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Economic Multi-Objective Dynamic Optimization (EMODO) as a Decision-Making tool in Biomethanation Process

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In biological methanation, the methane produced by anaerobic digestion (AD) is upgraded with the addition of syngas. The successful implementation of biomethanation requires the optimization of the production to be competitive in economic terms against chemical processes. Optimization is an arduous task, especially when it is desired to optimize multiple objectives that can be conflicting, such as yields, productivities, process times, and profit gains, among others. This work aims to implement an Economic Multi-Objective Dynamic Optimization (EMODO) approach as a decision-making tool for adequately operating the biomethanation process. The proposed EMODO strategy was based on a previously developed dynamic model for biomethanation. This strategy effectively optimized the $Gain$ and the $Profit\ margin$ by manipulating the inlet flow rates of gas (q_{gas}^{in}) and liquid (q_{liq}^{in}). The strategy also highlights the conflicting behavior of economic objectives and the dependence on substrates. The dynamic optimization improves the response time of the model smoothing the transitions between stages and achieving well adaptation to disturbances regarding the cost of the substrates and the selling prices of the products.

1. Introduction

The successful implementation of biological processes requires optimization to be competitive against chemical processes in economic terms. Emerging bioprocesses such as biological methanation can benefit from multi-objective optimization by maximizing or minimizing multiple variables of interest simultaneously.

Biological methanation or Biomethanation is a process in which the biogas produced through the well-known Anaerobic Digestion (AD) is upgraded by the biological conversion of CO_2 using syngas (a combination of H_2, CO, and CO_2) to obtain high-purity CH_4 (Rafrafi et al., 2020). The biogas produced in the AD contains between 50 - 75% of CH_4, 25 – 50 % of CO_2, and 2–7% water vapor (Laguillaumie et al., 2022). Through biomethanation, the biogas can be upgraded into biomethane (95 – 99 %) while removing CO_2 with the addition of H_2 or syngas (CO/H_2) (Sun et al., 2021). The hydrogenotrophic methanogens with CO_2 consumption transform the H_2. The CO can be transformed indirectly into H_2 by carboxydotrophic hydrogenogenesis, then into acetate by CO-acetogenesis and CO-homoacetogenesis, and finally transformed into CH_4 through hydrogenotrophic and acetoclastic methanogenesis (Guiot et al., 2011). Other works have shown that biomethanation can also be used to produce acetate (Laguillaumie et al., 2022), a molecule of interest that could help make this process more economically profitable.

Based on this complex biological system, managing the biomethanation process is still an arduous task. Therefore, achieving desired objectives such as high productivities, high-profit margins, or low flow rates remains difficult at an industrial scale, especially when it is desired to optimize several variables simultaneously. Multi-Objective Optimization (MOO) involves optimizing problems where there is more than one objective to be optimized simultaneously, and these objectives are usually conflictive.

The use of dynamic models plays a crucial role in designing control strategies. For instance, Model Predictive Control (MPC) (Morales-Rodelo et al., 2020) is implemented to maintain or optimize several variables simultaneously (e.g., productivities and yields). MPC refers to control actions that optimize a criterion in the

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system's future behavior, which is determined by the dynamic model (Camacho & Bordons, 2007). Economic MPC (EMPC) has recently been proposed incorporating a general cost function or performance index in its formulation to consider economic criteria in process optimization (Ellis et al., 2017).

MOO has been applied in bioprocess to find the trade-off between yields and productivities (Nimmegeers et al., 2018). In the AD considering the determination of Pareto fronts to find the trade-off between the environmental impact and net present value as economic aspect (Li et al., 2018). In biomethanation, MOO has been applied to minimize energy consumption and maximize the green degree and CH_4 production (Yan et al., 2016). However, these works not consider the dynamic optimization of the process, improving the performance of economic objectives.

