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Nonlinear Model Predictive Substrate Feed Control of Biogas Plants

Daniel Gaida, Christian Wolf, Thomas Bäck, and Michael Bongards

Abstract—**Optimal substrate feed control of biogas plants is a complex and challenging task due to the nonlinearity of the anaerobic digestion process, which produces biogas from biodegradable input material. In this paper a nonlinear model predictive control (NMPC) scheme is applied to optimally control the substrate feed of an agricultural biogas plant. The implemented algorithms are investigated in a simulation study using a validated simulation model of a full-scale biogas plant. Process states are estimated using a recently developed state estimator. Results show that this approach is very feasible providing the plant operator with a gain of 550 € per day compared to previous operation.**

I. Introduction

The digestion of energy crops as well as organic degradable waste in so-called biogas plants to produce biogas has proven to be a very promising technology for renewable electrical and thermal energy production [1, 2]. Biogas is a mixture of methane, carbon dioxide and a few other gases and is produced in digesters, which provide an anaerobic environment.

Due to the fact that valuable resources such as energy crops are fed to the digesters to produce biogas, an efficient use of the available substrates should be the primary goal. It is a valid assumption that an efficient use of substrate is more likely if a mix of several substrates is fed to a digester instead of solely one substrate [3]. But, as the anaerobic digestion process is high dimensional and has a nonlinear behavior, predicting the biogas yield of different substrate mixtures is a challenging task. Nevertheless, a reliable estimator for biogas production is needed so that control algorithms can be applied to optimally control the substrate feed of biogas plants.

In 2002, the Anaerobic Digestion Model No. 1 (ADM1) [4] was introduced, a complex mathematical model which can be used for predicting biogas production on the basis of substrate mixtures [5]. Using a model of a biogas plant, which is based on ADM1, a nonlinear model predictive control (NMPC) algorithm was developed, which allows an optimal substrate feed control for biogas plants [6]. In [6] optimality was defined as a balance between substrate/energy costs and the revenue from the electrical/thermal energy produced. Furthermore, constraints ensure stable plant operation, while maintaining a high organic loading rate. These criteria satisfy the above stated goal of an efficient use of substrates and furthermore increase the economic benefit of biogas plant operation. Nevertheless, the proposed approach is independent of the defined measure of optimality, meaning that this measure can be defined arbitrarily to address special requests from plant operators.

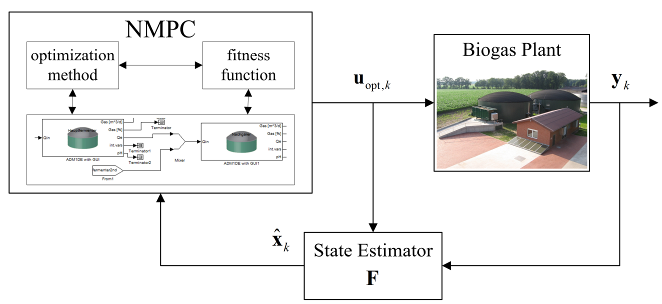

Fig 1. Nonlinear Model Predictive Control scheme for substrate feed control of biogas plants. The symbols used in this figure are defined in section I.

In Fig. 1 a standard NMPC scheme is sketched, which visualizes the control loop developed and used in this paper. The NMPC uses a mathematical model of the controlled biogas plant for prediction, a ‘fitness function’ defining optimality, and an optimization method used to solve the substrate feed optimization problem. As optimization methods stochastic, population based methods are employed, such as Covariance Matrix Adaptation Evolution Strategy (CMA-ES) [7], Differential Evolution [8] or Particle Swarm Optimization (PSO) [9]. These methods have the advantage that they do not get easily stuck in local optima when being applied to non-linear optimization problems. On the other hand, there is no guarantee that they will find the global optimum or even return a solution close to the global optimum. The substrate feed optimization problem is solved by evaluating different substrate mixtures, chosen by the optimization method, using the simulation model of the biogas plant.

