­­­Multi-stage Model Predictive Control of Agricultural Biogas Plant with Uncertain Substrate Characterization

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# Highlights

* AD process operated demand-oriented despite uncertain influent concentrations
* Multi-stage MPC controller satisfies safe operational gas storage filling levels
* Time-variant setpoints of methane production are tracked and disturbances rejected
* Orthogonal collocation enables fast computation for real-time application of MPC

# Abstract

Anaerobic digestion (AD) plants process organic substrates and provide renewable electricity and heat. Revenues of AD plants can be increased by generating biogas and electricity on demand or by pursuing biogas upgrading. However, suitable control procedures for individual applications are required to guarantee optimal process conditions at all time. In this contribution, a robust nonlinear model predictive control (NMPC) procedure was designed to optimize substrate feedings under uncertain substrate characterization. Simulation studies demonstrate the ability of NMPC to provide biogas for a flexibly operated combined heat and power unit, while ensuring save gas storage filling limits. Additionally, the NMPC successfully tracked changing setpoints of constant methane production for biogas upgrading, and rejected disturbances posed by measured disturbing feedings of very high uncertainty. By exemplifying demand-oriented operation of AD plants despite uncertain substrate characterization, the present study showcases ecologically and economically sustainable strategies for AD plant operation.

*Keywords:* Biogas Technology, ADM1, Robust Control, Influent Uncertainty, Flexibilization, Gas Storage, Demand-oriented operation

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# Introduction

To achieve the United Nations’ ambitious goals of the Paris agreement and shift towards renewable energy sources, anaerobic digestion (AD) could play an important role in ensuring electricity grid stability (Purkus et al., 2018). Unlike wind and solar energy, power generated from biogas through AD is not dependent on fluctuating weather conditions. Instead, the AD process can produce and buffer biogas for demand-oriented generation of sustainable electricity and heat (Theuerl et al., 2019).

To remain economically competitive with other renewable energy sources, AD plants must adopt innovative strategies to increase revenues and decrease operational costs, especially as state subsidies are fading out (Daniel‐Gromke et al., 2018). In this context, three promising strategies are (i) demand-oriented cogeneration of power and heat, (ii) biogas upgrading to biomethane and (iii) flexibility to utilize alternative substrates (Jordan et al., 2023; Daniel‐Gromke et al., 2018; Theuerl et al., 2019).

In demand-oriented cogeneration biogas is converted to electricity during peak load times, offering higher selling prices but also entailing high investment costs (Purkus et al., 2018). This is conventionally pursued by increasing installed capacities of combined heat and power (CHP) units and expanding gas storage (GS) volumes. Alternatively, demand-oriented feed optimization manipulates amount and composition of utilized substrates. This can align biogas and electricity production with anticipated electricity prices, and thereby minimizes the need for additional GS capacities while sustaining high revenues (Mauky et al., 2016). However, it requires reliable process models to accurately predict both anaerobic biogas production and electricity prices.

The second strategy is to equip existing AD plants with biogas upgrading units to produce biomethane for direct injection into the natural gas grid (Schröer and Latacz‐Lohmann, 2024), which is increasingly pursued internationally (Schmid et al., 2019). Since biogas upgrading units typically operate under stationary conditions for optimal efficiency, biogas production must typically be maintained at constant setpoints (Jønson et al., 2022).

The third strategy lies in reducing substrate costs and utilizing organic waste or low-cost feedstocks (Jordan et al., 2023). While for the majority of biogenic feedstocks there yet exist profitable value chains in Germany, there is still ample unused potential for use in AD plants (Steindl et al., 2025).

All three strategies require suitable control procedures to guarantee optimal process conditions at all time. Pursuing model-based control with variable, uncertain feedstocks requires reliable AD models and sound knowledge of substrate characterization.

While there exist sophisticated AD models, such as the well-established Anaerobic Digestion Model No. 1 (ADM1) proposed by Batstone et al. (2002) and its extensions (Kegl et al., 2025), their application to control studies is limited due to the manifold model parameters which need to be calibrated (Giovannini et al., 2018), and limited data availability at full-scale plants (Cruz et al., 2021). Instead, Bernard et al. (2001) proposed a model explicitly designed for monitoring and control. Due to lower system order and fewer parameters, this model has been successfully applied to monitoring and control of AD processes in lab- and pilot scale (García-Sandoval et al., 2016), (Raeyatdoost et al., 2023). However, the semi-empirical model of Bernard et al. lacks a clear stoichiometry foundation (compared to the ADM1) and is based on chemical oxygen demand (COD), typically applied for process characterization in wastewater engineering. Therefore, Weinrich and Nelles (2021) systematically simplified the ADM1 by summarizing degradation pathways and converting it from COD to mass base reference unit. This simplification eased deployment in agricultural settings and has been validated in different lab- and full-scale settings (Tisocco et al., 2024; Weinrich et al., 2021).

A critical aspect of AD modeling is reliable estimation of influent concentrations, which depends on accurate substrate characterization (Jimenez et al., 2015; Lübken et al., 2015). This generally involves extensive laboratory measurements to determine concentrations of particulate nutrients and soluble organic compounds (Liebetrau and Pfeiffer, 2020). One established way to quantify substrate degradability is by assessing the substrate's biochemical methane potential (BMP) through batch experiments (Dandikas et al., 2018; Koch et al., 2020). However, in practice BMP measurements are subject to significant measurement errors (Hafner et al., 2020). Moreover, in full-scale AD operation time-consuming batch experiment are often omitted in favor of literature values of comparable substrates. While nutrient compositions of common agricultural substrates are well-documented (especially for silages and manure) (Fisgativa et al., 2020; Lübken et al., 2015), there still exists substantial variations to determine anaerobic degradability across individual samples and seasons (Weinrich et al., 2018). In this study, uncertain influent concentrations are thus modeled as a consequence of underlying measurement uncertainties. These uncertainties diminish the confidence in resulting model inputs and lead to unreliable simulation results (Gehring et al., 2013; Tisocco et al., 2024). In model-based feed control of AD, these uncertainties can potentially lead to process instability (Kegl et al., 2025). To this end, robust model-based control approaches explicitly consider these uncertainties to safeguard operational constraints, such as GS limitations.

There exist numerous approaches in literature to control the AD process (Gaida et al., 2017), many of which have been applied to wastewater treatment plants (Alcaraz-González et al., 2021; Méndez-Acosta et al., 2008). In the context of agricultural AD, one powerful approach is model predictive control (MPC). MPC was originally developed in the petrochemical industry in the 1970s, and is valued for its intuitive concept and ability to handle nonlinear models and constraints on states and inputs (Qin and Badgwell, 2003). Hence, it has since been applied in a wide range of fields (Mayne, 2014), including biological systems (Kim et al., 2023) and AD (Körber et al., 2022). Mauky et al. (2016) proposed a nominal MPC scheme for demand-oriented CHP operation of an agricultural AD plant, and validated it experimentally in pilot- and full-scale. However, their process model did not include process inhibition and their MPC disregarded model uncertainties.

