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Mathematical approach for improving the reliability of parameter calibration in modeling of anaerobic digestion processes

Konrad KOCH[1)], Tito GEHRING[2)], Manfred LÜBKEN[2)], Marc WICHERN[2)] and Harald HORN[3)]

1) Institute of Water Quality Control, Technische Universität München, Am Coulombwall, 85748 Garching, **Germany**.
2) Institute of Environmental Engineering, Ruhr-Universität Bochum, Universitätsstraße 150, 44780 Bochum, **Germany**.
3) Water Chemistry and Water Technology, Karlsruhe Institute of Technology, Engler Bunte Ring 1, 76131 Karlsruhe, **Germany**.

wga@bv.tum.de

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The Nash-Sutcliffe model efficiency coefficient (E_{NSC}) has been modified in order to assess the quality of simulations compared to observed data from the mesophilic monofermentation of grass silage. By applying the E_{NSC} it is not only possible to find parameter sets with the best fit, but also to analyze the sensitivity of each parameter. For modeling the concentration of hydrogen, both the maximum uptake rate for hydrogen k_{m_H2} and half-saturation coefficient of hydrogen K_{S_H2} are equally sensitive. Modeling the concentration of organic acids as acetate, propionate and butyrate, maximum uptake rate k_m as well as the free ammonia inhibition constant for acetate uptake K_{I_NH3} and hydrogen inhibition constants K_{I_H2}, respectively are much more sensitive than their corresponding half-saturation constants K_S. Only changes of hydrogen inhibition constants and maximum uptake of acetate compared to the ADM1 suggested values (for mesophilic sludge digestion) were necessary to fit the measurements.

Matematički pristup za unapređenje pouzdanosti podešavanja parametara u modeliranju procesa anaerobne digestije *

Izvorni znanstveni članak

Model Nash-Sutcliffe koeficijenta efikasnosti (E_{NSC}) primijenjen je u svrhu procjene kvalitete simulacija u usporedbi s promatranim podacima mezofilne monofermentacije travne silaže. Primjenom E_{NSC} nije moguće pronaći najbolje moguće odgovarajuće skupove parametara, isto tako nije moguće analizirati osjetljivost svakog parametra. Za modeliranje koncentracije vodika, jednako su osjetljivi maksimalna stopa unosa vodika k_{m_H2} kao i poluzasićenost vodikom $K_{S\_H2.}$ Modeliranje koncentracije organskih kiselina kao acetata, propionata i butirata, maksimalni unos k_m jednako kao i konstanta inhibicije bez amonijaka za unos acetata K_{I_NH3} i konstanta inhibicije vodika $K_{I\_H2,}$ mnogo više su osjetljiviji u odnosu na njihove odgovarajuće poluzasićene konstante $K_{S.}$ Za odgovarajuća mjerenja samo su bile potrebne promjene konstante inhibicije vodika i maksimalnog unosa acetate u usporedbi s ADMI predloženim vrijednostima (za mezofilnu digestiju taloga).

1. Introduction

Anaerobic digestion is a complex biological process requiring the involvement of a variety of microorganisms. Nowadays, biogas plants are usually operated at relatively low organic loading rates due to fear of overload and failure and the subsequent financial consequences. For example, ten medium-sized agricultural biogas plants in Germany have an average organic loading rate (OLR) of 2.5 $kg_{VS}/(m^3 \cdot d)$ with a range between 1.5 and 3.8 $kg_{VS}/(m^3 \cdot d)$ [1]. However, wet fermentation systems could reach OLRs of up to 4 $kg_{VS}/(m^3 \cdot d)$ [2]. A model based tool which provides plant operators with suggestions concerning ongoing operation may be helpful. Achievement of a stable process at higher organic loading rates would consequently increase the ecological and economical effectiveness of agricultural biogas production.

Mathematical models can be useful for understanding the numerous processes or microorganisms involved. Thereby, the influences of parameters on the process can be identified and approaches for optimization are revealed. After successful calibration, a mathematical model is able to predict reactor behavior even under varying conditions. Originally, modeling of the anaerobic digestion process was performed with respect to synthetic substrates such as acetate [3], waste material (e.g. animal manure [4]), and waste water sludge [5]. Up to the end of the 20th century, a large

variety of models already existed, however most of them are designed for specific substrates or reactor types. In order to consolidate the mathematical description of the anaerobic process, the IWA task group on the Mathematical Modeling of Anaerobic Digestion Processes was founded in 1997 and resulted in the publication of Anaerobic Digestion Model No. 1 (ADM1) in 2002 [6]. In contrast to most of the parent models, ADM1 is universally applicable and nowadays it is the most complex model for anaerobic digestions modeling and is therefore widely used. But as the model was developed for treatment of activated and primary sludge, model parameters are calibrated for these kinds of substrates. Nevertheless, there is an increasing trend of simulations being used for agricultural substrates [7]. Examples include cattle manure [8, 9], cattle manure and maize [10], cattle manure and co-substrates [11] and grass silage [12, 13]. Due to this development, calibration of kinetic parameters to both different substrates and conditions are required. Especially when using a complex model with several kinetic parameters such as ADM1, sensitivity analyses are valuable in reducing parameter calibration to the sensitive one.

