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# SENSITIVITY ANALYSIS USING ADM1 MODEL FOR BIOGAS PRODUCTION

ABHILASH NAIR[a], ALEXANDRINA ZUZA[a*], PAUL-ŞERBAN AGACHI[a], ARPITA DAS[a], MARIUS BREHAR[b], GYŐZŐ FERENCZ BARABÁS[c]

**ABSTRACT.** This study is aimed for a sensitivity analysis to understand the effects of various stoichiometric and kinetic parameters, input composition, carbon and nitrogen composition in the Anaerobic Digestion Model No. 1 (ADM1). The ADM1 has been modified based on the design parameters and process conditions from Cluj-Napoca WWTP. It has to be further calibrated to simulate the steady-state anaerobic digestion of activated sludge at municipal wastewater. For this purpose, it is extremely important to understand the effect of various model parameters on the output variables. The modified model is able to predict the output with 2% error in biogas flow rate and 10% error in the digester pressure. The sensitivity analysis performed identifies the parameters that have a major impact over the output. This report also presents a list of parameters that have to be modified to calibrate the ADM1 model.

***Keywords:*** *ADM1, WWTP, activated sludge, sensitivity analysis, simulation, calibration*

## INTRODUCTION

Anaerobic processes have been widely used for the treatment of municipal and industrial wastewater through the fermentation of activated sludge, particularly in Europe [1]. The ADM1 structured model initially includes multiple steps describing complex biochemical and physico-chemical processes. The biochemical steps include breakdown from homogeneous particulates to carbohydrates (CHO), proteins (PRO) and lipids (LIP); extracellular hydrolysis of these particulate substrates to sugars, amino acids (AA), and long chain fatty acids (LCFA),

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[a] *Faculty of Chemistry and Chemical Engineering, Babes-Bolyai University of Cluj-Napoca*
[b] *Waste Water Treatment Plant Cluj-Napoca*
[c] *Waste Water Treatment Plant Budapest*
[*] *Corresponding author: alexandrinazuza@chem.ubbcluj.ro*

respectively; acidogenesis from monosaccharides (MS) and amino acids (AA) to volatile fatty acids (VFAs): propionic (HPr), butyric (HBu) and valeric acid (HVa) along with $H_2$; acetogenesis of LCFA and VFAs to acetate ($C_2H_3O_2^-$); and separate methanogenesis steps from $C_2H_3O_2^-$ to $H_2$ and $CO_2$ into $CH_4$ (Figure 1). These complex bio-chemical and physico-chemical reactions are implemented mathematically to analyze the amount of methane that can be generated from anaerobic digestion. There is also a need to analyze how much of the energy content in the produced methane could be used to generate heat and electricity.