At the core of MPC lies the process model, which serves to predict the future system behavior. To this end, nominal MPC does not explicitly consider model uncertainties. However, since each model is only an approximation of reality, real-world applications usually face a plant-model mismatch (Qin and Badgwell, 2003). Compared to nominal MPC, this mismatch is explicitly addressed in advanced MPC schemes (Piceno-Díaz et al., 2020), e.g., min-max MPC, stochastic MPC or tube-based MPC. When dealing with a parametric plant-model mismatch (i.e., assuming a structurally suitable model), multi-stage MPC, proposed by Lucia et al. (2013), offers a promising solution. It has been successfully demonstrated in multiple applications, and is accessible as the open-source Python library *do-mpc* provided by Fiedler et al. (2023).

The present study investigates the performance of multistage MPC for robust and dynamic operation of AD plants in the presence of uncertain substrate characterization. For this purpose, the AD process was modeled by a simplified ADM1 which includes process inhibition, and was applied in a simulative case study covering biogas upgrading. Additionally, the AD model was augmented by a GS model and applied in a second case study covering cogeneration with a CHP unit. In different operational configurations the system performance was assessed, as well as the satisfaction of constraints imposed by the capacity limits of the GS. This study thereby illustrates the capabilities of model-based feed control for more competitive AD operation and underscores the importance to explicitly consider uncertainties of substrate characterization.

# Materials and methods

## 2.1 Dynamic AD model: ADM1-R3

Due to the complexity of the original ADM1 (Batstone et al., 2002) with 34 states and 52 time-variant parameters, the present study applied the mass-based simplification ADM1-R3 proposed by Weinrich and Nelles (2021). The ADM1-R3 describes the AD process in two steps: (i) a combination of hydrolysis, acidogenesis and acetogenesis, and (ii) methanogenesis. Characteristic model equations are described in Hellmann et al. (2023). In the present study, the model was slightly extended by splitting carbohydrates (CH) into two fractions of slowly and fast degradable CH and with corresponding hydrolysis constants and . The influent CH were allocated to the fast fraction and distributed by an additional fraction parameter . The state vector is comprised by 18 states, cf. supplementary information (SI). The setup of the AD model and the simulation is illustrated in Fig. 1a.

### 2.1.1 Gas storage model

The ADM1-R3 was extended by a model of the GS and a CHP unit. The operating schedule of the CHP unit was taken from Mauky et al. (2016) and is shown in Fig. 1b. In accordance to Dittmer et al. (2022), the GS was modeled as membrane enclosure with a variable volume, which is connected to a fixed-roof AD digester of constant liquid and headspace volumes and . Isobaric conditions at a slightly elevated pressure of 1.014 bar were assumed within the GS. Further, a constant elevated temperature of 323 K (Stur et al., 2022) was assumed as a conservative estimate of the GS capacity during the summer months with high sun radiation.

The GS was assumed to be homogeneously filled with biogas from the AD digester (CH4, CO2 and H2O, all modeled as ideal gases). It is depleted through the CHP unit, whose thermal power supply is given through its electrical capacity and efficiency , as well as the lower heating value (LHV) of CH4 . The volume flow of CH4 to the CHP unit can be derived via the specific gas constant of methane as

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|  |  | (2.1) |

Two additional states describe the volume of CH4 and CO2 in the GS. An additional state for H2O could be avoided by assuming saturated water vapor at . Under isobaric and isothermal conditions, mass balances simplify to volume balances for

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| --- | --- | --- |
|  |  | (2.2) |

The volume flow of CH4 required for a specific electrical CHP output entails the outflow of the remaining gases proportionate to their volume fraction within the GS

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|  | , | (2.3) |
|  | , | (2.4) |

where denotes the volume fraction of component in the total GS volume. Inserting (2.4) into (2.3) delivers an expression independent of

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|  | . | (2.5) |

It was assumed that the volume flow from the AD process into the GS changes pressure and temperature instantaneously (from and to and ). Conservation of mass requires the outflow of the AD process to match the inflow into the GS. Applying the ideal gas law gives

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|  |  | (2.6) |

Inserting (2.6) into (2.2) delivers the ordinary differential equations (ODEs) of the two new GS states and

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| --- | --- |
|  | (2.7) |
|  | (2.8) |

### 2.1.2 Biogas plant dimensioning

Dimensions of the AD plant, GS and CHP unit were inspired by the research biogas plant at the German Biomass Research Center (Deutsches Biomasseforschungszentrum, DBFZ) as reported in Mauky et al. (2016) and summarized in Tab. 1. The CHP unit was assumed to have an electrical capacity of 50 kW and an electrical efficiency of 36%. To obtain a ratio between CHP unit and GS capacity in the range of Dittmer et al. (2022), the maximum GS capacity was set to 230 m³.

## 2.2 Uncertain substrate characterization

There exist analytical laboratory procedures to determine raw macronutrients of CH, proteins (PR) and lipids (LI) (Liebetrau and Pfeiffer, 2020). However, their anaerobic degradability can only be quantified heuristically, e.g. through batch tests (Jimenez et al., 2015). Thus, in this study, the three influent macronutrients CH, PR and LI were assumed to be uncertain since they describe only degradable fractions of raw macronutrient values (Weinrich et al., 2021). Other parametric or structural uncertainties were ignored. The following agricultural substrates were considered: grass silage (GrS), maize silage (MS), sugar beet silage (SBS) and cattle manure (CM).

### 2.2.1 Nominal computation

ADM1-R3 influent concentrations, denoted as , were computed according to Delory et al. (2025). To compute individual concentrations of dissociated components of acetic acids, carbon dioxide and ammonia nitrogen typical pH values for silages and manure were taken from Weißbach (Weißbach and Strubelt, 2008a, 2008b, 2008c) and Fisgativa et al. (2020), respectively.

Total solids () were assumed to consist of crude ash and crude macronutrients (crude carbohydrates , crude proteins and crude lipids ), which are given in percentage of , therefore it holds (Weinrich et al., 2021)

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|  |  | (2.9) |

Influent concentrations of degradable macronutrients can be computed based on crude macronutrients, their corresponding degradability quotient , , and the mass density of fresh matter (Lübken et al., 2015)

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|  |  | (2.10) |

PR and LI were assumed to be fully degradable, i.e. (Lübken et al., 2015), therefore all non-degradable macronutrients were attributed to CH. This is considered sufficiently accurate for the investigated agricultural substrates due to their low LI and PR concentrations, as shown in Tab. 1. The degradability of CH was derived from the total degradability of individual substrates

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|  |  | (2.11) |

To this end, total degradabilities were estimated by the ratio of substrates’ BMP and the widely accepted theoretical BMP for agricultural substrates of 420 L kg-1 degradable VS (DVS) (Weißbach, 2009). A fresh matter density of 1000 kg m-3 was assumed for all substrates.