Symbols/Oznake

ADM1	- Anaerobic Digestion Model No. 1 - Model anaerobne digestije Br. 1	k_{m_Pro}	- Maximum uptake rate propionate, $kg_{COD}/(kg_{COD}\cdot d)$ - Maksimalna stopa unosa propionata, $kg_{COD}/(kg_{COD}\cdot d)$
COD	- Chemical oxygen demand, mg/l - Kemijska potrošnja kisika, mg/l	K_{S_Ac}	- Half-saturation coefficient of acetate, kg_{COD}/m^3 - Koeficijent poluzasićenja acetata, kg_{COD}/m^3
E_{NSC}	- Nash-Sutcliffe model efficiency coefficient - Model Nash-Sutcliffe koeficijenta efikasnosti	K_{S_C4}	- Half-saturation coefficient of hydrogen, kg_{COD}/m^3 - Koeficijent poluzasićenja vodika, kg_{COD}/m^3
IWA	- International Water Association - Međunarodna udruga za vode	K_{S_H2}	- Half-saturation coefficient of valerate and butyrate, kg_{COD}/m^3 - Koeficijent poluzasićenja smjese I butirata, kg_{COD}/m^3
$K_{I\_H2\_C4}$	- Hydrogen inhibition constant for valerate and butyrate uptake, kg_{COD}/m^3 - Inhibicija konstante vodika za smjesu i unos butirata, kg_{COD}/m^3	K_{S_Pro}	- Half-saturation coefficient of propionate, kg_{COD}/m^3 - Koeficijent poluzasićenja propionata, kg_{COD}/m^3
$K_{I\_H2\_Pro}$	- Hydrogen inhibition constant for propionate uptake, kg_{COD}/m^3 - Konstanta inhibicije vodika za unos propionata, kg_{COD}/m^3	*OLR*	- Organic loading rate, $kg_{VS}/(m^3\cdot d)$ - Organska stopa unosa, $kg_{VS}/(m^3\cdot d)$
K_{I_NH3}	- Free ammonia inhibition constant for acetate uptake, $kmol_N/m^3$ - Konstanta inhibicije bez amonijaka za unos acetata, $kmol_N/m^3$	*TS*	- Total solids, % - Ukupne tvari, %
k_{m_Ac}	- Maximum uptake rate acetate, $kg_{COD}/(kg_{COD}\cdot d)$ - Maksimalna stopa unosa acetata, $kg_{COD}/(kg_{COD}\cdot d)$	*VFA*	- Volatile fatty acids - Hlapljive masne kiseline
k_{m_C4}	- Maximum uptake rate valerate and butyrate, $kg_{COD}/(kg_{COD}\cdot d)$ - Maksimalna stopa unosa smjese i butirata, $kg_{COD}/(kg_{COD}\cdot d)$	*VS*	- Volatile solids, % TS - Hlapljive tvari, % TS
k_{m_H2}	- Maximum uptake rate hydrogen, $kg_{COD}/(kg_{COD}\cdot d)$ - Maksimalna stopa unosa vodika, $kg_{COD}/(kg_{COD}\cdot d)$		-

2. Methods

2.1. Database and model set-up

Application of the modified Nash-Sutcliffe coefficient (E_{NSC}) is exemplarily demonstrated on data from the mesophilic treatment of grass silage. Two reactors were run as duplicates, indicated in the following as reactor L and reactor R. Details about the reactor set-up and operation can be found in [14] and information concerning modeling in [13]. Simulations and sensitivity analyses were executed with SIMBA 4.2 based on Matlab/Simulink (Version 7.0.4).

2.2. Calibration of kinetic parameters

Most of the kinetic parameters of the ADM1 cannot be estimated independently from others. During anaerobic digestion, hydrogen and in particular volatile fatty acids (VFA) play a central role. An accurate reproduction of both in this respect is important for the whole simulation, as the concentration influences a multitude of other processes. Degradation of acetate, propionate, and butyrate/valerate, respectively, is characterized by the half-saturation coefficient K_S, the maximum uptake rate k_m and the inhibition constant K_I for free ammonia (Acetate) and hydrogen (propionate and butyrate/valerate). For example, Equation 1 shows the rate for butyric acid as applied in ADM1. It is assumed that butyric and valeric acid are degraded by the same type of microorganism. Consequently, both parameters are summarized as C4.

$$\rho_j = k_{m\_C4} \cdot \frac{S_{Bu}}{K_{S\_C4} + S_{Bu}} \cdot X_{C4} \cdot \frac{1}{1 + S_{Va}/S_{Bu}} \cdot \frac{1}{1 + S_{H2}/K_{I\_H2\_C4}} \cdot I_{pH} \cdot I_{IN} \quad (1)$$

Where ρ_j is the rate of process j [$kg_{COD}/(m^3 \cdot d)$], k_{m_C4} is the maximum uptake rate for butyrate/valerate [$kg_{COD}/(kg_{COD} \cdot d)$], S_{Bu} is the concentration of dissolved butyric acid [kg_{COD}/m^3], K_{S_C4} is the half-saturation coefficient of butyrate/valerate [kg_{COD}/m^3], X_{C4} is the concentration of butyrate/valerate-utilizing bacteria [kg_{COD}/m^3], S_{Va} is the concentration of dissolved valeric acid [kg_{COD}/m^3], S_{H2} is the concentration of hydrogen [kg_{COD}/m^3], $K_{I\_H2\_C4}$ is the hydrogen inhibition constant for butyrate/valerate [kg_{COD}/m^3] and I_{IN} and I_{pH} are inhibition terms for inorganic nitrogen and pH value, respectively. The biomass decay rates were not changed in the simulations presented here (k_{dec} = 0.2 d^{-1} for all biomass groups).