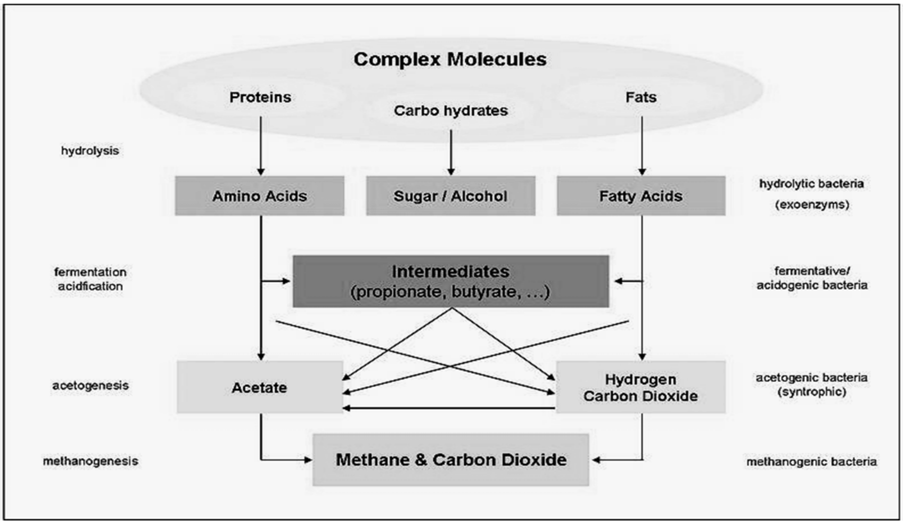

**Figure 1.** Anaerobic digestion conversion processes [2]

The ADM1 [3] has been used for the mathematical simulation of the fermentation of different substrates [4]. Since its development in 2002 and up to now the ADM1 has been tested and used on different substrates where a great number of research works are reported in the literature. Amongst others, investigations were done on mathematical simulation of special substrates of international interest, like starch [5], blackwater [6] or olive pulp [7]. Boubaker and Cheikh Ridha [8] investigated on the mesophilic anaerobic co-digestion of olive mill wastewater with olive mill solid waste. Page, DI. et al. [9], has modified the kinetic parameters of ADM1 in order to simulate dairy manure anaerobic digesters and thermophilic anaerobic co-digestion of olive mill wastewater and olive mill solid waste. Zaher, U. et al. [10], has developed a general integrated solid waste co-digestion model, for optimization and assessment of co-digestion of any combination of solid waste streams. This very important tool estimates particulate waste fractions of carbohydrates, proteins, lipids and inerts and thus generates inputs for ADM1, which subsequently predicts biogas generation. In fact, anaerobic digestion of the organic fraction of the municipal solid wastes alone or combined with organic sludge can contribute efficiently to solid waste reduction and biogas production as described by many researchers: Zuza et al. [11], Bolzonella et al. [12], Mace et al. [13] and Bolzonella et al. [14], for solid waste treatment under mesophilic or thermophilic conditions.

Since the introduction of activated sludge models (ASMs) by Henze et al., [15] the activated sludge processes have been studied using dynamic simulations in order to design, upgrade and optimize a range of configurations of the activated sludge unit in wastewater treatment plants (WWTPs). Later, the introduction of the anaerobic digestion model [3] extended the modeling further to the sludge line.

## EXPERIMENTAL SECTION

### ADM1 in the treatment of activated sludge at municipal wwtp context

In this current study, primary sludge from the primary settling tank and secondary sludge from the secondary clarifier are treated dried and mixed with polyelectrolyte and ferric chloride (Q), which are pumped subsequently into the digesters for the anaerobic digestion and biogas production. To maintain an inner constant process temperature of the digester, the sludge is recycled through heat exchangers. After the production of sufficient biogas, 20-25% of biogas is being recirculated into the digester for mixing purposes (Figure 2).

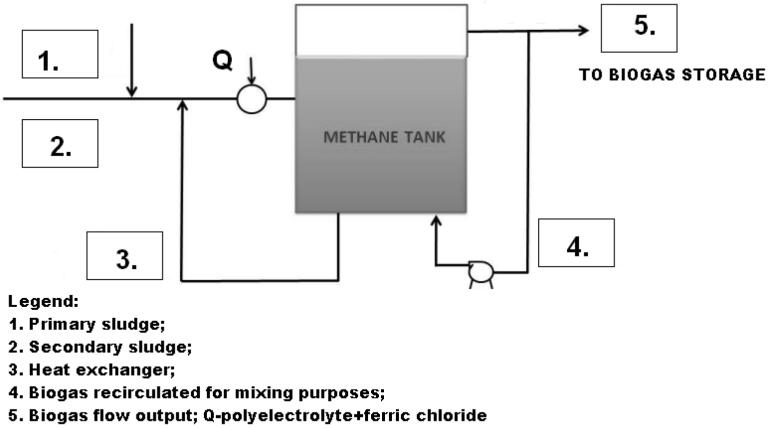

**Figure 2.** Sludge and biogas process lines

## Materials and methods

The main process parameters of the anaerobic digestion: flows, temperature, pressure and concentrations are presented in Table 1.