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D. Gaida is with the Institute of Automation & Industrial IT, Cologne University of Applied Sciences, Gummersbach, D 51643 Germany (corresponding author, phone: 0049-(0)2261-81966359; fax: 0049-(0)2261-819676469; e-mail: daniel.gaida@fh-koeln.de).

C. Wolf, and M. Bongards are with the Institute of Automation & Industrial IT, Cologne University of Applied Sciences, Gummersbach, D 51643 Germany (e-mail: christian.wolf@fh-koeln.de, michael.bongards@fh-koeln.de).

T. Bäck is with the Leiden Institute of Advanced Computer Science, Leiden University, Leiden, CA 2333 the Netherlands, (e-mail: baeck@liacs.nl).

The compulsory state estimator [10] in Fig. 1, estimating the current states of the controlled biogas plant, is needed so that the simulations performed during the optimization process can be started from the current estimate of the biogas plant's state. Here, the state of a biogas plant is defined by the state vector of the ADM1 implementation. In [11] a state estimator for biogas plants was developed using pattern recognition methods. This state estimator is used in this paper to provide the NMPC with up-to-date estimates of the state of the controlled biogas plant.

There are many contributions in the literature on closed-loop control of biogas plants or substrate feed optimization (e.g. [12–15]). But, to the authors' knowledge the approach proposed in this paper is the only one, which allows for an optimal substrate feed closed-loop control for biogas plants by optimizing a user-defined optimality criterion. Using this approach, it becomes possible to adapt the substrate feed composition in advance, e.g. in case one substrate runs out, to get a smooth transition between changing substrate feeds. Furthermore, the substrate mix is changed automatically in cases when substrate parameters or the fermentation biology changes, such that an optimal operating state for the anaerobic digestion process is maintained.

The ADM1 based simulation model, the developed NMPC and the state estimator are presented in the following section I. In section II these algorithms are investigated in a simulation study using a validated simulation model of a full-scale agricultural biogas plant. Section III concludes this paper with a discussion and summary of results.

I. Methods

A. Biogas Plant Modeling

The ADM1 is a very popular and the most complex mathematical model used to simulate the anaerobic digestion process (for a review see [16]). Recent work has shown that using this model full-scale agricultural biogas plants can be reliably modeled [17–19]. ADM1 is a structured model incorporating disintegration and hydrolysis, acidogenesis, acetogenesis and methanogenenesis steps.

In this paper a MATLAB® implementation of the ADM1 is used, operating in a 37 dimensional state space. All implementations in this paper were done in an environment provided by a MATLAB toolbox for biogas plant modeling, optimization and control published by Gaida et al. [20]. In this toolbox ADM1 is implemented as a stiff differential equation (DE) system, solved with MATLAB's ode15s solver. Both for the model predictive control and the state estimator a model of the biogas plant to be controlled is needed. Therefore using this MATLAB toolbox a sophisticated model of a biogas plant can be built, calibrated and validated, and used in the context of this paper. The model is implemented using Simulink® [21].

B. Nonlinear Model Predictive Control

In this paper basically the NMPC implementation presented in [6] is used to achieve all results. In Fig. 2 the pseudo-code of this NMPC method for optimally controlling biogas plants is sketched. In this implementation a detailed model of a biogas plant, incorporating the ADM1, is used for prediction. In Fig. 2 this model is represented by the nonlinear state vector function $\mathbf{f}_{\text{ADM1}} : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^n$. In this Simulink model not only the anaerobic digestion process is modeled but also components such as combined heat and power plants, a heating to heat the digesters and pumps to feed the substrates and pump the sludge. Based on this extensive model of a biogas plant the needed process values

Let $m \in \mathbb{N}^+$ be the number of available substrates and $n \in \mathbb{N}^+$ the dimension of the modeled state vector. Here, due to the ADM1, $n = 37$.
Set control horizon $T_C \in \mathbb{R}^+$ and prediction horizon $T_P \in \mathbb{R}^+$ with $0 < T_C \le T_P$.
Set substrate feed lower $\mathbf{LB} \in \mathbb{R}^m$ and upper boundaries $\mathbf{UB} \in \mathbb{R}^m$ with $\mathbf{UB} \ge \mathbf{LB}$.