### 2.2.2 Linear uncertainty propagation

In this study, uncertainties of influent macronutrients were derived from uncertainties of the underlying laboratory measurements by applying linear uncertainty propagation (Ku, 1966). This allows to compute the standard deviation (SD) of a variable which is a function of independently distributed variables , i.e. , as

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|  |  | (2.12) |

With (2.10) and (2.11), SDs of influent macronutrients are propagated as

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|  |  | (2.13) |
|  |  | (2.13) |
|  |  | (2.14) |

SDs were based on variation coefficients and nominal values of individual substrates, which are both summarized in Tab. 1. Resulting SDs of influent macronutrients are provided in the SI.

## 2.3 Model predictive control

MPC is an advanced model-based control approach that optimizes system performance by using a mathematical model to predict the system’s behavior over a future time horizon. This horizon is divided into equidistant time intervals, during which inputs (here substrates’ volume flows) are commonly assumed to be constant. The interaction between controller, plant and an estimator are shown in Fig. 1d. At each time step, the MPC solves an optimal control problem (OCP). This delivers the optimal input trajectory for the entire prediction horizon, of which only the first entry is applied to the plant (or a simulator). Afterwards, the horizon is shifted forward by one time step and the OCP is re-initialized with updated estimates of the process state based on the latest measurements . This is known as the receding horizon approach.

### 2.3.1 Multi-stage nonlinear model predictive control

Multi-stage nonlinear MPC is a control scheme aimed at robust controller performance with respect to parametric model uncertainties (Lucia et al., 2013). At the core of this method is the creation of a scenario tree in which all explicitly defined uncertainty realizations are combined with each other (Fig. 1d and Fig. 2). Creation of individual branches is repeated at each time step until a specified robust horizon , after which the branches maintain constant values until the end of the prediction horizon. Multi-stage MPC then minimizes the weighted sum of the cost functions across all scenarios in the scenario tree. In this study, each scenario was weighted equally, reflecting equal probabilities of all scenarios.

### 2.3.2 Simplified scenario tree design for AD model

Lucia and Engell (2014) stated that constraint satisfaction can only be guaranteed if parametric uncertainties assume the discrete values considered in the scenario tree. Yet they report that even for nonlinear systems scenario tree design with upper and lower limits of uncertain parameters often leads to constraint satisfaction for possible uncertainty realizations within the limits.

In this study, only macronutrient inlet concentrations were considered uncertain. While these uncertainties are on a continuous scale in real life (dotted line within the Plant block in Fig 1d), it often suffices to consider a limited number of uncertainty realizations (Lucia et al., 2013). These realizations were modeled as positive or negative deviations from their nominal values, while the deviations were chosen as a certain number of SDs based on the underlying uncertainty propagation, as shown in Fig. 2 (right).

Four substrates were considered for this study. Since each of them contained three macronutrients (CH, PR, LI), this would result in 12 discrete uncertain values. Even for robust horizons of 1 this would lead to different multi-stage scenarios, which was deemed computationally infeasible. Instead, in a first step the uncertain values for all macronutrients were grouped and varied simultaneously for all substrates. This led to a total of different multi-stage scenarios and is illustrated in Fig. 2 (left). Sensitivity analysis (cf. Sec. 3.2) though revealed that the most significant influence on model predictions was caused by uncertain influent CH. Therefore, the scenario tree was reduced to two scenarios as illustrated in Fig. 2 (right).

Robust horizons larger than one were not applied due to the scenario tree’s exponential growth and associated computational costs (Lucia et al., 2013), and by assuming uncertainty realizations as unknown but approximately time-invariant across the prediction horizon (Fig. 2).

## 2.4 Case studies

Two case studies were considered in this investigation, shown as two different pathways in Fig. 1a. Case study 1 addresses constant methane production through the AD process for subsequent biogas upgrading and feed-in into the natural gas grid. In practical applications, this requires separating CO2 from the generated biogas in a biogas upgrading unit, which is not modeled here. Since biogas upgrading processes are typically run at steady state (Jønson et al., 2022), the aim was to track piecewise constant setpoints of methane flow rate. Case study 2 considers cogeneration with a CHP unit and a GS for buffering, whose filling levels must remain within safe operational limits. Both case studies were investigated with and without disturbances, which model the feeding of a large amount of highly uncertain substrate (case study 1 and 2) as well as GS measurement noise (case study 2 only).

### 2.4.1 Constant methane production (case study 1)

The ADM1-R3 was used without an additional GS and simulated for a total of 30 days. Three different setpoint changes of methane volume flow were imposed at days 3, 6 and 9, followed by 21 days of constant operation. The setpoints were heuristically chosen as 350, 550, 450 and 350 m3 CH4 d-1. The MPC was not informed on upcoming setpoint changes, which reflects that in real-life scenarios non-foreseeable setpoint changes may suddenly be required.

In the framework of MPC, case study 1 was modeled through a cost function which penalizes squared deviations between the realized and required methane production across the prediction horizon of length as shown in Eq. (2.15). An additional terminal cost term puts emphasis on the end of the horizon and is used to ensure controller stability. Furthermore, the feed volume flow of substrates (system input ) is incorporated to incentivize economic substrate usage. Their total amount is penalized proportionally to their respective cost, where denotes the number of substrates. Both linear and quadratic input weighting were tested, with quadratic weighting delivering significantly smoother setpoint tracking during initial tests. Moreover, the squared changes of substrate feed volume flow are penalized to prevent the controller from acting too erratically. Otherwise, initial trials showed that this erratic controller behavior led to deep pH drops, from which the AD process did not recover. To consider the individual cost function components in similar orders of magnitude, they were normalized to their setpoint and maximum substrate cost, as described in Eq. X and X respectively~~, cf. (2.15(2.17)~~.

The AD model equations were discretized by orthogonal collocation on finite elements (OCFE, cf. Sec. 2.5) and denoted as discretized dynamic and measurement equations and . Enforcing positive states through non-negativity constraints proved to be unnecessary during initial tests, which was thus omitted. Normalized inputs were constrained between 0 and 1. The cost function for a single multi-stage scenario and the resulting OCP are shown in Eq. (2.15) and (2.16). Tab. 2 summarizes required coefficients used for case study 1.