This work aims at implementing an Economic Multi-Objective Dynamic Optimization (EMODO) strategy as a decision-making tool for the biomethanation process to guarantee the maximization of the $Gain$ and $Profit\ margin$. The $Profit\ margin$ was calculated based on changes in market prices using as substrates glucose, H_2, and CO and as products CH_4 and acetate. The $Gain$ was calculated with the price of CH_4 and acetate production.

Pareto optimal sets associated with three process stages were determined through MOO. Each Pareto fronts solution is considered a Pareto Optimal Point (POP). The Pareto optimal set is considered the first part of the decision-making tool, where it is necessary to select the best POP that maximizes the $Gain$ and $Profit\ margin$. In dynamic optimization is used an MPC, which is referred to as the second part of the decision-making tool that optimizes the performance of economic objectives with two control variables corresponding to q_{gas}^{in} and q_{liq}^{in}. To verify the efficacy of the EMODO strategy, the biomethanation process is simulated considering disturbances of ±20 % in the substrates, sugar, H_2, and CO cost, and the selling price of the products CH_4 and acetate.

2. Economic Multi-Objective Dynamic Optimization (EMODO)

Several variables can be optimized in the biomethanation process: yields, productivities, process times, etc. Most of these variables are often conflicting. A Multi-Objective Dynamic Optimization (MODO) strategy was proposed in previous work (Acosta-Pavas et al., 2022) in order to address the mentioned problem. However, this methodology does not consider any information about market evolution. Formulating a cost function could directly or indirectly reflect the process economics to consider economic optimization. Therefore, in this study, the MODO strategy is modified to consider economic aspects such as substrates costs or prices market through the Economic Multi-Objective Dynamic Optimization (EMODO) as the following five steps:

Step 1 - Model definition

Biological methanation was modeled by a dynamic model based on an extension of the Anaerobic Digestion Model No. 1 (ADM1_ME) (Acosta-Pavas et al., 2023). This model considers the uptake of sugar, volatile fatty acids, such as butyrate, propionate, and acetate, the uptake of H_2 and CO, and the decay of biomass and *in-situ* syngas addition. The ADM1_ME describes three types of variables: soluble ($S_{liq,j}$), particulated biomass (X_k) and gas $\left(S_{gas,i}\right)$ components. The ADM1_ME is summarized as Eqs. (1) – (3).

$$\frac{dS_{liq,j}}{dt} = \frac{q_{liq}^{in}}{V_{liq}}\left(S_{liq,j}^{in} - S_{liq,j}\right) + \sum_{k} Y_k f_{j,k} \mu_k - N_i \tag{1}$$

$$\frac{dX_k}{dt} = \frac{q_{liq}^{in}}{V_{liq}}\left(X_k^{in} - X_k\right) + Y_k \mu_k - \mu_{k,dec} \tag{2}$$

$$\frac{dS_{gas,i}}{dt} = \frac{q_{gas}^{in}}{V_{gas}} S_{gas,i}^{in} + N_i \left(\frac{V_{liq}}{V_{gas}}\right) - \frac{q_{gas}}{V_{gas}} S_{gas,i} \tag{3}$$

Sub-index j ϵ [1,8] represents glucose, butyrate, propionate, acetate, H_2, CH_4, CO, and CO_2 in the liquid phase. The H_2, CH_4, and CO are expressed in $gCOD/L$, and CO_2 is expressed in mol/L. Chemical Oxygen Demand (COD) is the amount of oxygen needed to degrade the organic matter into CO_2 and H_2O. It is important to mention that CO_2 is expressed in mol instead of COD, as suggested by Batstone et al. (2002). Sub-index k ϵ [1,6] denotes for the biomass that degrade glucose, butyrate, propionate, acetate, H_2, and CO, respectively. For the gas phase, the sub-index i ϵ [1,4] corresponds to H_2, CH_4, CO, and CO_2. The inlet flow rates of liquid and gas are represented by q_{liq}^{in} and q_{gas}^{in}, respectively, while q_{gas} denotes the outlet gas flow rate. V_{liq} and V_{gas} are the liquid and gas volumes, respectively. $S_{liq,j}^{in}$, $S_{gas,i}^{in}$ and X_k^{in} represent the inlet concentration of the component j in the liquid phase, the inlet concentration of component i in gas phase, and the inlet concentration of biomass