Set optimal substrate feed, at $k = 0$, $\mathbf{u}_{\text{opt},0} \in \mathbb{R}^m$ to the current substrate feed of the biogas plant.

For $k = 1, 2, 3, \ldots$

1. Estimate the current operating state of the real biogas plant $\hat{\mathbf{x}}_{k-1} \in \mathbb{R}^n$ [11].

2. Define substrate feed boundaries $\mathbf{lb} \in \mathbb{R}^m$ and $\mathbf{ub} \in \mathbb{R}^m$ such that:
$\mathbf{lb} := \max\left((1-c) \cdot \mathbf{u}_{\text{opt},k-1}, \mathbf{LB}\right)$,
$\mathbf{ub} := \min\left((1+c) \cdot \mathbf{u}_{\text{opt},k-1}, \mathbf{UB}\right)$,
$c \in (0,1)$, satisfying $\mathbf{lb} \le \mathbf{ub}$

3. Find optimal substrate feed $\mathbf{u}_{\text{opt},k}$ minimizing the fitness function $F : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}$:

$$\mathbf{u}_{\text{opt},k} := \arg\min_{\mathbf{u} \in \mathbb{R}^m} F\left(\mathbf{x}\left(T_P\right), \mathbf{u}\right)$$

w.r.t. $\mathbf{lb} \le \mathbf{u} \le \mathbf{ub}$
$\mathbf{x}'(\tau) = \mathbf{f}_{\text{ADM1}}\left(\mathbf{x}(\tau), \mathbf{u}(\tau)\right)$
$\mathbf{x}(0) = \hat{\mathbf{x}}_{k-1}$
$\mathbf{u}(\tau) = \mathbf{u} = \text{const.} \forall \tau \in \left[0, T_P\right]$

4. Apply optimal constant substrate feed $\mathbf{u}_{\text{opt},k}$ to the real biogas plant for control horizon T_C.

End For

Fig 2. Pseudo-Code of NMPC for biogas plants to evaluate the fitness function (such as costs, energy production, etc…) can be calculated [17]. In the current NMPC implementation there are a few particularities that will be discussed in the next two paragraphs.

As can be seen in the third step of the pseudo-code currently the fitness function F is only evaluated at the end of the prediction horizon T_P, thus the stage cost, as defined in [22], is set to zero. This is done, because in the end only the fitness of the steady-state solution matters. This is because biogas plants are usually operated in steady-state and the primary control goal is to keep the biogas plant at its optimal steady-state. To circumvent possibly occurring problems in the not observed time period $\tau \in [0, T_P)$, such as a too high variation in the substrate feed, in the second step of the pseudo-code the substrate feed boundaries $\mathbf{lb}, \mathbf{ub} \in \mathbb{R}^m$ are centered around the current substrate feed $\mathbf{u}_{\text{opt},k-1}$ such that the substrate feed range is always smaller as the maximal range defined by $\mathbf{LB}$ and $\mathbf{UB}$. Looking at this implementation one could raise the question why we use a dynamical and not a steady-state model for prediction. A dynamical model is used because in a future implementation a stage cost will be included, which also contains a penalty term for the control variable. So the current implementation is just a work-around until the final one, currently under development, is available.

As a second particularity (in step 3) it can be seen that the substrate feed $\mathbf{u}(\tau)$ is kept constant over the control and prediction horizon, T_C, T_P respectively. This restriction due to the current implementation of the NMPC algorithm will be removed in the near future as well.