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|  |  | (2.15) |
|  |  | (2.16) |

### 2.4.2 Cogeneration (case study 2)

Case study 2 addresses demand-oriented cogeneration. For this purpose, the ADM1-R3 was augmented by the GS model described in Sec. 2.1. Since CHP units typically have an operation point of optimal electrical efficiency, the CHP unit was assumed to be either turned on at 100% capacity or turned off. A weekly CHP operating schedule inspired by Mauky et al. (2016) was repeated for a total of 30 days, as illustrated in Fig. 1b.

To keep the GS filling level within the specified bounds, the cost function (2.17) penalizes the squared deviation between the actual filling level and a constant setpoint level (Mauky et al., 2016). This deviation was additionally penalized by the power of four to increase the steepness of the deviation function close to the GS limits. Initial tests revealed good results for filling level setpoints just below 50%. The normalized GS filling level was computed from the sum of its individual normalized components, i.e. the GS states and , as well as (cf. Sec. 2.5.3). A linear substrate cost term was added for the same reason as in case study 1. Initial tests showed no necessity to penalize the rate of input changes, nor for a terminal cost, which were thus omitted.

Constraints to the OCP are posed by the system equations. The ODE system contains two additional equations due to the GS states, which were constrained to be non-negative. The normalized GS filling level was further soft-constrained between 5% and 95% by adding slack variables and (Fiedler et al., 2023). (2.17) and (2.18) show the cost function and constraints of a single multi-stage scenario. Tab. 2 summarizes the parameters used for case study 2.

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| --- | --- |
|  | (2.17) |
|  | (2.18) |

### 2.4.3 Modeled disturbances

#### 2.4.3.1 Disturbance feeding

The first of two modeled disturbances is called disturbance feeding which addresses the following context. Operational cost of AD plants can be reduced by feeding low-cost substrates, such as manure and organic waste (Daniel‐Gromke et al., 2018), which might only be available irregularly and in small amounts. Conducting detailed substrate characterizations for such additional substrates might therefore not be economically viable, resulting in even higher uncertainties than for regular substrates. Therefore, occasional dosages of cattle manure with 2.5 times the regular SDs were added, acting as a fixed and known disturbance to the controller at specified times and flow rates. Tab. 2 summarizes volume flow rates, resulting additional organic loading rates (OLRs) and time windows of the simulated disturbance feedings. OLRs are based on nominal cattle manure.

#### 2.4.3.2 Gas storage measurement noise

For case study 2 an additional noise was imposed on the GS states in (2.7) and (2.8). This aims to reflect measurement noise of the GS filling level, which typically suffers from low accuracy and resolution (Stur et al., 2022). At every time step both GS states were independently imposed with a random uniform noise of ±1% of the respective GS state. Additionally, every five hours the magnitude of this noise was increased to ±3%.

## 2.5 Numerical implementation

### 2.5.1 Orthogonal collocation on finite elements

The *do-mpc* toolbox used in this study requires the model ODEs to be discretized at equidistant time steps of the prediction horizon (Fiedler et al., 2023). For this purpose, orthogonal collocation on finite elements (OCFE) was used (Finlayson, 1980). This method divides continuous time into discrete elements and approximates the ODE solutions with polynomial trial functions. Accuracy is ensured via predefined collocation points within the finite elements. This converts the differential equations into a set of algebraic equations which depend on the trial function parameters. Their solution delivers the system trajectory and thus replaces the ODE integration.

For simulations in this study, a time step of 0.5 h was used with one finite element per time step. A Gauss-Radau collocation scheme of order 2 was applied (Biegler, 2010).

### 2.5.2 Initialization of simulations

All dynamic MPC simulations were preceded by a 500 d open-loop simulation to achieve a steady-state. During open-loop simulation, a constant mix of all four substrates was fed continuously, consisting of 0.25 m3 d-1 of each silage and 0.75 m3 d-1 of cattle manure. Based on nominal substrate characterization, this resulted in an OLR of about 1.5 kg VS m-3 d-1.

### 2.5.3 Normalization

To improve numerical stability of the MPC, states and inputs were normalized. All 18 AD states and influent concentrations of the extended ADM1-R3 were normalized to their maximum absolute value observed during the preceding steady-state simulation. Both GS states and were normalized to the total GS volume . Substrate feed inputs were normalized to the maximum feeding values assumed for the respective conveyor augers or pumps, which operate differently for solid and liquid substrates, as illustrated in Tab. 1 (Substrate feeding).

### 2.5.4 Soft- and hardware

Multi-stage MPC was implemented in *do-mpc* (Fiedler et al., 2023), version 4.6.4. Note that in *do-mpc*, control and prediction horizon have the same length. As a nonlinear solver, *ipopt* (Wächter and Biegler, 2006) was used, which was accelerated by embedding the linear solver *MA27* of the coin-HSL library. All procedures were implemented in Python 3.10.12. Simulations were run on a MacBook pro (macOS Sequoia 15, Apple M1 chip, 8 GB of RAM).

# Results and discussion

## 3.1 Distributions of substrate characterization

Individual influent macronutrient concentrations were obtained for each substrate based on substrate data available at DBFZ and nominal calculations. These are illustrated as boxplots in Fig. 3 with individual sample sizes in the legend. Additionally, normal distributions based on linear uncertainty propagation of measurement errors are shown. Distributions are discussed with respect to nominal (mean) values; this is followed by resulting error bands, both theoretical and measured, based on linear uncertainty propagation and measurement data, respectively.

Clearly CH form the largest macronutrient fraction, which holds for silages (by an order of magnitude), but also for manure. All substrates distinctly differ in CH and PR. SBS exceeds all other substrates in CH but is very low in PR and LI. CM is generally low in all macronutrients compared to silages, and is only subceeded by SBS in PR and LI. GrS is comparably high in LI, followed by MS. GrS and MS show similar LI concentrations.

The theoretical CH uncertainty is smallest for CM despite the large sample size. This can be attributed to the generally low macronutrient concentrations due to its high water content, as illustrated in Tab. 1. For CH, the theoretical uncertainty delivers SDs of similar orders of magnitude for all three silages in the range of 36-50 g L-1. CH of CM, by comparison, only show a SD of around 5 g L-1. For PR and LI, small theorical SDs were obtained for all macronutrients with a range of 0.5-2.5 g L-1 for PR and 0.06-0.82 g L-1 for LI.

Within the investigated substrate samples, the results for CM compare well among boxplots and normal distributions, both for mean values and error bands. For SBS, mean and median of SBS differ substantially for CH and PR, which may indicate an outlier within the small sample size of 3. Nevertheless, measured error bands are estimated well by linear error propagation, especially for LI, with little underestimation for CH and PR. For MS and GrS, theoretical and measured error bands of PR are in the same range with SDs of 1.5-3 g L-1. Linear error propagation, however, underestimates the measured LI error bands in MS and GrS.