**Table 1.** General plant design and process parameters

| **PROCESS PARAMETERS** | **SLUDGE LINE** | **ANAEROBIC FERMENTERS** |
|---|---|---|
| | *Primary sludge* | |
| Fermentation temperature: 37-39 °C | Flow: 260 $m^3$/day | Unit: 4 |
| Working Pressure: 20-25 mbar | Content of MS[7]: 27% | Volume: 3500 $m^3$ |
| HRT[1]: 21-25 days | Content of VS[8]: 73% | Type: Monostadium |
| Influent/Effluent Flow: | Fixed residue: ~1800 mg/L | with recirculation |
| 2500-13000 $m^3$/h | | Height: 12 m |
| Heat exchangers thermal agent | *Secondary sludge* | Diameter: 19 m |
| input/output temperature: 80/60 °C | Flow: 280 $m^3$/day | Biogas production: |
| Procentage of OMT[2]: 30-50% | Content of MS: 29% | average of 3000 |
| OL[3]: <<2 kg VSS/$m^3$ | Content ofVS: 71% | $m^3$/day |
| pH: 7-8 | Fixed residue: ~35000 mg/L | |
| Turbidity: <35 mg/L | | |
| Ortho-P[4] influent/effluent: 8 -1 mg/L | *Fermented sludge* | |
| D.O.[4]: 2-3.5 mg/L | Flow: 540 $m^3$/day | |
| Nitrates: <40 mg/L | Content of MS: 40% | |
| Ammonia influent/effluent: 70/1 mg/L | Content ofVS: 60% | |
| TSS[5]: 7500-9000 mg/L | Fixed residue: ~19000 mg/L | |
| TOC[6]: <125 COD/L | | |
| *Nomenclature:* | | |
| | *[5]Dissolved Oxygen* | |
| *[1]Hydrolic Retention Time* | *[6]Total Suspended Solids* | |
| *[2] Organic Matter Transformation* | *[7]Total Organic Carbon* | |
| *[3] Organic Load* | *[8] Mineral substances* | |
| *[4]Ortho*-Phosphates | *[9] Volatile Substance* | |

## Simulink model

The ADM No.1 Simulink model [16], has been modified based on the process conditions presented in the previous table. The balance equations presented [3] has been modified slightly to include the sludge recycle and the gas recycles into the digester. The original ADM1 model is built under the assumption that the reactor is a thermodynamically isolated system. But under industrial conditions, a heating system has to be provided to maintain the digester temperature within the desired range. This is done by continuously recycling the digester fluids through a heat exchanger. This recycle of internal fluids could have a certain influence on the compositions and hence this recycle has to be included in the model. The ADM 1 model equations consider the system to be a CSTR. In an actual plant operation, these CSTR conditions are achieved either by a mechanical action of a stirrer or by pumping gas through the digester. In this model under consideration, a bio-gas recycle is used to achieve this condition. This recycle has serious effects on the digester pressure, methane concentration in the biogas and quantity of biogas produced. Hence, the effects of the gas- recycle has to be included to make the mathematical model close to the industrial condition.

The first equation, Eq. (1) and Eq. (2), presents the change in the process conditions that are incorporated in the ADM1 model. Since the tank has been modelled as a perfectly mixed vessel, the influence of these recycles on physical conditions of mixing and other hydrodynamic effects can be ignored. Figure 3 presents the model that has been build up to study the digester section of WWTP. The 4 digester model has been converted to a single digester system, to produce an equivalent model; this can be done by simple addition of all the process conditions because in real situation all the 4 digesters work parallel, under uniform flow conditions.

For Liquid stream:

$$\frac{dS_i}{dt} = \frac{q_{in}S_{in,i}}{V_{liq}} + \frac{q_{rec,s}S_i}{V_{liq}} - \frac{q_{out}S_i}{V_{liq}} - \sum\nolimits_{j=1-19} \rho_j \, v_{i,j} \tag{1}$$

$S_i$ (i=1:24) – State variables
$\rho_j$ – Kinetic rates
$v_{i,j}$ – Stoichiometric coefficients
$q_{rec,s}$ – Sludge recycle flow
$q_{in}$ – Sludge input
$q_{out}$ – Sludge output
$V_{liq}$ – Volume of the liquid fraction

