Evolutionary Algorithm Application for Parameter Estimation of the Anaerobic Digestion Model No.1

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Abstract—The paper present an application of evolutionary algorithms in environmental sciences. It describes the Anaerobic Digestion Process and a suitable mathematical model (Anaerobic Digestion Model No.1). The Anaerobic Digestion Model No.1 is adopted on a real waste water treatment plant digestion process. The paper shows how the fitting the Anaerobic Digestion Model No. 1 onto the real digestion process can be solved by the use of evolutionary algorithms.

I. INTRODUCTION

This paper is based on the work of the European Eureka research project APROMOCS¹. APROMOCS is a common Eureka research project between the Technical University of Kaunas, the University of Applied Sciences Schmalkalden and industrial partners from Lithuania and Germany. The project aims are the development of improved waste water treatment monitoring and control systems. Necessary for the development of advanced control strategies are simulations of the system behavior. The simulations are based on mathematical models which described the internal reactions of the biological wastewater treatment process and the digestion process. One of the most powerful but nonlinear models is the Anaerobic Digestion Model No. 1 (ADM1). This paper deals with the adaption of the ADM1 on a real anaerobic digestion process of the Bamberg² waste water treatment plant. To achieve this goal is an estimation of the ADM1 parameters essential. This has to be done in a high dimensional parameter space based on the available measurements of the Bamberg waste water treatment plant.

II. ANAEROBIC DIGESTION MODEL NO. 1

A. Anaerobic Digestion - Theoretical Background

The inlet of a waste water treatment plant contains heavily loaded waste water. The loaded content will be metabolized during the waste water treatment process into sludge. This activated sludge has to be stabilized with an anaerobic digestion process to reduce the organic content, the smell building content, the suspended solids and pathogen and also to improve the dewatering ability. [4]

The anaerobic digestion process consists of four main steps which are shown in Fig. 1.

Hydrolysis

The sludge input to the digester consists of a homogeneous mixture of undissolved complex carbohydrate, proteins and lipids. In the hydrolysis step, the complex compound will be disintegrated and metabolized by enzyme into dissolved compounds with a simple molecular structure like monosaccharide, long chain fatty acids or amino acids. [4] [6]

Acidogenesis

During the acidogenesis, carbohydrate, protein and lipid will be metabolized by anaerobic bacteria into low chain organic acids, alcohol, hydrogen, carbon dioxide and acetic acid. [4] [6]

Acetogenesis

In the acetogenisis step, the alcohol and low chain organic acids are metabolized by special anaerobic bacteria into acetic acid. [4] [6]

Methanogenesis

In the last step, the methane bacteria metabolized the acetic acid and some part of the hydrogen and carbon dioxide from the acidogenesis step into methane. [4] [6]

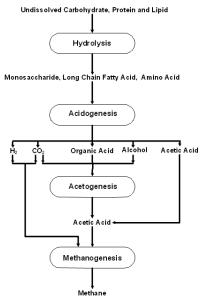


Figure 1. Anaerobic Digestion Process [4]

¹ Advanced Process Monitoring and Control Systems for Wastewater Treatment Plants

² The town of Bamberg has 70.000 inhabitants and it is located in the north of Bavaria, Germany.

B. Anaerobic Digestion Model No. 1

Several approaches were published to describe the behavior of an anaerobic digester. To name but a few there are the approaches of [2], [7], [13] and [14]. The authors decided to work with the approach of [2], the Anaerobic Digestion Model No. 1 (ADM1), because of the following reasons:

- The model is based on a huge scientific knowledge, because scientist form all over the world developed together the model on the platform of the International Water Association.
- The ADM1 represents the complex internal reaction of an anaerobic digester in an adequate accuracy.
- In the ADM1 publication is a implementation of the ADM1 as a single stage continuous-flow stirred-tank reactor shown.
- A large number of suggested parameters for the process equations are given in the ADM1 publication.
- Implementations of the ADM1 into MatLab are published. [2] [10] [11]

The used ADM1 implementation, with the extension published in Rosen [10], consists out of differential and algebraic equations which model the internal relations. There are 19 biochemical kinetic processes and 3 gas liquid transfer kinetic processes to calculate 26 dynamic state concentration variables. Implicit algebraic equations describe the acid-base and hydrogen kinetics. The model also takes process inhibition by pH, hydrogen and free ammonia and death of biomass in account.

Furthermore the ADM1 includes the temperature influences on the digestion processes, the calculation of the particular pressure in the headspace and the gas flow out of the digester. [1]

A full introduction into the ADM1 is beyond the scope of this paper. For more detailed information are the publications of [2] and [10] recommended.