The most significant difference between the implementation used in this paper compared to [6] can be found in step 1 of the pseudo-code. In this paper the biogas plant's state is estimated using [11], whereas in [6] the biogas plant's state was not estimated but just taken from the controlled model of the biogas plant. This was possible because in [6], as well as in this paper, a biogas plant model and not a real biogas plant is controlled, as can be seen in the results section below.

C. State Estimation of Biogas Plants

In [11] a state estimator for biogas plants was developed. The implemented state estimator is a nonlinear transfer function, whereas the functional connection between in- and outputs is created using machine learning methods. In [11], four different classification and feature extraction methods were applied, namely LDA [23], GerDA [24], a linear classifier, and Random Forest [25]. In this paper, we just present the results obtained with Random Forest. Random Forest forms an ensemble of unpruned decision trees [26], whereas classification is performed by taking the majority vote of the decision trees.

The transfer function $\mathbf{F} : \left(\mathbb{R}^p\right)^{M+1} \times \left(\mathbb{R}^m\right)^{N+1} \to \mathbb{R}^n$ used for state estimation has the form

$$\hat{\mathbf{x}}_{k-1} = \mathbf{F}\left(\left(\mathbf{y}_i\right)^{k-M-1,k-1}, \left(\mathbf{u}_{\text{opt},i}\right)^{k-N-1,k-1}\right) \qquad (1)$$

using the notation $\left(\mathbf{y}_i\right)^{k-M-1,k-1} := \left\{\mathbf{y}_{k-M-1}, \ldots, \mathbf{y}_{k-1}\right\}$ with $\mathbf{y} \in \mathbb{R}^p$ being the vector of $p \in \mathbb{N}^+$ measured process variables obtained from the biogas plant. Thus, to estimate the current state of the plant $\hat{\mathbf{x}}_{k-1}$ the last $M+1$, $M \in \mathbb{N}^+$, measurement values of the process variables are taken into account, such as the substrate feeds, which were applied to the plant for the last $N+1$, $N \in \mathbb{N}^+$, instances. As measurements the following $p = 4$ process variables are assumed to be measurable for each digester separately:

- pH value in the liquid phase of the digester [-]
- biogas production [m³/d]
- methane concentration of the biogas [%]
- carbon dioxide concentration of the biogas [%].

For each of these process variables standard measurement equipment is commercially available and is often already installed on biogas plants [27].

An important difference between the state estimator formulated in (1) and the conventional state estimation algorithms such as the Extended Kalman Filter (EKF) is, that an EKF needs an initial state estimate and the state estimator in (1) does not [10]. For the application of biogas plant control using ADM1 this is an advantage because giving a plausible initial state estimate for a real biogas plant is very difficult if feasible at all.

Random Forest learns a pattern between the given input, namely the measured process values and substrate feeds, and the needed output data, namely the state estimate of the biogas plant. Therefore, a dataset of corresponding input/output samples has to be produced. As the state of a biogas plant, defined by the ADM1, is very complex, as stated above, it is impossible to measure the state in a feasible way. Therefore, the dataset has to be produced doing exhaustive simulations with a validated model of the biogas plant to be controlled. To simplify the pattern recognition process, the range for each state vector component $\hat{x}_{j,k}$ is clustered into 10 equally spaced classes, $\hat{\mathbf{x}}_k := \left(\hat{x}_{1,k}, \ldots, \hat{x}_{j,k}, \ldots, \hat{x}_{n,k}\right)^T$. Splitting this new dataset into a training and a test dataset Random Forest can learn the functional behavior of the state estimator $\mathbf{F}$. Evaluating the Random Forest based state estimator, using the test dataset, it was shown in [11] that mean classification error rates below 13 % can be achieved.