k in the liquid phase, respectively. Y_k is the yield of biomass k, $f_{j,k}$ corresponds the stoichiometric coefficients; μ_k and $\mu_{k,dec}$ refer to the growth and decay rate of biomass k, and N_i to the mass transfer rate of component i. The simulations of the biomethanation process were carried out using the ADM1_ME considering a bubble column reactor (BCR) with a working volume of 37.5 L and a hydraulic retention time (HRT) of 20 days operating at 37°C for 330 days. The organic loading rate (OLR) was varied over time in all stages, according to Table 1. The reference stage corresponded to the simulation without gas addition, with a q_{liq}^{in} of 1.88 L/d. The flow rates q_{liq}^{in}, q_{gas}^{in}, and the gas loading rate (GLR) will be optimized by the EMODO strategy for stages I – III.

Table 1:Stages and OLR simulated with the ADM1_ME.

Stage	**Time (Day)**	$\boldsymbol{OLR\ (gCOD/L/d)}$
Reference	1-30	0.53
I	30-130	1.07
II	130-230	1.60
III	230-330	2.13

To propose economic variables, literature values of 3.40×10^{-4},1.63×10^{-4}, 5.96×10^{-4}, and 1.63×10^{-3} $EUR/gCOD$ were suggested for the cost of sugar, syngas, the selling price of CH_4, and selling price of acetate, respectively. Then, to verify the efficacy of the EMODO strategy, selling prices were simulated, considering disturbances in the price. First, an increase of 20% (+20%) in the selling price of CH_4 and a reduction of 20% (-20%) in the selling price of acetate were considered from 70-100 days (Disturb 1). Then, an increase of 20% in the cost of syngas was simulated from 190-210 days (Disturb 2). Finally, a decrease of 20% in the selling price of CH_4 and an increase of 20% in the cost of syngas were considered from 260-290 days (Disturb 3).

Step 2 - Definition of the optimization problem

The definition of economic optimization corresponds to the maximization of the gain of CH_4 and acetate ($Gain$), and the profit margin of CH_4 and acetate ($profit\ margin$) by modifying the q_{gas}^{in} and q_{liq}^{in}. The economic multi-objective optimization to find the Pareto optimal set was proposed as,

$$\max_{\{q_{gas}^{in},\, q_{liq}^{in}\}} (Gain, profit\ margin) \tag{4}$$

$$subject\ to \begin{cases} dy/dt = \xi(x,u,p,v) \\ 1 \le q_{gas}^{in} \le 100\ L/d \\ 1.875 \le q_{liq}^{in} \le 10\ L/d \end{cases} \tag{5}$$

The objective variables are,

$$Gain = \frac{acetate\ selling\ price \cdot S_{liq,ac}}{HRT} + \frac{CH_4\ selling\ price \cdot q_{gas,CH4} \cdot 64}{22.4 \cdot V_{liq}} \tag{6}$$

$$Profit\ margin = \frac{(CH_4\ sales + acetate\ sales\ ) - Substrates\ cost}{CH_4\ \text{sales} + acetate\ sales} \cdot 100\% \tag{7}$$

In these equations, $\xi(x,u,p,t)$ represents the ADM1_ME, which depends on the state variables x, the control variables u, the parameters p, and the disturbances in the inputs v. $Substrates\ cost$ refers to the cost of glucose and syngas (Eq (8)). $CH_4\ sales$ and $acetate\ sales$ are the gains in EUR for selling all the CH_4 and acetate produced, Eq (9)-(10).