In literature, a wide spectrum of substrate characterizations is reported for comparable substrates. This holds especially true for degradable macronutrient concentrations because of the manifold ways to determine them (Koch et al., 2020; Lübken et al., 2015; Fisgativa et al., 2020). For example, Weinrich et al. (2021) determined ADM1-R3 influent concentrations for CM well comparable to this study, while Fisgativa et al. (2020) report significantly higher ones with CH, PR and LI in the range of 84, 4 and 5 g L-1. Likewise, for MS, CH concentrations reported by Fisgativa et al. (2020) are in the same range, whereas PR are much lower and LI much higher than in the present study. Furthermore, Weinrich et al. (2021) determined a comparable PR concentration for SBS as in this study, but lower CH (178 g L-1) and much higher LI concentrations (6 g L-1).

In summary, ADM1 influent characterization of agricultural substrates results in starkly different macronutrient values for comparable substrate types. This can be attributed to seasonal fluctuations, sampling and measurement errors and different assumptions on degradability. Linear uncertainty propagation based on measurement uncertainties results in substantial error bands, which realistically reflect measured uncertainties of ADM1 substrate characterization, but for LI in MS and GrS rather represent lower estimates. ~~Moreover, among the considered substrates, SBS by far shows the highest CH concentrations, and the largest measured error band.~~ The impact of uncertain substrate characterization on model predictions is therefore discussed in the following.

## 3.2 Sensitivity analysis of uncertain macronutrients

Influence of uncertain macronutrient influent concentrations becomes evident when considering them in model simulations according to the block diagram shown in Fig. 1d. Two simulators were run in parallel and provided with the same controller input (feed volume flows), but with different influent concentrations: one with nominal and the other with elevated values (nominal + 1 SD). The first simulator was updated by an ideal estimator (assuming no plant-model mismatch) at each time step, the second one was run in open loop. This approach was applied for all three macronutrients individually. Sensitivity analysis is discussed by means of case study 1, while the corresponding controller performance shall be discussed in Sec. 3.3.1.

Model simulations for different realizations of influent CH, PR and LI concentrations (nominal and elevated) are shown in the SI. The feed volume flows are almost identical for the three cases. Thus, only the feed volume flows of the first case (differing CH) are shown.

The strongest discrepancy between the two parallel simulations is lies in different CH values. This may be explained with the high CH content of used substrates relative to PR and LI, and hence the high absolute values of a single SD. The normalized root mean squared error (NRMSE)[[1]](#footnote-2) between the two resulting trajectories (nominal & elevated) of methane production is 0.130 and 4.3E-3 for pH. In comparison, varying influent concentrations of PR and LI by one SD delivers NRMSEs of 9E-3 and 1.3E-3 for methane production and 4E-3 and 4.2E-5 for pH, respectively.

It was laid out that practical influent uncertainty of LI is underestimated by linear uncertainty propagation. However, even when heavily increasing the corresponding number of SDs for LI to 5, the outcome remains of the same quality: NRMSEs of methane production and pH are 0.020 and 2E-4, which is still an order of magnitude lower than for a single SD of CH. Consequently, only CH were considered for constructing uncertain multi-stage scenarios due to their substantial impact on model predictions. In turn, PR and LI were set constant at their nominal levels, resulting in a scenario tree as shown in Fig. 2 (right).

## 3.3 Multi-stage MPC performance

### 3.3.1 Setpoint tracking of constant methane production

Fig. 4 shows controller performance for setpoint tracking of methane production. 1.5 SDs were assumed for influent uncertainty realizations. Dashed graphs show controller predictions 3 time steps (1.5h) ahead of each given optimization time instance. Further, plant simulations were based on elevated values of the scenario tree according to Lucia et al. (2013) and illustrated in Fig 1d (plant block).

As can be seen in the magnification of the central plot window, convergence for increasing setpoints is reached almost instantaneously ( d) and without overshoot in response to sudden, heavy feedings of manure and silages (top plot window). In turn, the controller reacts to decreasing setpoints by entirely stopping the feeding (days 6, 9), which suffices to deliver convergence within 1d. Constant setpoints are maintained by a constant feeding of substrate with almost identical shares in silages and about 5 times as much manure. While co-digestion with constant substrate proportions is common in practical AD operation (Mata-Alvarez et al., 2011), continuous feed volume flows are rather uncommon. Instead, quasi steady-state methane production is typically approximated through small substrate dosages in short intervals (Bonk et al., 2018), which leads to slightly fluctuating gas productions. The obtained simulation results are, however, a consequence of the formulation of the OCP, which allows the controller enough degrees of freedom to deliver indeed constant methane productions.

The pH can be maintained approximately constant, with a pH in the range of 7.3-7.7, and the most significant drop at a feeding spike at time day 3. Moreover, the process is constantly in a state of ammonia inhibition, with an ammonia inhibition factor (inhibition 3 in bottom subplot) of about 0.3. However, since the other two inhibition factors of nitrogen limitation and pH (inhibition 1 and 2) are retained at about 1, the process remains stable. Stable process operation at diminished levels of ammonia inhibition factors have also been reported by Weinrich et al. (2021).

Disturbance feedings (2nd subplot) could be rejected well through the controller by adequately reducing the feeding of silages, as can be seen in the magnification in the top subplot. Note that the total gas production diminishes during disturbances. However, the control error of methane production remained in the range of 0-2 m3 d-1 which occurred during the strongest disturbance feeding (days 13-17), shown in the corresponding magnification. The run time for the entire simulation of 30 d took only 2 min. This would clearly allow real-time application and underscores the numerical efficiency through orthogonal collocation as discretization and the HSL solver.

Overall, the controller successfully tracked changing setpoints of methane production in a stable fashion with fast convergence and despite disturbance feeding of varying amplitude. This in turn requires that continuous inflow of substrates is technically feasible. Moreover, state feedback was assumed, which would require a high model fidelity (and thus a low plant-model mismatch) in reality.

### 3.3.2 Save gas storage levels during cogeneration

System performance during cogeneration is shown in Fig. 5 by means of optimized substrate feeds, disturbance feedings and GS filling level as well as characteristic AD process variables (such as gas production, pH and microbial inhibition). The GS filling limits are maintained despite process uncertainty and disturbances, hence constraints are robustly satisfied. Uncertainty values of controller and plant were assigned as described in Sec. 3.3.1 with hyperparameters as per Tab. 2.