For Gas section:

$$\frac{dS_i}{dt} = \frac{q_{rec,g}S_i}{V_{gas}} - \frac{q_{out}S_i}{V_{gas}} + k_L a_{gas}(S_{gas,liq} - K_{H,gas}P_{gas}) \tag{2}$$

gas – biogas composition ($S_{CO2}$+$S_{CH4}$+$S_{H2}$)
$k_L a_{gas}$ – Gas Liquid mass transfer coefficient
$K_{H,gas}$ – Henrys Constant for the corresponding gas
$q_{rec,s}$ – Gas recirculation flow rate
$P_{gas}$ – Partial pressure of the biogas
$V_{gas}$ – Volume of the gas fraction

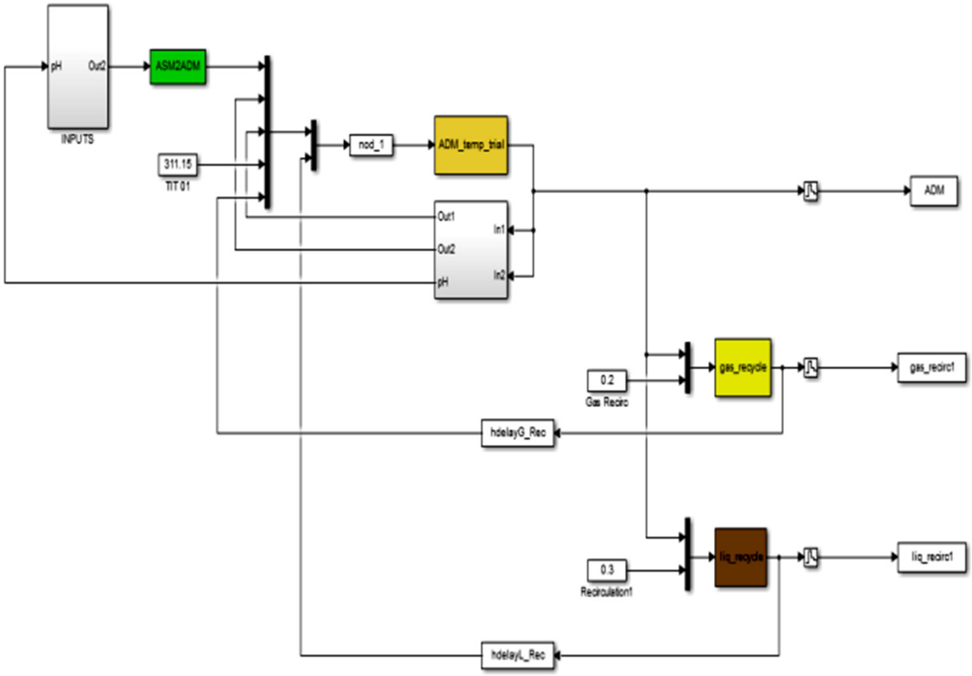

**Figure 3.** Simulink model with sludge and gas recycle

## ASM-ADM1 Simulink® interface

The ADM No.1 model is often connected to an ASM-ADM converter [17] which provides a detailed algorithm to convert the ASM1 model parameters to ADM1. Attaching a converter to the ADM No 1 has two major advantages. Firstly this provides the need for having less complex ASM 1 input variables compared to the ADM 1 input which has about 25 input state variables. Secondly it also would be convenient to link it to the Waste Water treatment model to create a Benchmark for a complete Waste Water Treatment Plant (BSM No.2).

Even after the implementation of ASM-ADM interface in the digester model, the input variables used are completely different from the values that are regularly monitored in the industry. There are no available methods for direct measurement of these input variables. The values of these inflow composition provided in the literature [18] cannot be directly used in a digester model, due to the huge variations in waste-water sludge composition. Apart from the immeasurable input parameters, there is also a possibility of various parameters that could be different from those used in the ADM No. 1 [3].

The default values of influent sludge composition, conversion parameters of the ASM-ADM converter, stoichiometric and kinetic parameters presented in the ADM1 fails to give the required tank pressure and methane production rates. Hence there is a need for calibrating these values to match the values obtained from the WWTP.