For the uptake of acetate, the inhibition term for hydrogen is substituted by one for free ammonia. Furthermore, the term which affects the competitive inhibition by the concurrence of butyrate and valerate disappears. Already from the equation, the parameters that will probably be sensitive when enough substrate is present ($X_{C4} >> 0$) can be deduced. The change of k_m will always have an influence on simulation results; however K_S will only affect the process when the concentration of the corresponding acids is quite low. In high concentrations, the influence of K_S is not as great because the Monod term is converging to 1. The K_I Monod term is reacting the opposite way. Its sensitivity increases when the concentration of hydrogen (or free ammonia in case of acetate) increases.

2.3. Modified Nash-Sutcliffe coefficient

Besides a mathematical description of important processes, the calibration of model parameters is fundamental for a successful simulation. The quality of the model results depends strongly on the calibration of kinetic parameters, whose estimation is usually done manually by visual comparison to experimental results [9, 15, 16, 17]. This procedure however is quite subjective and requires experience. It is possible that two people, given the same experimental data set, would estimate parameters differently. The question whether the parameter calibration is non-ambiguous still has to be clarified. Nevertheless, a more objective assessment tool is advised. One possibility is the definition of a fitness function by minimizing the sum of the differences between the measurements and the simulation results (least squares method):

$$E = \sum_{i=1}^{n} (X_{i,measured} - X_{i,simulated})^2 \quad (2)$$

where E is the sum of errors between measured and simulated values, and $X_{measured}$ and $X_{simulated}$ are measured and the simulated values.

The advantage of this method is the possibility to quantify the goodness of fit, whereas low values show less differences and hence good agreement. A disadvantage is the lack of comparability of E concerning two simulations with different parameter dimensions. For example, E is significantly different when a fictitious concentration is used such as 1,000 mg/L compared to 1 g/L. Furthermore, individual outliers are much more sensitive to the results in contrast to a continuous discrepancy due to squaring. At least E has no explanatory power and an assessment is only possible in relation to a

simulation with the same reference parameter.

Assessment of the quality of a simulation with reference to the measurements is necessary for every kind of model. Calculation possibilities are as numerous as complex. In the field of hydrology, the so called Nash-Sutcliffe model efficiency coefficient [18] is widely used in order to assess the quality of simulations compared to observed data. By dividing the sum of differences by the average of measurements, it is not only possible to find the parameter set with the best fit,

but also to quantitatively describe the accuracy of the model outputs. In its modified version, the term of the squared differences is replaced by their absolute values to avoid sensitivity to the outliers. This modification guarantees that a difference is as dominant as two differences, each with half the value:

$$E_{NSC} = 1 - \frac{\sum_{i=1}^{n} \left| X_{i,measured} - X_{i,simulated} \right|}{\sum_{i=1}^{n} \left| X_{i,measured} - \overline{X}_{measured} \right|} \quad (3)$$

Where $X_{measured}$ and $X_{simulated}$ are the measured and simulated values respectively, and $\overline{X}_{measured}$ is the average of all measurements.

An efficiency of 1 corresponds to a perfect match of the modeled parameters to the observed data, where an efficiency of 0 indicates that the model prediction is as accurate as the mean of the observed data. The values below 0 imply that the simulation was worse than the simple average of the measurements.

3. RESULTS AND DISCUSSION

3.1. Application of E_{NSC}

The applied methodology to adapt ADM1 to grass silage followed a two-step procedure. First, all kinetic parameters were set to the suggested ADM1 values for mesophilic sludge digestion. Second, simulations were run by varying the kinetic parameters (maximum uptake rate k_m, half-saturation coefficient K_S and inhibition constant K_I) of the corresponding component. The agreement of the simulation results compared to measurements has been evaluated on the basis of the modified Nash-Sutcliffe coefficient. Figure 1 depicts the measured data for the two reactors and the simulation results with two different hydrogen inhibition constants $K_{I\_H2\_C4}$.