Compared to setpoint tracking described previously, the resulting optimal feeding pattern differs significantly: most of the time, the substrate feed is zero. Only at distinct times, large dosages of CM and SBS are added within short intervals. The other two available substrates GrS and MS are not fed at all. CM often reaches the upper limit of the allowed feed volume flow of 450 m3 d-1, especially during the first five days. Right after feeding peaks, the gas production increases sharply, while SBS leads to more distinct increases in gas production than CM. Most of the time, feeding peaks occur at the beginning of CHP operation, which depletes the GS. The GS is emptied due to CHP operation twice a day and 3 times on Sundays (Fig. 1b). Moreover, the GS is depleted less on the weekend than during the week, with around 14 vs. 9 h of CHP on-times. Therefore, it is plausible that the highest GS filling levels can be observed on the weekends, i.e. at multiples of 6 and 7 days, as the simulation starts with Monday.

However, this predictable feeding pattern is distorted by disturbance feedings, e.g. around day 6.5: the GS approaches the filling limit almost up to the soft constraint at 95% (as shown in the magnification) when the CHP unit is turned on. However, as the disturbance feeding continues the feeding onset is delayed until its end at around day 7, which results in a small drop in gas production. Feeding is resumed with a large amount of both SBS and CM. The positive contribution of gas production by the disturbance feedings becomes even more apparent at the highest amplitude of disturbance feedings during days 15 and 19. Clearly the feeding of ordinary CM and SBS is decreased to almost 50% compared to times without disturbance feeding. However, disturbance rejection was primarily successful because the controller was informed on upcoming disturbance feedings as well as their associated uncertainty. In case of random, unpredicted disturbances, GS filling constraints might be violated. Nevertheless, the controller ensured safety margins from the lower GS constraints of about 20% and about 10% from the upper GS constraint (without disturbance feeding). Soft constraints are violated at day 6 due to disturbance feeding. Hard constraints, by contrast, are never violated, and thus the safety margin is large enough to compensate for measurement noise on GS states.

The pH is retained in a stable range of around 7.5 with minor fluctuations of 0.1 after feedings. pH drops are deeper upon feeding of SBS than CM, which occurs in line with more pronounced increases in gas production.

Process inhibition is dominated by ammonia inhibition, with a corresponding factor of about 0.3 (bottom plot). The other two inhibition factors are almost at 1. Only minor fluctuations are visible during feedings, but the controller manages to sustain inhibition at stable levels.

## 3.4 Comparison of robust and nominal MPC

The superior performance of multi-stage MPC over nominal MPC is illustrated in Fig. 6. Clearly, nominal MPC (on the left) fails to ensure stability and leads to massive constraint violations, whereas multistage MPC (on the right) maintains safe GS filling levels and an overall stable process. For the simulations, no additional disturbance feeding was considered, nor measurement noise on GS states. Instead, influent uncertainties were varied at 2 SDs (cf. Tab. 2) to challenge the controller performance. As before, multi-stage scenarios of the robust MPC were based on upper and lower uncertainty value; the nominal MPC was supplied with nominal values; and the plant assumed elevated values (plant block in Fig 1d).

The inferior performance of the nominal controller becomes apparent when considering the differences between controller predictions (dotted lines) and plant realizations (solid lines) of gas production (center subplot and magnifications therein): the controller – assuming nominal influent concentrations – systematically underestimates the gas production of substrates, and thereby slowly drives the system towards the upper GS filling limit. While initially GS constraints can be ensured, at around day 22.3 the soft constraint (grey dashed line) is violated for the first time. By then, the controller still predicts decreasing GS filling levels, but the plant in fact exceeds the maximum GS filling level soon after (day 22.4). Since state feedback was assumed (i.e., the controller initializes its state at the beginning of the prediction horizon with the exact plant state), the instable plant behavior also affects the controller predictions, underscored by the predicted constraint violations around day 22.6. If the optimization solver fails to determine a solution that satisfies constraints, it reverts to solving an approximate problem with relaxed constraints (Qin and Badgwell, 2003). This approximate solution, however, cannot lead the system back into a stable operating point. Instead, it further destabilizes the system, which is apparent from the erratic feed volume flows (top subplot) and thus fails to restore stability. Consequently, gas production, pH and inhibition also assume clearly instable or even unphysical values. In real-life, such a plant behavior would require to release or flare off excess biogas from the headspace, resulting in opportunity cost and avoidable greenhouse gas emissions (Reinelt et al., 2016). Remedies could be longer prediction horizons to better anticipate prospective CHP down-times (Qin and Badgwell, 2003), or lower maximum allowed feed volume flows to restrict the erratic feeding behavior.

By comparison, the robust multi-stage MPC controller (on the right) acts more conservatively. It thereby delivers stable plant operation and safe GS filling levels, with a safety margin of around 15% to both lower and upper GS constraints, as well as stable pH and inhibition values. The rare peaks in pH predictions are caused by numerical noise during orthogonal collocation. They can be reduced with higher numbers of collocation points or higher degrees of orthogonal polynomials, though at the expense of increased run times. Otherwise, the overall system performance is very similar as in the previous section, and therefore not further detailed here.

The increased robustness of multi-stage MPC, however, comes at a price: the runtime is significantly longer than for nominal MPC provided the solver does not need to revert to suboptimal solutions with constraint relaxation. This has been tested for the same scenario as discussed here but with only 1 SD for influent uncertainty and a slightly reduced target filling level of 35% (plots not shown). The run time for nominal MPC was 547 s vs. 964 s for multi-stage MPC. With a simulated time of 30 d, the multi-stage controller is, however, still real-time capable.

## 3.5 Limitations and outlook

The presented results are based on simulations, which assumed state feedback, i.e. perfect knowledge of the plant’s dynamic state. Moreover, the considered uncertainties were limited to influent macronutrients within known bounds. Further, disturbance feedings were considered predictable and of known uncertainty. Only agricultural substrates were considered, in which PR and LI were assumed to be fully degradable. Lastly, independent feeding of five substrates was assumed, which is uncommon (Fachagentur Nachwachsende Rohstoffe e. V., 2021), though technically not impossible.

Future research should therefore address a state observer to estimate the process state from available measurements, experimental validation including non-agricultural substrates (e.g., organic wastes), and analysis of expected surplus revenues through demand-oriented feeding.

# Conclusions

A robust multi-stage MPC framework was developed to optimize substrate feedings with uncertain influent macronutrients to an agricultural biogas plant. In two case studies, the MPC delivered successful setpoint tracking of constant methane production; and ensured that GS capacity constraints were met during demand-oriented CHP operation despite GS measurement noise. The robust MPC rejected disturbance feedings of especially high uncertainty and maintained process stability where nominal MPC resulted in plant failure. Simulation runtimes confirmed real-time capability for a resolution of 0.5 h. Future work should incorporate a state observer and address experimental validation.

# Appendix A. Supplementary Information

E-supplementary information of this work can be found in the online version of the paper.