### Sensitivity analysis

Before we tune the model parameters to obtain the desired output, it is necessary to understand the effect of various parameters (Table 2) on the output variables.

**Table 2.** Inflow Composition [18]

| PARAMETER | PARAMETER ABBREVIATION | Value |
|---|---|---|
| Soluble inert organic matter | $S_I$ | *30* |
| Readily biodegradable substrate | $S_S$ | *68.22* |
| Particulate inert organic matter | $X_I$ | *7148.21* |
| Slowly biodegradable substrate | $X_S$ | *27987.36* |
| Active heterotrophic biomass | $X_{B,H}$ | *4043.27* |
| Active autotrophic biomass | $X_{B,A}$ | *8.49* |
| Particulate products arising from biomass decay | $X_P$ | *26.02* |
| Soluble biodegradable organic nitrogen | $S_{ND}$ | *0.1* |
| Particulate biodegradable organic nitrogen | $X_{ND}$ | *0.19* |

These parameters used to describe the model, have been obtained by experimentations and have been successfully implemented in various WWTPs, but as mentioned before, some of them still have a possibility of change. With such a huge list of variables that could be varied to fit in the data, a suitable choice has to be made to select the ones that can provide significant influence in the output variable. It has to be taken into account the parameters chosen that are most likely to be affected by the change in feed composition. Table 3 shows the list of variables that are most likely to represent the parameters that is depended on the type of sludge. The parameters such as Henry's law coefficients, acid-base equilibrium constant, acid-base rate constant are considered dependent completely on temperature and hence remain constant. The same is the case with the specific Monod maximum uptake rate, first order decay rate for biomass death, Monod half saturation constant, which are maintained same as the default values due to its extremely complex dependency function on the output variables.

**Table 3.** Stoichiometric and kinetic parameters

| Parameter | Description | UNIT |
|---|---|---|
| $C_i$ | carbon content of component | kmoleC/kgCOD |
| $k_La$ | gas–liquid transfer coefficient | days |
| $N_i$ | nitrogen content of component i | kmoleN/kg COD |
| $Y_{substrate}$ | yield of biomass on substrate | kgCOD_X/kgCOD_S |
| $f_{product,substrate}$ | yield of product on substrate | $kgCOD/kgCOD^{-1}$ |

where,

i - Components/state variables used in the ADM1
(Batstone *et al.* 2002)

## RESULTS AND DISCUSSION

The simulation outputs: in Figures 4-6 it is presented the simulation output for biogas production rate, methane concentrations and tank pressure from the initial conditions to the time it reaches steady state. These graphs present a preliminary idea of the time taken for the process to reach steady state conditions. The comparison of the simulated variables and the industrial data is provided in Table 4. The table clearly shows that the methane concentration clearly matches the values of the design parameters, but the flowrate and the digester pressure varies from the design values. Hence a tuning of parameters has to be done to match the values.

**Table 4.** Output parameters

| OUTPUT | units | SIMULATED VALUE | INDUSTRY VALUE |
|---|---|---|---|
| Steady state pressure | mbarg | 49.42 | 25 |
| Methane concentration | dimensionless | 69.37 | 70% |
| Biogas flowrate | $m^3$/day | 3312 | 3000 |

The values given in Table 5 are the base operating condition. Which implies that the model has been run based on the stoichiometric values from the literature. Now these values from the literature are increased by 10 times and are used to run simulations until it reaches the steady state conditions. The final values of biogas flowrate (q) and tank pressure (P) have been recorded at the end of each run. The values of % P and % q can be mathematically explained by the flowing equation.

$$\%P = \frac{P_{new} - P_{base}}{P_{base}} \tag{3}$$

where,

$P_{new}$ – the value of tank pressure after the change in the selected parameter
$P_{base}$ – the value of tank pressure obtained with literature data parameter simulation

$$\%q = \frac{q_{new} - q_{base}}{q_{base}} \tag{4}$$

where,

$q_{new}$ – the value of biogas flowrate after the change in the selected parameter
$q_{base}$ – the value of biogas flowrate obtained with literature data parameter simulation

The value of methane concentrations has shown extremely low sensitivity to the variation in inflow sludge composition, stoichiometric and kinetic parameters. Hence the prime focus has been put to study the influence on biogas flowrate q and methane tank pressure p.