The ADM1 is implemented into Visual Studio.Net with C#. For more detailed information about the ADM1 implementation is [16] recommended.

III. APPLICATION OF THE ADM1 ONTO THE BAMBERG WASTE WATER TREATMENT PLANT DIGESTION PROCESS

A. Bamberg Waste Water Treatment Plant (WWTP)

The digestion process of the Bamberg WWTP consists of three coupled digesters which operate in a two stage parallel-serial structure. Table 1 shows the digester characteristics. In the first stage the digesters one and the digester three are parallel feed with the activated sludge. Both feed there partial digested sludge into the digester two in the second stage.

The produced biogas form all three digester is collected in two gas tanks and then converted by three combined heat and power units.

To represent the real digestion structure are two different approaches used. The first Approach, Approach A, merge the three digesters together into one 7000m³ digester. This Approach can be simulated with one ADM1. This is an enormous simplification in comparison to the second Approach, Approach B. This Approach uses for every digester one single ADM1 and link them

TABLE I.
DIGESTER CHARACTERISTICS

	Digester One	Digester Two	Digester Tree
Digester Volume	2000m³	2000m³	3000m³
Digester Form	Egg	Egg	Cylinder
Recirculation Method	Stirring Unit	Stirring Unit	Pump

together. This Approach is more precisely but it increases the complexity and the simulation time.

B. Database

The ADM1 needs 24 input parameters. The most of these parameters determine the chemical oxygen demand (COD). The outcome of the ADM1 contains more then 30 values that describe the digester state. Previous works, like [3] and [5], deals with the adaption of the ADM1 on a down scaled laboratory digester. The use of a laboratory digester has the advantages that the digester inlet and outlet can be easy analyzed (COD composite) and controlled, a lot of measurement possibilities are available and the digester can operate in borderline situations.

In this paper the ADM1 is adapted to a real WWTP digestion process. The bases for the adaption are historical measurements. The ordinary measurement doesn't contain detailed information about the digester inlet and outlet, can be disturbed and is not so extensive like a laboratory digester. The measurement consists out of the daily values over the year 2006. A very huge problem is the calculation of the COD composite and the corresponding ADM1 input out of the measured data, but this topic is beyond the scope of this paper.

C. ADM1 Parameter

The overall ADM1 consist out of more then eighty parameters. Based on the works of [3] and [5] the parameters, which are shown in Table 2, are identified as the main influence parameters. Using Approach B makes the estimation of nine parameters for every ADM1 necessary. Because of the high dimensionality in the parameter space and the nonlinearity of the ADM1 requires the uses of stochastic parameter estimation techniques.

TABLE II. SIGNIFICANT ADM1 PARAMETERS

Parameter	Name	Value [2]	Value [3]	Value [5]
k _{dis}	Disintegration Parameter	0,4	1,0	1,5839
k _{hyd,ch}	Hydrolytic Parameter Carbohydrates	0,25	n.i.a	0,00099
k _{hyd,pr}	Hydrolytic Parameter Proteins	0,2	n.i.	n.i.
$k_{hyd,li}$	Hydrolytic Parameter Lipids	0,1	n.i.	n.i.
$k_{dec,all}$	Decay Rate	0,02	n.i.	0,0092
k _{m,pro}	Monod maximum specific uptake propionate	13	9	n.i.
$K_{S,pro}$	Half saturation value propionate	0,3	0,2	n.i.
k _{m,ac}	Monod maximum specific uptake acetate	8	9	352,0085
$K_{S,ac}$	Half saturation value acetate	0,15	0,15	20,0903

