegradable substrates could be used to optimize the operating conditions of a continuous biogas plant to meet the required methane flow rate production by using a simplified dynamic model of the anaerobic digestion and an optimization algorithm based on a sequential quadratic programming method. The architecture was successfully tested in a simulation environment where the AD model was also used to mimic the real plant measurements.

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