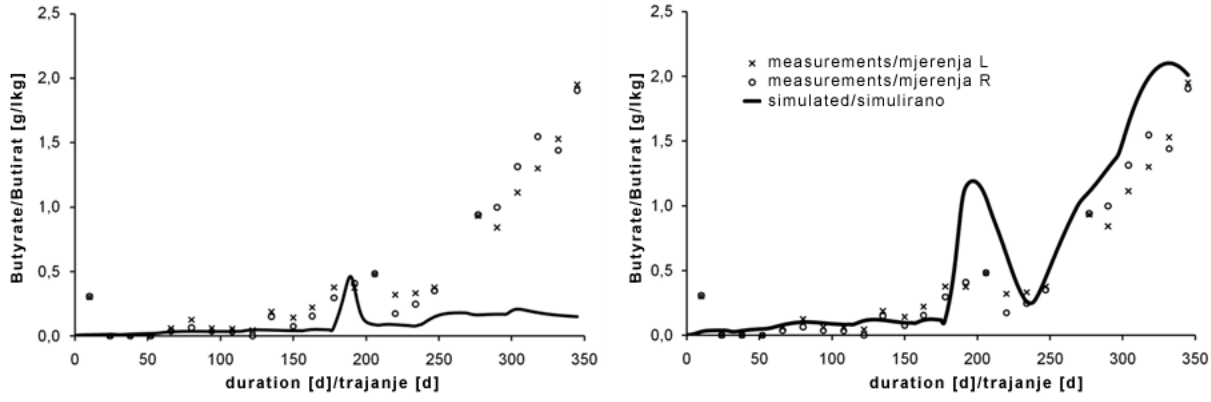

Figure 1. Simulation results and measured data for the concentration of butyrate for two different hydrogen inhibition constants $K_{I\_H2\_C4}$.

Slika 1. Rezultati simulacije i mjerene vrijednosti koncentracije butirata za dvije različite konstante inhibicije vodika $K_{I\_H2\_C4}$.

It is obvious that the simulation on the right expresses the dynamics of the measurements much better than the left one. Applying the modified E_{NSC} results in a value of 0.24 (0.15) for the left picture and a value of 0.67 (0.57) for the right with reference to reactor L (reactor R). The visual impression could hence be quantified by the coefficient.

3.2. Identification of kinetic parameters

If the determination of the modified Nash-Sutcliffe coefficient is implemented in the model software, a value is obtained for every combination of parameters. In principle, all influencing parameters can be varied and a coefficient is obtained for every combination. For a better visualization, a variation of only two parameters is advisable.

The following simulation studies have been done based on the measurements for reactor L treating grass silage under mesophilic conditions. Graphs are structured in such a way that on the abscissa and ordinate, the variation of one kinetic parameter around a default value (multiplication by 1.0) is displayed and the agreement (as E_{NSC}) is depicted in grey. As it is impossible to visualize more than two parameters, the third one remained at its default value (may already be adapted). To emphasize the highest values, the negative values have been zeroed (equal to white) and the maximum value was set to black. Therefore, grey scale differs between each figure. Furthermore, only highly dynamic areas are presented.

The concentrations of hydrogen and the organic acids depend first of all on the production of the corresponding component itself and in addition to those factors discussed in the following chapter, on the decay rate of the utilizing bacteria. All biomass decay rates remained at their suggested ADM1 values.

3.2.1. Hydrogen

The concentration of hydrogen is only influenced by the maximum uptake rate k_{m_H2} and the half-saturation coefficient K_{S_H2}. For creation of Figure 2, k_{m_H2} has been varied around its suggested value (35 d^{-1}), while K_{S_H2} has already been adapted to $5.6 \cdot 10^{-5}$ kg_{COD}/m^3 (suggested ADM1 value: $7 \cdot 10^{-6}$ kg_{COD}/m^3). The range is quite similar to previous studies [12], where it has already been stated that the hydrogen inhibition constant applied for propionate and valerate/butyrate uptake for grass silage is up to two orders of a magnitude lower than that for activated sludge digestion. The colour gradient reveals that both parameters are similarly sensitive. Because as few as possible parameters should be modified and K_{S_H2} has already been changed, k_{m_H2} should remain at the suggested value. Hence, the optimum can be found by multiplication with 1.0 (white line). The highest value and hence, the highest degree of agreement is achieved for about $1.0 \cdot K_{S\_H2}$, which justifies the previously realized modification by a factor of 8. Nevertheless, several other combinations resulted in comparably high coefficients. Although a couple of maxima (not only in the depicted area) exist, a tupel of parameters needs to be chosen for running a simulation. In order to limit the amount of combinations, as few as possible parameters are calibrated. Finally, the suggested ADM1 parameter values are based on widespread research reflecting the complex biological processes, and any unnecessary change should be avoided.

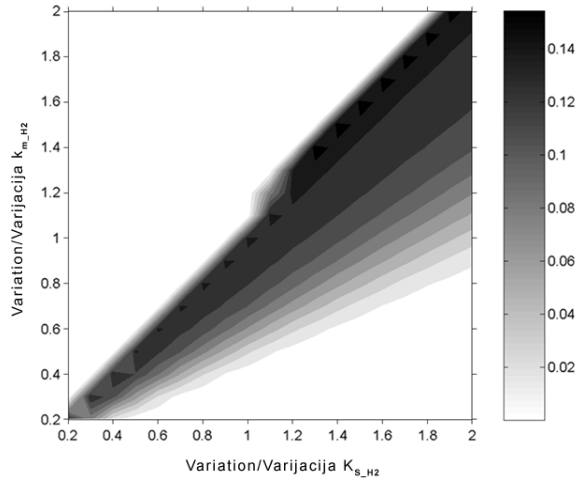

Figure 2. Sensitivity analysis for the concentration of hydrogen by varying k_{m_H2} and K_{S_H2}.

Slika 2. Analiza osjetljivosti koncentracije vodika promjenom k_{m_H2} i K_{S_H2}.