$$Substrates\ cost = \big((Sugar\ cost \cdot OLR) + (Syngas\ cost \cdot GLR)\ \big) \cdot V_{liq} \tag{8}$$

$$CH_4\ sales = \frac{CH_4\ selling\ price \cdot\ q_{gas,CH4} \cdot 64}{22.4} \tag{9}$$

$$acetate\ sales = \frac{acetate\ selling\ price \cdot S_{liq,ac}\ \cdot V_{liq}}{HRT} \tag{10}$$

Step 3 - Selection of the Pareto optimal point (POP)
In this study, the simulations were run using an Intel® Core i7 8665U 2.11 GHz, 16 GB RAM computer. The *paretosearch* function from MATLAB® was used to obtain the Pareto optimal set for each stage. Figure 1 presents the three Pareto fronts computed for each stage, where 60 POP were calculated.

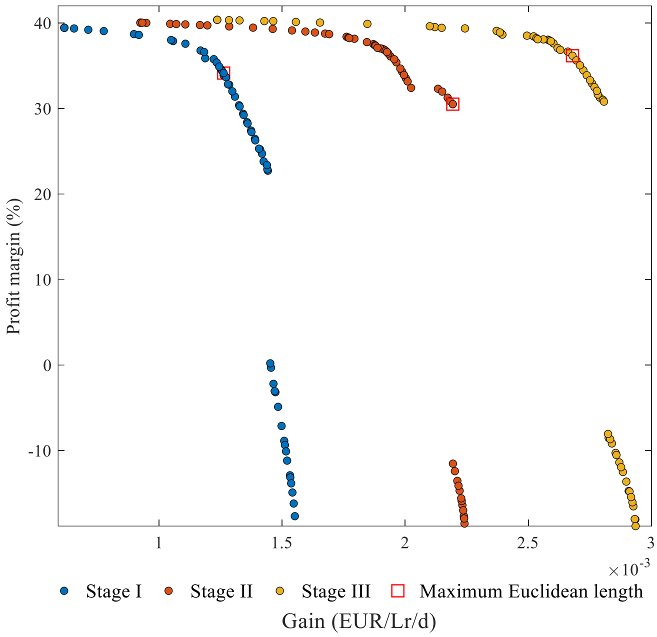

Figure 1: Pareto optimal sets for stages I-III, and maximum Euclidean length.

At each stage, one POP was selected, which corresponded to the maximization of the Euclidean length (d_{max}) for the $Gain$ and the $Profit\ margin$ (red squares in Figure 1). For all the stages, d_{max} was calculated as the distance from the origin, using a normalization as in Eq. (11).

$$d_{max} = max\left(\sqrt{\left(\frac{Gain^* - min(Gain^*)}{max(Gain^*) - min(Gain^*)}\right)^2 + \left(\frac{Profit\ margin^* - min(\ Profit\ margin^*)}{max(\ Profit\ margin^*) - min(\ Profit\ margin^*)}\right)^2}\right) \quad (11)$$

Step 4 - Definition of the dynamic problem with a single weighted objective
In order to consider a dynamic optimization, the two previously defined objectives and their optimal points (POP) were merged into one objective function and solved based on an MPC problem. The proposed dynamic optimization determines the input variables that minimize the following objective function,

$$\min_{\{q_{gas}^{in}, q_{liq}^{in}\}}\left(\sum_{j=t}^{t+H_p}\left(\frac{|Gain^* - Gain(t)|}{Gain^*}\right)^2 + \left(\frac{|Profit\ margin^* - Profit\ gain(t)|}{Profit\ gain^*}\right)^2 + \sum_{j=t}^{t+H_c} W_{u,1}\,\Delta q_{gas}^{in}(t)^2 + W_{u,2}\,\Delta q_{liq}^{in}(t)^2\right) \quad (12)$$

Eq. (12) is subject to the constraints in Eq (5). $Gain^*$ and $Profit\ margin^*$ denote the POP values for $Gain$ and $Profit\ margin$ computed by the MOO, $\Delta q_{gas}^{in}(t)^2$ and $\Delta q_{liq}^{in}(t)^2$ are the differences between q_{gas}^{in} and q_{liq}^{in}, respectively, before and after each step of the dynamic optimization. $W_{u,1}$ and $W_{u,2}$ are the parameters that weight the importance of the control effort term in the optimization. The initial values for both manipulated variables, q_{gas}^{in} and q_{liq}^{in} were $1\ L/d$ and $1.875\ L/d$, respectively.