As the state estimator just returns a class label for each state vector component $\hat{x}_{j,k}$ based on the input variables, the real value for each component is in between a lower and upper boundary defined by the previously applied splitting of the state vector components into 10 classes. Instead of using the center values in between these lower and upper boundaries (named $\mathbf{lb}_\mathbf{x} \in \mathbb{R}^n$ respectively $\mathbf{ub}_\mathbf{x} \in \mathbb{R}^n$) we use that state vector as current state estimate, whose maximum norm of its derivative is minimal. Thus the current state estimate $\hat{\mathbf{x}}_{k-1}$ is defined as:

$$\hat{\mathbf{x}}_{k-1} := \arg \min_{\mathbf{lb}_\mathbf{x} \leq \mathbf{x} \leq \mathbf{ub}_\mathbf{x}} \left| \mathbf{f}_{\mathrm{ADM1}} \left(\mathbf{x}, \mathbf{u}_{\mathrm{opt},k-1} \right) \right|_\infty . \tag{2}$$

In (2) we try to find a steady-state solution for all states $\mathbf{x}$ inside the allowed range $\mathbf{lb}_\mathbf{x} \leq \mathbf{x} \leq \mathbf{ub}_\mathbf{x}$. Thus, using this definition we try to increase the chance that simulations starting at $\hat{\mathbf{x}}_{k-1}$ (step 3 of the pseudo-code in Fig. 2) converge to a steady-state solution respectively converge at all.

II. RESULTS

In this chapter the results are presented. Therefore, the setup sketched in Fig. 1 is implemented in MATLAB. In the performed experiments, the simulation model of the biogas plant used for prediction is also used as a surrogate for the full-scale biogas plant. Thus, the results shown here reflect the results which could be obtained given perfect knowledge on the behavior of the real biogas plant. The NMPC and the state estimator are implemented as described above.

A. *The Biogas Plant*

The biogas plant under consideration is a full-scale agricultural biogas plant with an electrical power output of 750 kW located in Germany. The plant contains two digesters with a volume of about 3000 m³ each. Only the first digester is fed with substrates including maize, grass and manure.

B. *Experimental Setup*

With the experiments done, we tried to show that it is possible to control a model of a full-scale biogas plant using the developed NMPC and the state estimator. In [6] it was already shown that, using a perfect state estimator, which just returns the current state of the biogas plant model as its state estimate, it is possible to optimally control the substrate feed of the model of a full-scale biogas plant. Thus, in the experiments carried out in this paper we compare the control results that were obtained with the perfect state estimator with the performance of the NMPC equipped with the more realistic state estimator developed in [11]. Therefore two experiments were carried out with identical settings, one with the perfect and one with the real state estimator. In both experiments the settings shown in Table I were used. As substrates we used maize silage, manure and the solid fraction of manure, i.e., $m = 3$. The values given in $\mathbf{LB}, \mathbf{UB}, \mathbf{u}_{\mathrm{opt},k}$ (see Table I) are given in the same order as the substrates are named in the sentence above.

The operating state, in which the control is started, $\mathbf{u}_{\mathrm{opt},0}$, is suboptimal for the biogas plant at hand.

Table I: Control settings of the experiments

control settings	
$T_C = 7\ d$	$T_P = 250\ d$
$\mathbf{LB} = (20, 10, 0)^T\ \frac{m^3}{d}$	$\mathbf{UB} = (40, 30, 5)^T\ \frac{m^3}{d}$
$\mathbf{u}_{\mathrm{opt},0} = (30, 15, 3)^T\ \frac{m^3}{d}$	$c = 0.05$

Therefore, the task of the NMPC will be to find the trajectory to a better, if possible the optimal, operating state for the biogas plant.

A prediction horizon T_P of 250 days seems to be quite high, compared with the hydraulic retention time of the plant, which in this case is about 100 days. This is justified as follows. As the control operates the plant towards a high loading rate the VFA/TA (volatile fatty acids / total alkalinity) value is very near its allowed upper boundary, as it is defined in the fitness function. Thus, experiments carried out with a prediction horizon of 150 and 200 days resulted in equally good results over the prediction horizon. But, a steady-state simulation with the final substrate feed resulted in a slightly worse fitness value, because at equilibrium the VFA/TA value violated its upper boundary. The reason is that sometimes after 150 respectively 200 days the model is not yet in its steady-state, such that the final VFA/TA value could be underestimated. Using a prediction horizon of 250 days the final VFA/TA value is predicted more accurately resulting in better results.