3.2.2. Acetate

For this simulation study all three parameters remained at their suggested ADM1 values. As can be seen in the top graphs of Figure 3, K_{S_Ac} is – in contrast to k_{m_Ac} and K_{I_NH3} – quite a non-sensitive parameter. This corresponds to the previous considerations based on Equation 1 that the half-saturation coefficient will only be sensitive at low concentrations of the associated acid. However, acetate reached concentrations of 5,000 mg/L during this experiment. If K_{S_Ac} remains unchanged and the two sensitive parameters are varied, the down graph is obtained. According to the convention that as the least possible parameters should be adapted, intersections with standard value (multiplication by 1.0) should be preferred. Furthermore, the change of a parameter should be as small as possible, too. As the Nash-Sutcliffe coefficient for $0.55 \cdot k_{m\_Ac}$ is higher as for $0.4 \cdot K_{I\_NH3}$ as well, a calibration of the maximum uptake rate k_{m_Ac} on 55 % of its suggested value is advised. However, other combinations ($1.8 \cdot k_{m\_Ac}$ and $0.2 \cdot K_{I\_NH3}$, for example) also lead to similar coefficients. A definitive calibration of parameters is once again not possible.

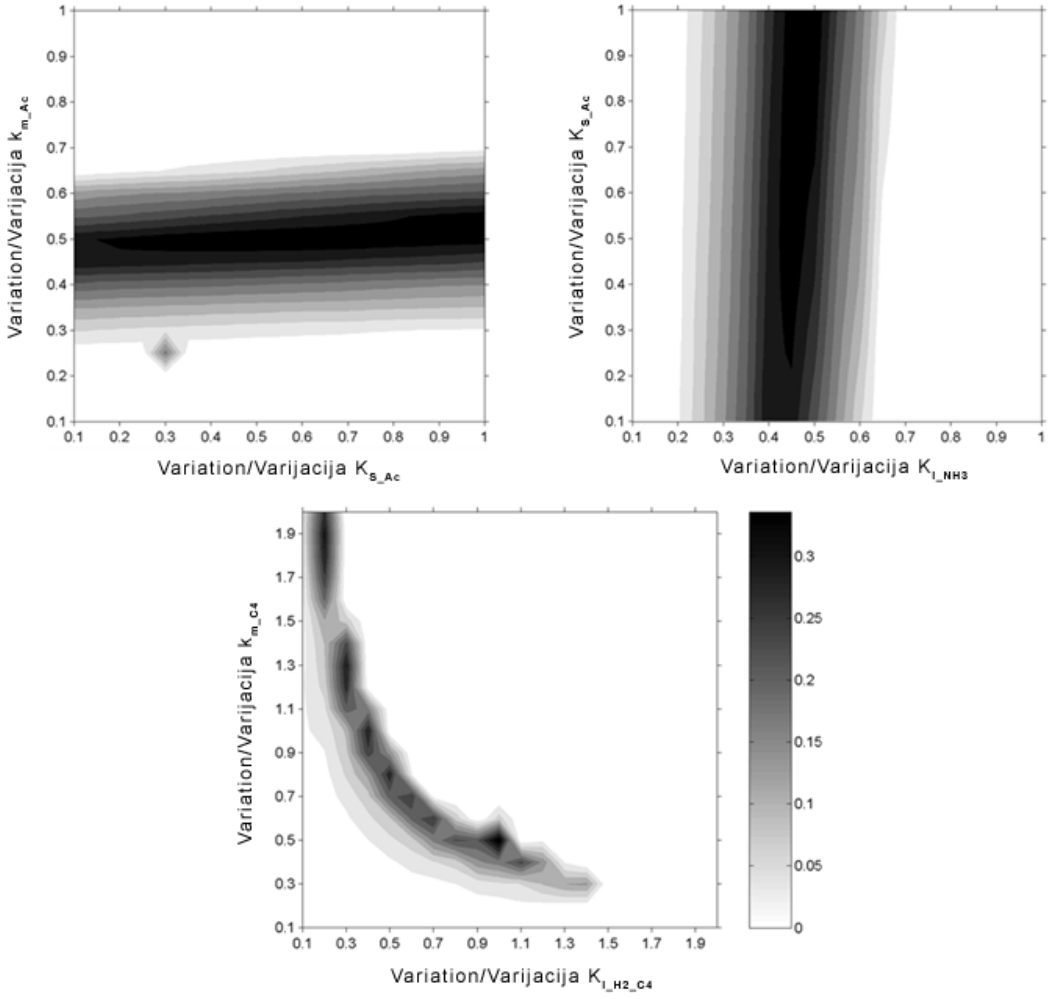

Figure 3. Sensitivity analysis for the concentration of acetate by varying k_{m_Ac}, K_{S_Ac} and K_{I_NH3}.

Slika 3. Analiza osjetljivosti koncentracije acetata promjenom k_{m_Ac}, K_{S_Ac} and K_{I_NH3}.

3.2.3. Propionate

In contrast to the simulation studies for acetate, the hydrogen inhibition constants for propionate and butyrate/valerate have already been adapted due to reasons of visualization. $K_{I\_H2\_Pro}$ has been reduced by a factor of 0.013 compared to its suggested value [13], but is set as the standard value (multiplication by 1.0) in the following graphs. Similar to Figure 3 and due to a high concentration of propionate (up to 8,000 mg/L) once more, the sensitivity of K_{S_Pro} is marginal as depicted in Figure 4 (top graphs). As an adaption of $K_{I\_H2\_Pro}$ was already necessary, k_{m_Pro} remains at its suggested value. Although the lower graph shows that the optimum should be rather in the field of $1.3 \cdot K_{I\_H2\_Pro}$ (white line), this discrepancy is due to the fact that both reactors were considered for parameter calibration, but this simulation study refers only to reactor L.