Step 5 - Implementation of the optimization
Two cases were analyzed. Case 1 corresponded to the use of the POP identified in step 3 and applied directly in the simulation with the ADM1_ME (Pareto results). Case 2 referred to dynamic optimization as a control strategy (Dynamic opt). The weights $W_{u,1}$ and $W_{u,2}$ were manually adjusted to values of 1×10^{-7}. The prediction (H_p) and control (H_c) horizons were considered with equal values and equivalent to the time length of each stage (Table 1). Optimization was performed with the *patternsearch* algorithm in MATLAB®.

The results of the optimization are displayed in Figure 2. In both cases, the $Gain$ increased at each stage change, while the $Profit\ margin$ varied between 30 and 35% (Figure 2-C). For both economic variables, it is observed that the dynamic optimization improved the model's response, smoothing the transition between stages, which is ideal in this type of biological process to avoid additional disturbances.

Additionally, the EMODO strategy responds satisfactorily to the three proposed disturbances regarding the cost of substrates and the selling price of products, especially with the disturbance presented between 190-210 days, where there was a 20% increase in syngas cost and subsequent transition between stages II and III (Figure 2-A).

In Figure 2-B, comparing case 2 to case 1 in terms of control variables, a slight reduction of 3.3×10^{-2} and 7.5×10^{-2} L/d was observed for q_{liq}^{in} in stages I and III, respectively. A slight increase of 3.6×10^{-2} L/d was observed in stage II. In contrast, q_{gas}^{in} showed an increase of 5.85 and 11.15 L/d in stages I and III, respectively, and a reduction of 9.49 L/d in stage II.