a not investigated

```
BEGIN
INITIALISE population
INITIALISE ancestor based on the ADM1 standard parameter
MUTATE ancestor
EVALUATE population;

WHILE (TERMINATION CONDITION not satisfied)

1 CALCULATE fitness
2 SELECT parents;
3 RECOMBINE pairs of parents;
4 MUTATE the resulting children;
5 EVALUATE new children;
6 SELECT individuals for the next generation;
7 CHECK termination condition
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Figure 2. EA Pseudo Code

IV. EVOLUTIONARY ALGORITHMS (EA)

The pseudo code in Fig. 2 shows a generalized EA procedure. The following subsections give explanations about the implementation of the single steps.

A. Object Function and Estimation Valudation

The research goal is the estimation of the ADM1 parameters that are shown in Table 2. The EA generates a possible version of these parameters. To determine the quality of the estimated parameters is an object function necessary. The object function aim is to measure the fitting of the ADM1 depending on the generated parameters. Therefore is a static simulation used with the annual mean of the digester input and the generated parameters. The simulation outcome is compared with the annual mean of six criteria that are shown in Table 3.

For the comparison of different solutions for the ADM1 parameter is an aggregation of the six criteria into one criterion required. For this purpose the method of Composite Programming (CP) [1] is used. CP is based on benefit analysis methods. The deviation between the simulated and the measured value of each criterion is transformed, like a fuzzy membership function, into a null to one space. Null represents a very low fitting and one represents a perfect fitting. The transformed values are aggregated into one value by use of a weighted Minkowski-Norm (1).

$$c = 1 - \left[\sum_{i=1}^{n} \alpha_{i} \cdot (1 - a_{i})^{p}\right]^{\frac{1}{p}}$$

$$c - \text{cumulative fitting}$$

$$\alpha_{i} - \text{weighting of the}$$

$$\text{individual fitting}$$

$$a_{i} - \text{individual fitting}$$

$$p - \text{aggregation factor}$$

$$(1)$$

To reduce the total simulation time is the evaluation of a whole population at one generation implemented as a parallel computer network. A master PC runs the EA. The other PC's represents one ADM1. The ADM1-PC's receives the phenotype from a master pc and returns the fitting values and there aggregation.

B. Initial Population

Our chosen genotype consists of three main parts, like the suggestion in [15]. The first part contains the state parameter of the evolutionary algorithm. This includes the fitness, the birth generation and the fitting values of the estimates ADM1 parameters. The second part contains the phenotype of the ADM1 parameters and the third part the standard deviation of the phenotype values.

Base of the initial population is an ancestor, one individual, with the phenotype values given in [2]. The initial standard deviations are set up to ten percent of the associated phenotype value. In the next step the ancestor is several times copied, mutated and the paste in then initial population.

C. Fitness, Selection, Crossover and Mutation

The EA-Routine starts with the calculation of the parent generation fitness. Base for the fitness computation is the aggregated fitting value. At this application are proportional fitness functions and order based fitness function implemented.

The fitness of each genome is the basis for the selection as parent for the next generation. The probability of a genome selection increases with the genome fitness. Implemented selection functions are the roulette selection, the stochastic universal sampling, the tournament selection and a uniform selection. Out of the selection pool are two parents randomly chosen and recombined. The recombination of the phenotype is done with a discrete or enlarged intermediate crossover method and the recombination of the standard deviation with an intermediate crossover method. The generated offspring is paste into the child population. The procedure repeats until a specified number of children are generated.

In the next step the whole child population is taken within a mutation operation. The phenotype of each child is mutated with a normal distributed probability based on the according standard deviation. The standard deviations are adaptive adjusted by a second mutation operation.

D. Reinsertion and Termination

There are three methods implemented to replace individuals of the parent population with individuals of the child population. The first method is to replace the whole parent population with the best individuals from the child population. The second approach is to merge the parent and the child population together and build with the best individual a new parent population. The third method only exchanges the worst twenty percent of the parent population with the best individual from the child population.

The EA-Routine stops after a defined number of generation or when the relative difference between the best individual over a defined number of generation is too small and the EA is converged.

TABLE III. FITTING CRITERIA

Criteria	Annual Mean	Unit	
gas flow digester one	1594.0	Nm³d-1	
gas flow digester two	1056.0	Nm³d-1	
gas flow digester three	2692.0	Nm³d⁻¹	
methane content	69.8	%	
рН	7,.11	[1]	
COD outlet digester two	14.4	kg m ⁻³ d ⁻¹	

V. SIMULATION RESULTS AND CONCLUSIONS

This section shows the results for the ADM1 approaches A and B based of one exemplified simulation. The example used a (μ,λ) -strategy with a population size of eleven parent individuals that create 77 child individuals. The fitness is calculated with an order based fitness function and the selection is done with stochastic universal sampling. The individuals were recombined with an enlarged intermediate crossover and mutated with the standard mutation method.