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## CRediT authorship contribution statement

**Simon Hellmann:** Conceptualization, Methodology, Investigation, Validation, Visualization, Writing - Original Draft. **Julius Frontzek:** Methodology, Software, Validation, Data Curation, Visualization, Writing - Original Draft. **David M. Zarate:** Methodology, Software, Data Curation, Visualization, Writing – Review & Editing. **Terrance Wilms:** Conceptualization, Methodology, Validation, Writing - Original Draft. **Konrad Koch:** Methodology, Writing Review & Editing, Supervision. **Steffi Knorn:** Writing - Review & Editing, Supervision, Funding acquisition. **Stefan Streif:** Writing - Review & Editing, Supervision. **Sören Weinrich:** Conceptualization, Resources, Writing - Review & Editing, Supervision, Project Administration, Funding acquisition

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## Tables

**Table 1:** Model parameters of AD process, CHP unit and GSa, b, as well as nominal values and variation coefficients required for substrate characterization and uncertainty quantification of macronutrients.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Category | Variable | | Value | | Unit | | Category | | Variable | | Value | | Unit |
| Operational AD parametersa,b |  | | 163 | | m³ | | Kinetic parameters | |  | | 2.5 | | d-1 |
|  | | 16.3 | | m³ | |  | | 0.25 | | d-1 |
|  | | 311 | | K | |  | | 0.4 | | - |
|  | | 1.013 | | bar | | Substrate feeding | |  | | 80 | | m3 d-1 |
| Gas Storagea |  | | 230 | | m3 | |  | | 450 | | m3 d-1 |
|  | | 323 | | K | |  | | 1000 | | kg m-3 |
|  | | 1.014 | | bar | | CHP unita | |  | | 50 | | kW |
|  | | 518.4 | | J kg-1 K-1 | |  | | 36 | | % |
|  |  | |  | |  | |  | | 50.01 | | MJ kg-1 |
| Substrate/VCa | | BMPa,c  [L kg-1 VS] | | TSa,d  [% FM] | | a,d  [% TS] | | a,d  [% TS] | | a,d  [% TS] | | number of samples | |
| corn silage | | 357 | | 33.73 | | 4.43 | | 7.81 | | 2.44 | | 50 | |
| grass silage | | 372 | | 31.74 | | 11.29 | | 13.93 | | 2.14 | | 5 | |
| sugar beet silage | | 389 | | 39.27 | | 9.39 | | 3.39 | | 0.19 | | 3 | |
| cattle manure | | 246 | | 8.08 | | 23.65 | | 16.63 | | 2.38 | | 24 | |
| VC [%]e | | 14.51 | | 1.94 | | 7.40 | | 5.52 | | 10.04 | | - | |

a AD: anaerobic digestion, CHP: combined heat and power, GS: gas storage, VC: variation coefficient, BMP: biochemical methane potential, TS: total solids, : measurements of raw ash, protein and lipids, VS: volatile solids, FM: fresh matter

b Individual values were inspired by the research biogas plant at DBFZ described in Mauky et al. (2016).

c BMP of sugar beet silage from Heidarzadeh Vazifehkhoran et al. (2016), all others from in-house measurements at DBFZ.

d Nominal values were determined from in-house substrate characterization at DBFZ with given sample size.

e VC of BMP taken as mean residual standard deviation of all four substrates in Hafner et al. (2020), Tab. 3, excluding cellulose. VC of , , , and were taken from Delory et al. (2025).

**Table 2:** Parameters of MPC problems for case study 1 and 2

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Category | Variable | Value | | | Unit |
| Substrate costs | Maize silage | 40 | | | € t-1 FM |
| Grass silage | 35 | | | € t-1 FM |
| Sugar beet silage | 50 | | | € t-1 FM |
| Cattle manure | 20 | | | € t-1 FM |
|  |  | Case study 1a | | Case study 2 b |  |
| MPC parameters |  |  | 0.5 | 0.5 | h |
|  |  | 15 | 40 | - |
|  |  | 1 | 1 | - |
|  |  | 1.5 (1) | 1 (2) | - |
|  |  | 10 | 0.5 | - |
|  |  | 100 | 50 | - |
|  |  | 0.1 | 10 | - |
|  |  | - | 40 | % |
| Disturbance feedingc | time window | 5-10, 13-17, 22-26 | | 5-7, 9-12, 15-19 | d |
| volume flow | 3.88, 7.75, 11.63 | | 2.91, 3.88, 5.82 | m3 d-1 |
| additional OLR | 1, 2, 3 | | 0.75, 1, 1.5 | kg VS m-3 d-1 |

a Differing values used for sensitivity analysis are given in parentheses.

b Differing values used for comparison between nominal and robust MPC are given in parentheses.

c Does not apply for sensitivity analysis and comparison between nominal and robust MPC.