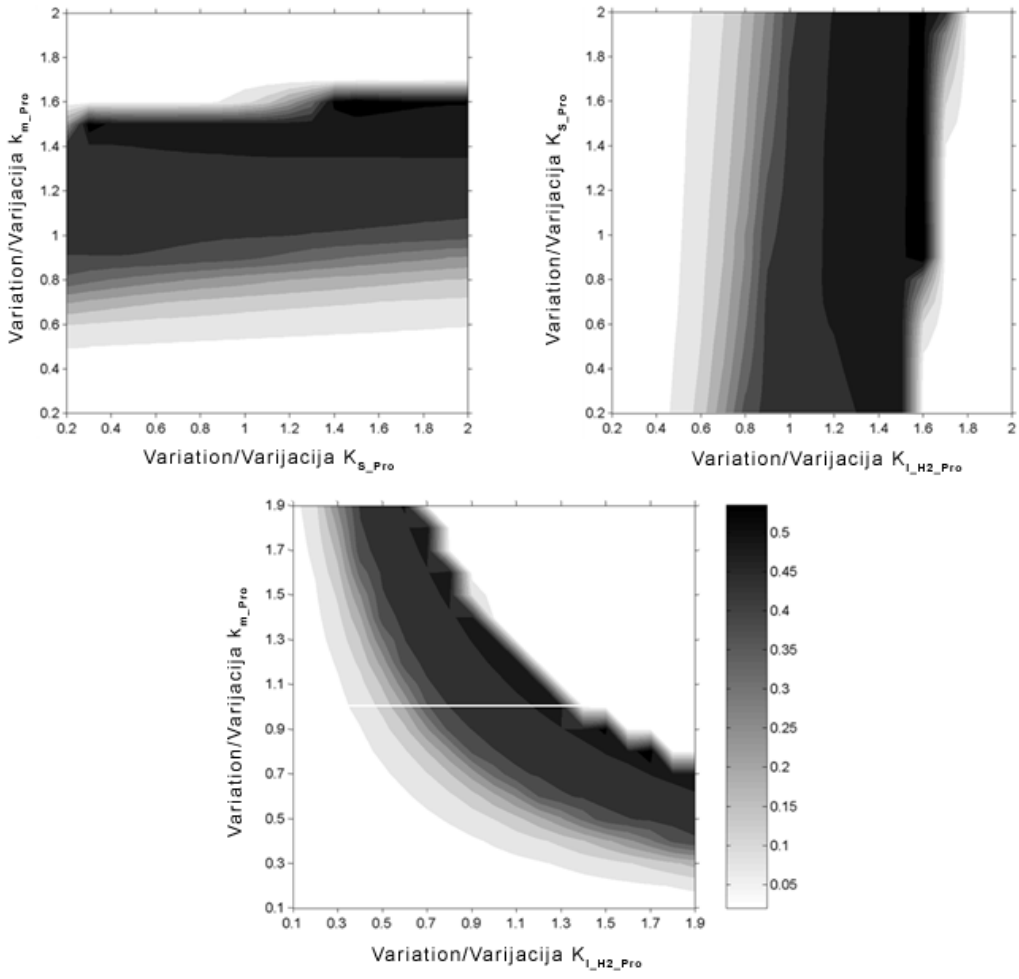

Figure 4. Sensitivity analysis for the concentration of propionate by varying k_{m_Pro}, K_{S_Pro} and $K_{I\_H2\_Pro}$.

Slika 4. Analiza osjetljivosti koncentracije propionata promjenom k_{m_Pro}, K_{S_Pro} and $K_{I\_H2\_Pro}$.

3.2.4. Butyrate

Similar to the studies of propionate, the hydrogen inhibition constant for butyrate and valerate uptake $K_{I\_H2\_C4}$ has been reduced by a factor of 0.005 compared to its suggested value, but is set as the standard value. Again this change overlaps with the ranges proposed by previous research for the adaption of ADM1 to grass silage [12]. The concentration of butyrate in reactor L acted as a reference for the calculation of the E_{NSC}. Once more, the maximum uptake rate k_{m_C4} and the hydrogen inhibition constant $K_{I\_H2\_C4}$ are the most sensitive parameters. Nevertheless, due to the relatively low concentration of butyric acid (less than 2,000 mg/L), the influence of K_{S_C4} increased as can be seen by the shift of E_{NSC} relative to the K_{S_C4}-axis. In contrast to Figure 3, where a variation of K_{S_Ac} had nearly no influence on the goodness of fit, changing K_{S_C4} by constant $1.2 \cdot K_{I\_H2\_C4}$ caused a change from nearly zero for low factors up to the maximum Nash-Sutcliffe coefficients for higher factors.