While calibrating the model, it is now known which parameters have to be varied. In case of a major deviation of model data from the industrial data, the results showing higher values of $\%P$ and $\%q$ could be varied and later the values with lower $\%P$ and $\%q$ could be further varied to fit the model.

**Table 5.** Parameters that have negative effects on pressure and biogas production

| Default value | Parameter | Description | mbarg | m³/day | %P | %q |
|---|---|---|---|---|---|---|
| 0.41 | f_ac_su | Yield (acetates from sugars) | 24.17 | 1631.8 | -2.36 | -50.87 |
| 0.08 | Y_aa | Yield of biomass on amino acids | 24.44 | 1649.4 | -2.33 | -50.34 |
| 0.007 | N_aa | Nitrogen contend of amino acids | 24.67 | 1665.5 | -2.31 | -49.86 |
| 0.13 | f_bu_su | Yield (butyrate from sugars) | 33.18 | 2239.4 | -1.51 | -32.58 |
| 0.27 | f_pro_su | Yield (propionate from sugars) | 34.50 | 2328.8 | -1.38 | -29.88 |
| 0.05 | f_pro_aa | Yield (Propionate from amino acids) | 36.71 | 2477.6 | -1.18 | -25.40 |
| 0.0217 | C_fa | Carbon content in fatty acids | 42.26 | 2852.7 | -0.65 | -14.11 |
| 0.03 | C_sI | Carbon content in soluble inert | 42.29 | 2854.9 | -0.65 | -14.04 |
| 0.1 | Y_su | Yield of biomass on sugar | 43.10 | 2909.3 | -0.57 | -12.41 |
| 0.02786 | C_xc | Carbon content in Composite | 44.24 | 2986.5 | -0.47 | -10.08 |
| 0.06 | Y_fa | Yield of biomass in fatty acids | 44.25 | 2986.9 | -0.47 | -10.07 |
| 0.04 | Y_pro | Yield of biomass on propionates | 44.83 | 3026.3 | -0.41 | -8.88 |

**Table 6.** Effect of changes in input composition

| Default value | Parameter | Description | mbarg | m³/day | %P | %q |
|---|---|---|---|---|---|---|
| 0.03 | C_pr | Carbon content in proteins | 865.4 | 58412.2 | 76.8 | 1658.7 |
| 0.022 | C_li | Carbon content in lipids | 222.9 | 15045.1 | 16.3 | 353.0 |
| 0.0313 | C_ch | Carbon content in carbohydrates | 196.4 | 13258.6 | 13.9 | 299.2 |
| 0.95 | f_fa_li | Yield (fatty acids from lipids) | 120.1 | 8109.1 | 6.7 | 144.2 |
| 0.0313 | C_ac | Carbon content in acetic acid | 77.7 | 5248.1 | 2.7 | 58.0 |
| 0.4 | f_ac_aa | Yield (acetic acid from amino acid) | 71.3 | 4813.9 | 2.1 | 44.9 |
| 0.26 | f_bu_aa | Yield (butyric acid from amino acids) | 61.6 | 4158.4 | 1.2 | 25.2 |

**Table 7.** Effect of 6 most important variables

| Default value | Parameter | Description | mbarg | m$^3$/day | %P | %q |
|---|---|---|---|---|---|---|
| 14024 | $X_S$ | Slowly biodegradable substrate | 140.1 | 7102.2 | 184.7 | 113.8 |
| 30315.3 | $X_{BH}$ | Active Heterotrophic biomass | 210 | 8904.7 | 326.7 | 168.1 |
| 744.6 | $X_{ND}$ | Particulate biodegradable organic nitrogen | 63 | 3489.4 | 28.0 | 5.0 |
| 1643.7 | $X_{BA}$ | Active Autotrophic biomass | 52 | 3364.8 | 5.6 | 1.3 |
| 33.3 | $S_S$ | Readily biodegradable substrate | 50.1 | 3321.9 | 1.8 | 0.2 |
| 3.6 | $S_{ND}$ | Soluble biodegradable organic nitrogen | 49.99 | 3315.5 | 1.5 | 0.1 |