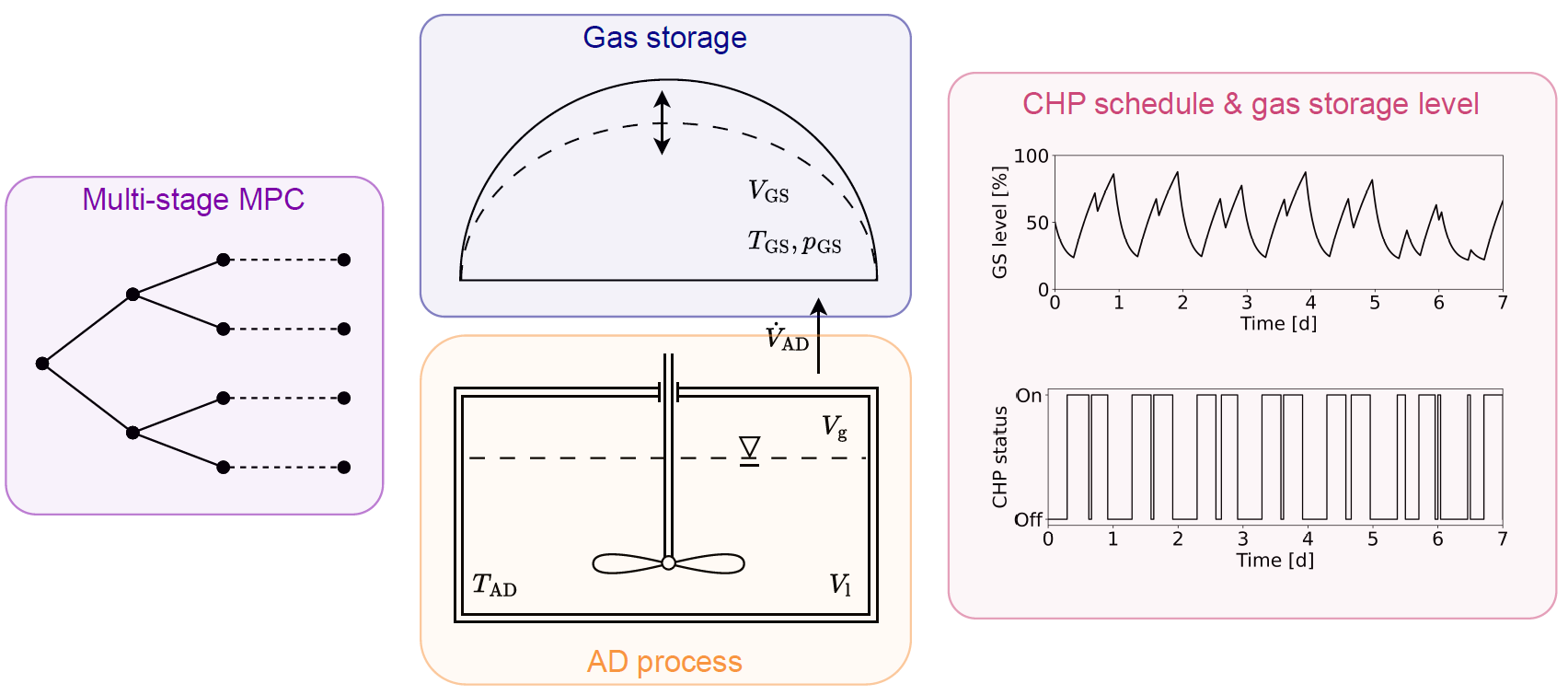
## Figures

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| |  | | --- | |  | | **(a)** | | | | |
| |  | | --- | |  | | **(b)** | | |  | | --- | |  | | **(d)** | | | |
| |  | | --- | |  | | **(c)** | |
| |  | | --- | |  | | **(e)** | | | | |
| **Figure 1**: Setup of simulated system **(a)**: AD process and controller (for constant methane production); as well as AD process, gas storage, CHP unit and controller (for cogeneration). Subfigures show the CHP operating schedule of Mauky et al. (2016) **(b)**, a schematic course of the resulting gas storage filling level **(c)**, a block diagram of controller, estimator and plant/simulator setup **(d)**, and a block diagram of the ADM1-R3 model components **(e)**. Subfigure **(d)** includes a second simulator based on nominal influent concentrations only used for sensitivity analysis. | | | |
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| **Figure 2**: Schematic illustration of scenario trees with grouping of uncertain macronutrients for all substrates (left) and with only two possible uncertain values for influent carbohydrates (right) | | |

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| **Figure 3**: Theoretical and measured distributions of degradable fractions of macronutrients. Theoretical distributions are shown by means of gaussian curves, measured distributions by means of boxplots. Sample sizes used for measured distributions are given in the legend. Note that y-axes only apply for theoretical distributions. |
|  |
| **Figure 4**: Setpoint tracking performance of methane production for biogas upgrading with disturbing feeding of very uncertain cattle manure. Controller predictions are shown for 3 time steps (1.5 h) into the future. The prediction horizon was 15 time steps (7.5 h). Note the different scales of fed substrates for silages (left) and manure (right). |
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| **Figure 5:** Dynamic feeding (1st subplot) for cogeneration with robust MPC controller delivers robust constraints satisfaction, i.e. safe gas storage filling limits (3rd subplot). Despite disturbing feedings of increasing amplitude and duration (2nd subplot) and random gas storage measurement noise, hard constraints of the gas storage are never exceeded. Note that the scale of fed substrates (1st subplot) differs for silages (left) and manure (right). CHP operating times are shaded out in grey (3rd subplot). The prediction horizon was 40 time steps (20 h). |

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| **Figure 6:** Comparison of nominal (left) and robust MPC (right) during cogeneration with plant-model mismatch. While nominal MPC becomes unstable at day 22, robust MPC maintains process stability and ensures save gas storage operating limits. Controller plots refer to 8 d ahead predictions. The prediction horizon was 40 time steps (20 h) for both cases. | |

## Graphical Abstract



## Supplementary Tables

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| **Table SI 1:** States, initial conditionsa and influent concentrations for ADM1-R3-frac and gas storage. For macronutrients, resulting standard deviations are provided. |
| |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | | Index | stateb | Init.a, c | maize silagec, d | grass silagec, d | sugar beet silagec,d | cattle manurec, d | | 1 |  | 0.05 | 10.32 | 10.44 | 8.17 | 4.54 | | 2 |  | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | | 3 |  | 4.97 | 0.00 | 0.00 | 0.00 | 0.00 | | 4 |  | 0.96 | 0.76 | 1.57 | 0.07 | 1.30 | | 5 |  | 957.00 | 662.71 | 682.59 | 607.25 | 919.16 | | 6 |  | 1.48 | 239.75±40.09 | 199.91±36.61 | 327.33±49.42 | 20.82±5.38 | | 7 |  | 1.48 | 0.00 | 0.00 | 0.00 | 0.00 | | 8 |  | 0.95 | 26.33±1.54 | 42.28±2.47 | 9.57±0.56 | 13.31±0.78 | | 9 |  | 0.41 | 7.99±0.82 | 7.63±0.78 | 0.61±0.06 | 2.01±0.21 | | 10 |  | 1.92 | 0.31 | 0.27 | 0.35 | 0.06 | | 11 |  | 0.52 | 0.02 | 0.01 | 0.02 | 0.00 | | 12 |  | 1.00 | 14.84 | 35.34 | 28.34 | 19.14 | | 13 |  | 0.05 | -0.03 | 0.00 | 0.01 | 0.02 | | 14 |  | 0.05 | 1.02 | 5.46 | 0.99 | 4.53 | | 15 |  | 4.54 | 0.00 | 0.00 | 0.00 | 0.00 | | 16 |  | 0.02 | 0.00 | 0.00 | 0.00 | 0.42 | | 17 |  | 0.36 | 0.00 | 0.00 | 0.00 | 0.00 | | 18 |  | 0.66 | 0.00 | 0.00 | 0.00 | 0.00 | | 19 |  | 46 | - | - | - | - | | 20 |  | 46 | - | - | - | - |   a Initial conditions before transition into steady-state (SS). Dynamic simulations start from SS conditions (except and ).  b States 19 and 20 are only used in cogeneration case study. Given initial values are also used to initialize dynamic simulations.  c Concentrations in kg m-3 except in kmol m-3, and and in m3  d pH of silages taken from Weißbach (2008), for manure from Fisgativa (2021) |

## Supplementary Figures

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| **Figure SI 1**: Sensitivity analysis of ADM1-R3 with respect to different influent macronutrient concentrations (top: CH, center: PR, bottom: LI) and effect on gas production and pH. For simulator 1, elevated values were used, and nominal ones for simulator 2, cf. Fig. 1d. For the used agricultural substrates, CH have the strongest influence, followed by PR and LI. | |

1. Computed as with mean operator [↑](#footnote-ref-2)