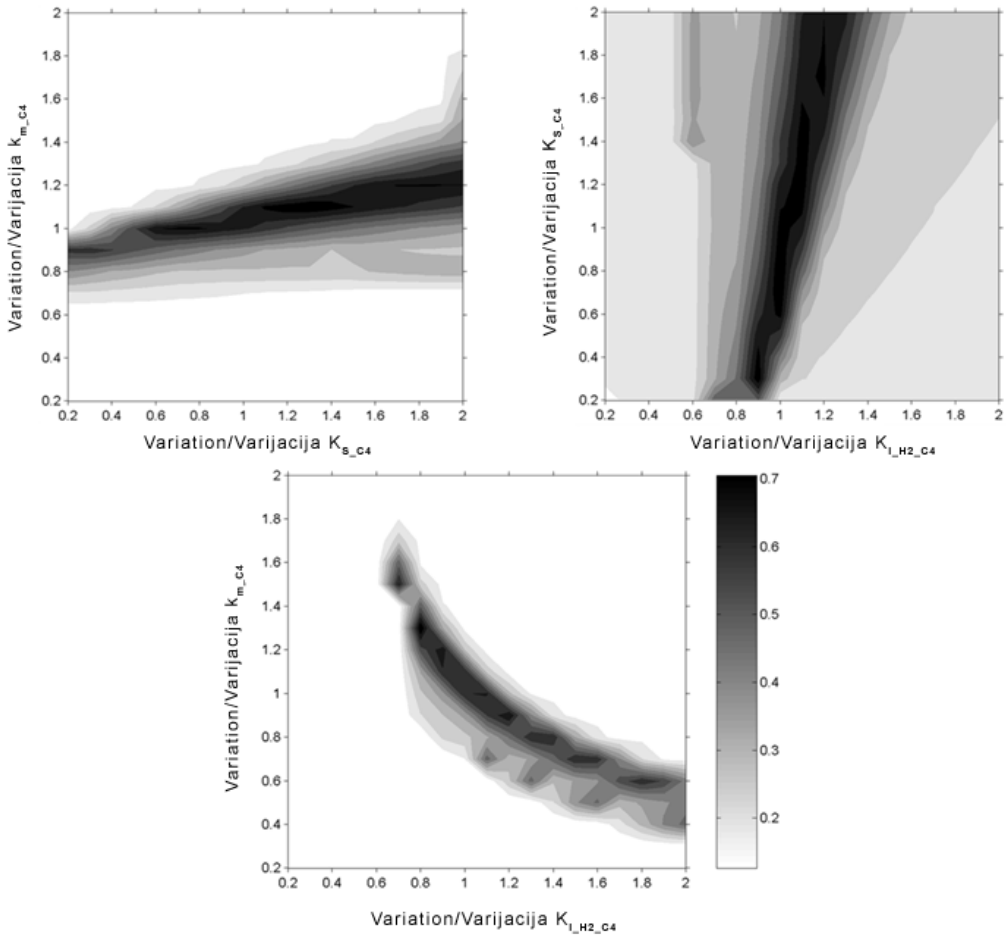

Figure 5. Sensitivity analysis for the concentration of butyrate by varying k_{m_C4}, K_{S_C4} and $K_{I\_H2\_C4}$.

Figure 5. Analiza osjetljivosti koncentracije butirata promjenom k_{m_C4}, K_{S_C4} and $K_{I\_H2\_C4}$.

3.2.5. Summary

Figures 2 to 5 clarify that the kinetic parameters have different impacts on the model results. They further indicate that the model results are not bijective. On the one hand, a pair of parameters led to a definitive E_{NSC} value. But on the other hand, an arbitrary E_{NSC} was reached by a couple of combinations of the parameters. The phenomenon that the same result can be achieved in different ways is called equifinality. This means that there is not simply one optimal parameter set that represents a system, but rather that several combinations of parameter values for a chosen model structure may fit the data equally well. On this account, several authors have already started to specify parameters not by single values, but by confidence regions [19, 20]. Thus, not the parameter value itself is important, but rather the combination. Knowledge on equifinality is insofar basically for modelling as calibration of parameters is usually not definite. It is hence possible that the model's output is equal although parameter sets were different. Maybe some parameters compensate for each other due to the overdetermined system. Proportional to its complexity, parameter calibration in ADM1 requires a large database. In further research, adapted parameters must be proven by independent datasets.

4. CONCLUSIONS

The modified Nash-Sutcliffe model efficiency coefficient was applied as an alternative methodology for the calibration of kinetic parameters of the ADM1. Sensitivity analyses highlighted different influences on the model's output by what the number of parameters for calibration could be reduced to the most sensitive ones. As has already been shown [13], only changes of hydrogen inhibition constants and maximum uptake of acetate compared to the ADM1 suggested values were necessary in order to fit the measurements.

The approach presented is universally applicable and hence transferable to any other model where a calibration of parameters is necessary and an independent determination is not possible. A quality assessment procedure based on the E_{NSC} implemented in the model allows the software to automatically search for the parameter combination with the best fit. In this context, the phenomena of equifinality should be considered.

Applying the Nash-Sutcliffe coefficient enables parameter sensitivity analysis and parameter estimation as well. Thereby,

- extensive manual analysis of model output is avoided,
- percentile quantification of the degree of agreement is enabled,
- comparison of the different goodness of fit values (independent of their units) is possible,
- a new approach for parameter sensitivity analysis is presented, and
- finally, the reliability of model calibration is significantly improved.