As optimization method Covariance Matrix Adaptation Evolution Strategy (CMA-ES) [7] is used. CMA-ES belongs to the family of evolution strategies, which are stochastic methods often used for numerical optimization of nonlinear optimization problems [28]. Therefore CMA-ES belongs to the population based methods; the population size here is set to 8 and the number of generations to 4. Due to the parameter c (see Fig. 2) the domain of the optimization variable used to solve the substrate feed optimization problem is very small. This is why such small numbers for the population size and the number of generations may be chosen. A parameter study performed in [6] showed that with such small numbers only slightly less good results are achieved, with the benefit of much less time spent for optimization.

The fitness function is defined to be a weighted sum of the net income (income from selling electrical and thermal energy less the operating energy and substrate costs) and a number of operating stability constraints. The constraints considered include a limit on the pH value inside the digesters, a maximum dry matter content of the substrate mixture (26 % FM), a maximum VFA/TA value of 0.4 [29] and a minimum methane fraction of 50 % inside the produced biogas.

The problem defined in equation (2) is solved using CMA-ES with a population size of 10 and 5 number of generations.

C. Results

In Fig. 3 the progress of the fitness values for both experiments are plotted. The total time available for the control to change from the current to the optimal substrate feed should be around 100 days. Using a control horizon T_C of 7 days k in Fig. 2 is running from 1 to 15, resulting in a total time of 105 days, called simulated period. All simulations (over control and prediction horizon) performed in each experiment are plotted in the figure. In Fig. 3 (a) all fitness values are plotted including outliers. Outliers are caused by particular simulations starting at the state estimates of the real state estimator and lead to a very slow simulation progress. Possible reasons are misclassification, sudden change in plant operation, etc. Therefore each simulation is stopped at the latest after 30 minutes to avoid an exhaustion of the available working memory. The fitness value then can be quite bad (so called outliers), e.g. such as in Fig. 3 in the neighborhood of the simulation number 200. In Fig. 3 (b) the range of the y-axis is limited to the interesting range of the fitness values. As can be seen the progress of the fitness values of both experiments is quite similar (correlation coefficient of r= 0.8 for the data without outliers). Thus it is shown that it is possible to optimally control the substrate feed of a biogas plant by only

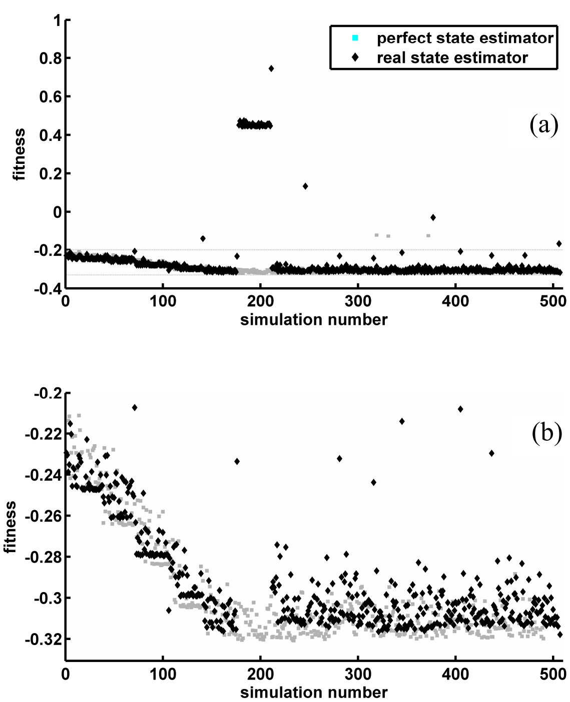

Fig 3. Comparison of the progress of optimization. (a) All fitness values, including outliers. (b) Same data as in (a) with zoom on y-axis, ignoring outliers. The range of the y-axis of (b) is visualized with two dotted lines in (a). The final fitness values of both experiments are the same and equal to -0.32.

measuring the four standard process values named in section I.C.