A. Approach A – One Digester

Fig. 3 presents the development of the cumulative fitting value of the best individual at each generation of approach A. The figure represents a typical shape of the cumulative fitting value at the research.

The cumulative fitting value starts at fitting level of 0.70 and converged until one hundred generations to an average fitting level of 0.78. After 270 generations the EA overcome the stagnation and begin to fluctuate. The EA reach a maximum fitting level of 0.86 at generation 279.

After such a long convergence phase and by such a high deviation of the cumulative fitting value must the best fitting value of 0.86 treated with special attention. Fig. 4 displays the gas flow on a static simulation with 500 days by using the estimated values at the fitting value of 0.86. Fig. 4 makes it obvious that the estimated cause an instable digester state. This makes a more detailed analysis necessary. For this purpose is a static simulation of the best individual at each generation done and standard deviation over one hundred days of the gas flow at a supposed stable digester state calculated. This is the base of a partial correlation analysis between the standard deviation of the gas flow and the estimated parameters.

The partial correlation analysis results that standard deviation depends only on the $k_{m,ac}$ parameter. The correlation coefficient is 0.86. The critical correlation coefficient with a probability of error of 0.1 percent and 293 degrees of freedom is 0,206 [17]. Therefore can the calculated correlation coefficient deemed to be significant. The dependency between the standard deviation and $k_{m,ac}$ is illustrated in Fig. 5.

The best fitting value at a stable state is estimated at generation 244 with a value of 0.79. The estimated values of the fitting criteria using the parameters of this best individual are illustrated in Table 4. It compares the annual mean of the fitting criteria with the best results of approach A and approach B.

B. Approach B – Three Digesters

The development of the cumulative fitting value of the best individual at each generation of approach B is shown in Fig. 6. Because of the higher simulation time of approach B as approach A were only 150 generations used. The cumulative fitting value starts at 0.55. Until the first 44 generations reach the EA an average fitting value of 0.62 except two non stable peaks at generation 4 (0.73) and generation 33(0.70). After generation 45 starts the EA convergence on an average fitting level of 0.73. The EA reach a maximum fitting level of 0.74 at generation 145. In different to approach A is the highest fitting value a stable solution.

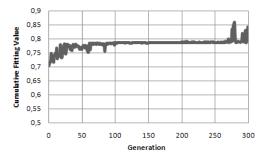


Figure 3. Cumulative Fitting Value of Approach A

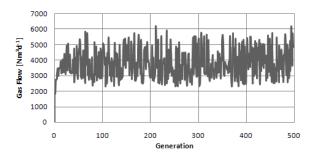


Figure 4. Gas flow at a static simulation

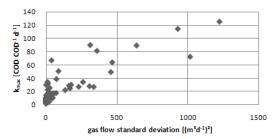


Figure 5. Gas flow standard deviation vs. k_{m,ac} value

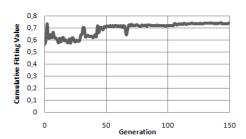


Figure 6. Cumulative Fitting Value of Approach B

TABLE IV.
FITTING OF THE APPROACHES

Criteria	Annual Mean		Approach A	Approach B
gas flow digester one	1594			1293
gas flow digester two	1056	5342	3817	971
gas flow digester three	2692			2671
methane content	69.8		64.8	65.4
pН	7.11		7.23	7.20
COD outlet digester two	14.4		11.8	6.24

The estimated values of the fitting criteria using the parameters of this best individual are illustrated in Table 4.

C. General Conclusions

The simulated values of both approaches don't achieve the targeted aims of the criteria. Both approaches reach an equal value at the methane content and the pH-value. But the approaches show a different behavior in the gas flow and the COD outlet. Approach A is more focusing on the COD outlet and approach B on the gas flow. This is caused in the effect that the ADM1-parameters have opposed influences on both criteria. In Fig. 7 is the development of the gas flow and the COD outlet at Approach A during the EA displayed. It becomes apparent that at the beginning the gas flow starts at a high level and the COD outlet on a low level. To achieve a higher COD outlet is it necessary that less COD is transformed during the digestion process into biogas. The EA tries to achieve sufficient fitting overall criteria. Hence the gas flow starts to fall and the COD outlet increases. With an improved balanced between the criteria the cumulative fitting value in Fig. 2 begin to rise.

The in the former section described method CP is responsible for a well-balanced fitting of the ADM1 overall criteria's. The method allows that the cumulative fitting increases when one hand some individual fitting values decrease and at the same time on the other hand another individual fitting value stronger increases. Hence that approach B contains three gas flow criteria in opposite to approach A with only one, is the center of the fitting quality more on the gas flow.

VI. OUTLOOK

In the further development of the research project are the following extensions on the EA planed.

First of all is a different approach for the creation of the initial population. Instead of an ancestor is a random based initialization of the phenotype parameter intend. Second of all is an upgrade of the mutation method. The new mutation method would be the Covariance Matrix Adaptation. Third of all is a reduction of the phenotype parameters space based on an extended partial correlation analysis between the phenotype parameters.

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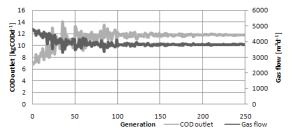


Figure 7. Gas flow vs. COD outlet at approach A