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REFERENCES

[1] EFFENBERGER, M.; LEHNER, A.; GRONAUER A.: *Performance Figures of Agricultural Biogas Plants for (Co-)Digestion of Energy Crops*, Vth International Symposium on Anaerobic Digestion of Solid Wastes and Energy Crops, Hammamet 2008.

[2] WEILAND, P.: *Biogas production: Current state and perspectives*, Applied Microbiology and Biotechnology 85(2010)4, 849-860.

[3] ANDREWS, J.F.: *Dynamic model of the anaerobic digestion process*, Journal of the Sanitary Engineering Division 95(1969)SA 1, 95-116.

[4] HILL, D.T.: *Simplified monod kinetics of methane fermentation of animal wastes*, Agricultural Wastes 5(1983)1, 1-16.

[5] SIEGRIST, H.; RENGGLI, D.; GUJER, W.: *Mathematical modelling of anaerobic mesophilic sewage sludge treatment*, Water Science and Technology 27(1993)2, 25-36.

[6] BATSTONE, D.J.; KELLER, J.; ANGELIDAKI, I.; KALYUZHNYI, S.V.; PAVLOSTATHIS, S.G.; ROZZI, A.; SANDERS, W.T.M.; SIEGRIST, H.; VAVILIN, V.A.: *Anaerobic Digestion Model No. 1*, International Water Association, London 2002.

[7] LÜBKEN, M.; GEHRING, T.; WICHERN, M.: *Microbiological fermentation of lignocellulosic biomass: Current state and prospects of mathematical modeling*, Applied Microbiology and Biotechnology 85(2010)6, 1643-1652.

[8] MYINT, M.; NIRMALAKHANDAN, N.; SPEECE, R.E.: *Anaerobic fermentation of cattle manure: Modeling of hydrolysis and acidogenesis*, Water Research 41(2007)2, 323-332.

[9] SCHOEN, M.; SPERL, D.; GADERMAIER, M.; GOBERNA, M.; FRANKE-WHITTLE, I.; INSAM, H.; ABLINGER, J.; WETT, B.: *Population dynamics at digester overload conditions*, Bioresource Technology 100(2009)23, 5648-5655.

[10] AMON, T.; AMON, B.; KRYVORUCHKO, V.; ZOLLITSCH, W.; MAYER, K.; GRUBER, L.: *Biogas production from maize and dairy cattle manure - Influence of biomass composition on the methane yield*, Agriculture, Ecosystems and Environment 118(2007)1-4, 173-182.

[11] LÜBKEN, M.; WICHERN, M.; SCHLATTMANN, M.; GRONAUER, A.; HORN, H.: *Modelling the energy balance of an anaerobic digester fed with cattle manure and renewable energy crops*, Water Research 41(2007)18, 4085-4096.

[12] WICHERN, M.; GEHRING, T.; FISCHER, K.; ANDRADE, D.; LÜBKEN, M.; KOCH, K.; GRONAUER, A.; HORN, H.: *Monofermentation of grass silage under mesophilic conditions: Measurements and mathematical modeling with ADM 1*, Bioresource Technology 100(2009)4, 1675-1681.

[13] KOCH, K.; LÜBKEN, M.; GEHRING, T.; WICHERN, M.; HORN, H.: *Biogas from grass silage - Measurements and modeling with ADM1*, Bioresource Technology 101(2010)21, 8158-8165.

[14] KOCH, K.; WICHERN, M.; LÜBKEN, M.; HORN, H.: *Mono fermentation of grass silage by means of loop reactors*, Bioresource Technology 100(2009)23, 5934-5940.

[15] BOUBAKER, F; RIDHA, B.C.: *Modeling of the mesophilic anaerobic co-digestion of olive mill wastewater with olive mill solid waste using anaerobic digestion model No. 1 (ADM1)*, Bioresource Technology 99(2008)14, 6565-6577.

[16] QU, X.; VAVILIN, V.A.; MAZÉAS, L.; LEMUNIER, M.; DUQUENNOI, C.; HE, P.J.; BOUCHEZ, T.: *Anaerobic biodegradation of cellulosic material: Batch experiments and modelling based on isotopic data and focusing on aceticlastic and non-aceticlastic methanogenesis*, Waste Management 29(2009)6, 1828-1837.

[17] RAMIREZ, I.; MOTTET, A.; CARRÈRE, H.; DÉLÉRIS, S.; VEDRENNE, F.; STEYER, J.-P.: *Modified ADM1 disintegration/hydrolysis structures for modeling batch thermophilic anaerobic digestion of thermally pretreated waste activated sludge*, Water Research 43(2009)14, 3479-3492.

[18] NASH, J.E.; SUTCLIFFE, J.V.: *River flow forecasting through conceptual models part I - A discussion of principles*, Journal of Hydrology 10(1970)3, 282-290.

[19] GE, H.; JENSEN, P.D.; BATSTONE, D.J.: *Pre-treatment mechanisms during thermophilic-mesophilic*

temperature phased anaerobic digestion of primary sludge, Water Research 44(2010)1, 123-130.

[20] BATSTONE, D.J.; KELLER, J.: *Variation of bulk properties of anaerobic granules with wastewater type*, Water Research 35(2001)7, 1723-1729.