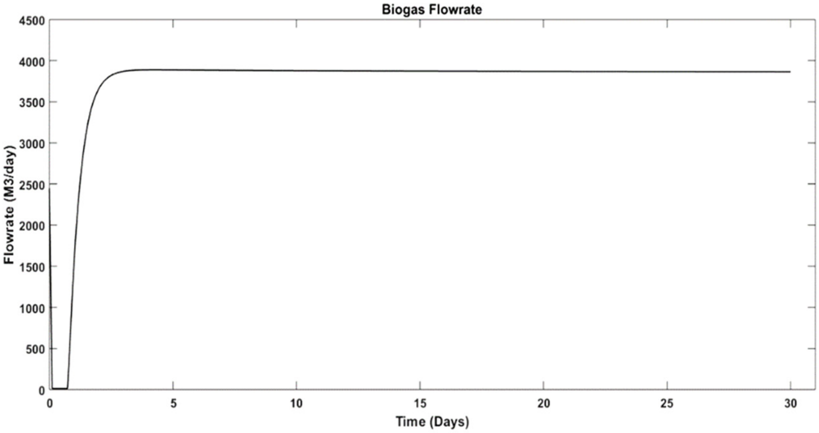

**Figure 4.** Biogas Flowrate in time

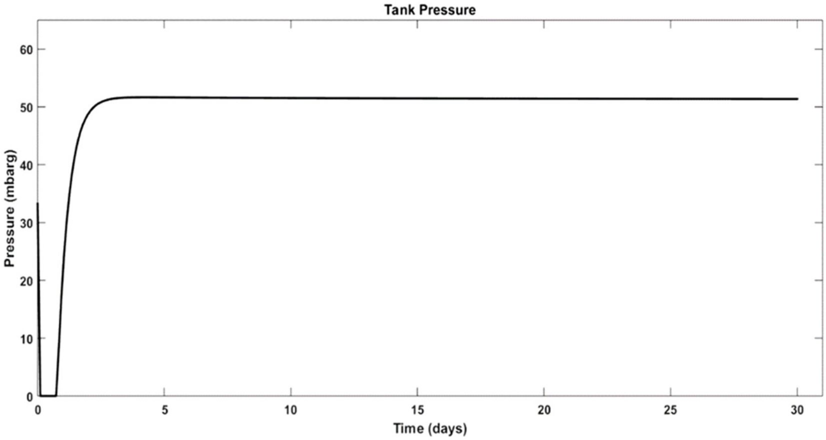

**Figure 5.** Pressure in time

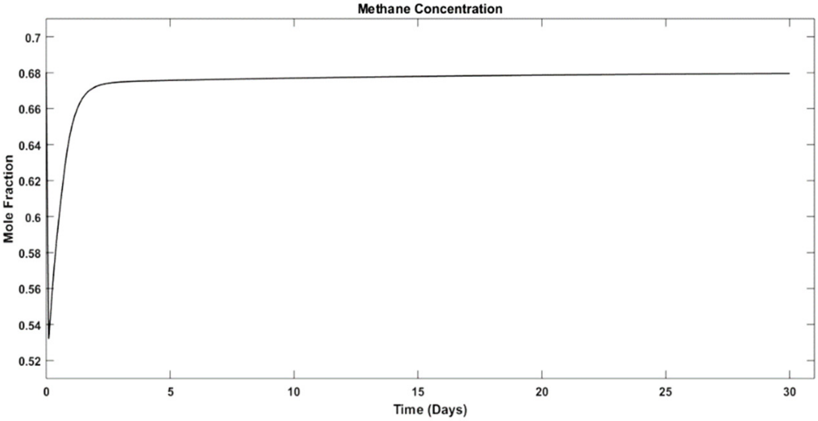

**Figure 6.** Methane concentrations in time

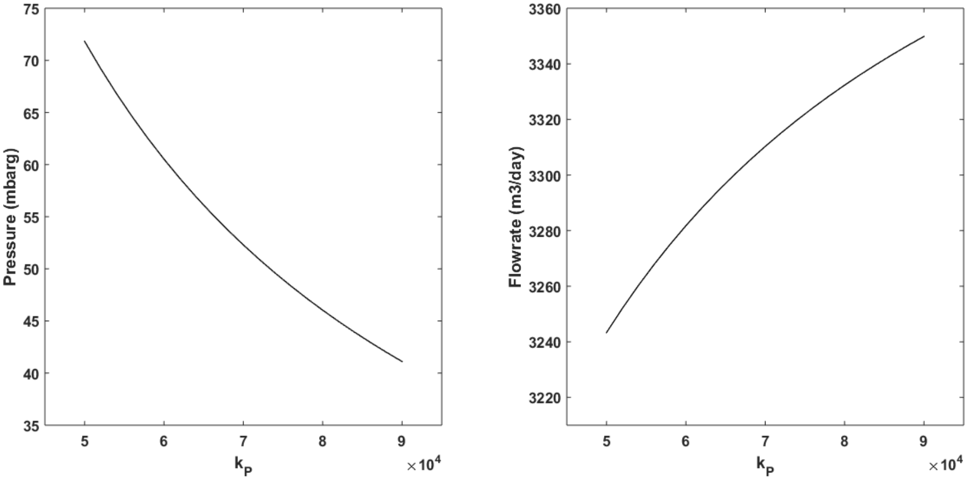

**Figure 7.** Effect of $k\_p$ on tank pressure and flowrate

The results of the sensitivity analysis that was performed has been presented in Table 5.

The first table presents the variables that have a positive influence on the pressure and biogas flowrate. The ones presented in Table 6 have a negative influence on the total output parameters. These parameters are presented in the descending order of their sensitivities to have an idea about the order in which they have to be varied to get fit the ADM1 model to an industrial digester.

Table 6 presents the effect of changes that has been presented in the input composition. It has been observed the inserts have no effect on the output variables, but the rest of the compositions show its effect. The effect of 6 most important variables has been presented in Table 7.

$$q = k\_p * (P\_digester - P\_atms) \tag{5}$$

The parameter $k\_p$ which is the correlation factor between the digesters pressure and the gas flowrate, as mentioned by equation (5), has a unique influence in the model. In the ADM 1, a change in $k\_p$ increases the biogas flowrate, this can be directly observed from the equation. But in this case study, analysing the simulation results, it has been observed to also reduce the tank pressure. This effect may be due to the presence of a gas recycle equations which has been included in the ADM model. These results are presented in Figure 7. Due to this unique property, this parameter could be of vital use in tuning the ADM1 model.

## CONCLUSIONS

ADM1 has been modified based on the design parameters and process conditions from Cluj-Napoca WWTP and has to be further calibrated to simulate the steady-state anaerobic digestion of activated sludge at municipal wastewater, in the production of biogas.

The sensitivity analysis performed identifies the parameters that have a major impact over the output.

The simulation outputs: biogas production rate, digester pressure and the methane concentration fit the industrial data. The methane concentration (69.37) clearly matches the values of the design parameters (70%), but the flowrate (3312 $m^3$/day) and the digester pressure (49.42 mbarg) varies slightly from the design values (3000 $m^3$/day and 25 mbarg respectively).

Parameter $k\_p$ which is the correlation factor between the digesters pressure and the gas flowrate has a unique influence in the model, because a rise in the digester pressure simultaneously decreases the flow rate. The model has to be calibrated to bring the simulation results within acceptable error margins of industrial data. The knowledge of calibration parameters and its effect on the output variables would act as a basis to either manually vary or develop an optimisation algorithm to perform the calibration exercise.

## ACKNOWLEDGMENTS

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