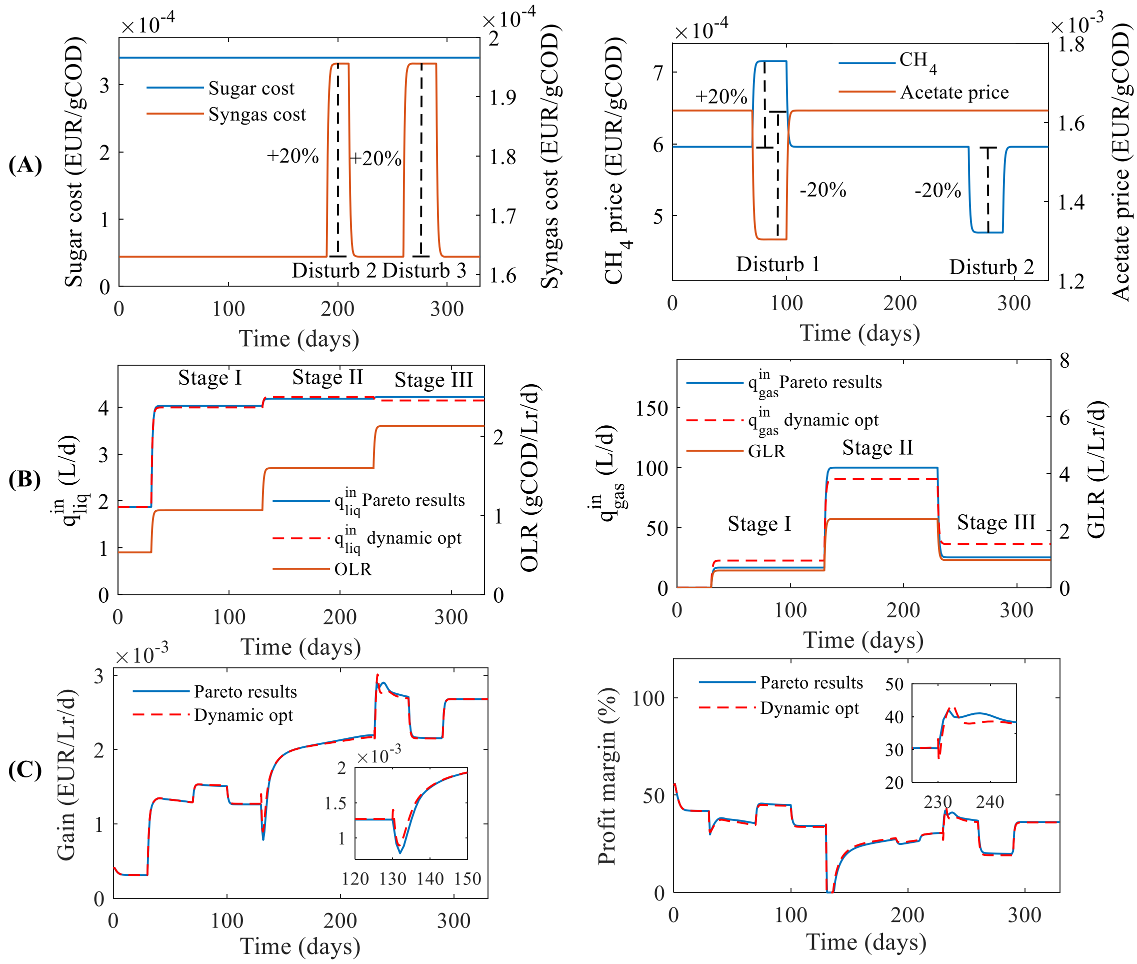

Figure 2: ADM1 ME inputs and outputs. (A) ADM1_ME Economic inputs (B) ADM1_ME inputs (C) ADM1_ME Economic outputs. Case 1: Pareto results, case 2: dynamic optimization as a control strategy (Dynamic opt). Disturbance 1-3 (Disturb 1-3).

If the EMODO strategy is considered as a decision-making tool in the biomethanation process, it is necessary to refer to the ADM1_ME inputs (Figure 2-B) and the ADM1_ME outputs at a steady state (Figure 2-C). For stages I and III, there were slight decreases in q_{liq}^{in}, while the OLR doubled, and the q_{gas}^{in} increased from 22 to 25 L/d, respectively, resulting in an increase in GLR from 0.60 to 0.97 $L/L_r/d$. This led to an increase in $Gain$ from 1.27×10^{-3} to 2.68×10^{-3} $EUR/L_r/d$, while the $Profit\ margin$ slightly increased from 33.8% to 36.0%.

From a $Gain$ point of view, it can be increased by maintaining similar $Profit\ margins$. However, it should be noted that a significant increase in q_{gas}^{in} is needed to achieve these changes, as in stage II, where values of 91 L/d were obtained.

3. Conclusions

The EMODO strategy demonstrates to be a good alternative to obtain the best $Gain$ and $Profit\ margin$ by manipulating q_{gas}^{in}, and q_{liq}^{in}. These variables played a key role and ranged between optimal values of 22 - 91 L/d and 4.00 and 4.22 L/d through all stages. The proposed strategy shows the conflicting behavior of both economic objectives and the high dependence of the substrates added to the process (the three Pareto fronts, clearly differentiated for each stage). The application of dynamic optimization improves the response, smoothing the transitions between stages. The efficacy of the EMODO strategy is demonstrated with a successful adaptation to three disturbances in the cost of the substrates and the selling price of the products. These results show the feasibility of the proposed methodology as a decision-making tool and its use for multiple control objectives.

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