In practical terms the -0.1 improvement in fitness value (from -0.22 to -0.32) achieved by the NMPC represents an additional gain of about 550 €/day for the biogas plant operator.

In Fig. 4 the optimal substrate feed trajectories $\mathbf{u}_{\text{opt},k}$, $k = 1,\ldots,15$, obtained during both experiments are visualized for each substrate separately. For the feed of maize silage both trajectories are almost equal. The feeds for manure are quite different, but the maximal difference of 1.6 m³/d is relatively small, compared to the mean manure inflow of about 15 m³/d. The substrate feeds for the solid fraction of manure in the beginning are very similar to each other but in the end there is a small difference between them. As the feed of maize silage has the highest influence on the fitness value it can be concluded, that both control algorithms return very similar results.

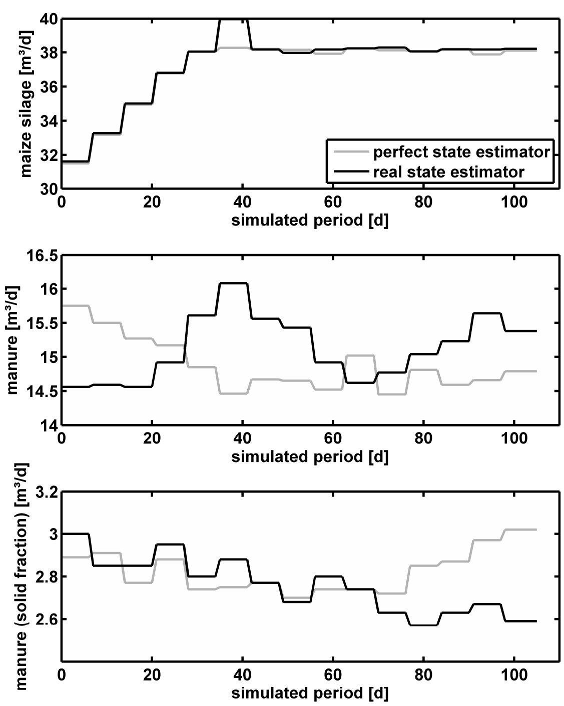

Fig 4. Comparison of the trajectories of the three controlled substrate feeds over the simulated period of about 100 days (exactly: $15 \cdot T_C = 105d$). Remark: A simulation number (see x-axis of Fig. 3) of 35 equals a simulated period of 7 days (control horizon). This is because CMAES evaluates 4 times 8 (number of generations times population size) simulations + 2 extra simulations during optimization and the 35th simulation is done over the control horizon.

Two further experiments starting at $\mathbf{u}_{\text{opt},0} = (1,\,1,\,1)^T \ \frac{m^3}{d}$ also resulted in very self-similar results (correlation coefficient of r= 0.9 for the fitness values without outliers). The final fitness value again is about -0.32. The latter two experiments demonstrate that the NMPC even can be used in the startup-phase, at least for the simulation model.

III. Conclusion

In this paper an online nonlinear model predictive control algorithm is evaluated using a validated simulation model of a full-scale agricultural biogas plant. The results show that using this mathematical model of the biogas plant, based on the ADM1, as predictor biogas plants can be optimally controlled by the sole measurement of these four standard process values: pH value, total biogas production and methane and carbon dioxide concentration of the biogas.

As the optimality criterion may be defined by the user using every modeled process this is a very general approach for optimal online control of biogas plants. It was shown that using the NMPC additional gains of hundreds of Euros per day can be achieved.

A trial of the proposed NMPC is scheduled for summer 2012 in order to optimally control a full-scale biogas plant.

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