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Anaerobic co-digestion in plant-wide wastewater treatment models

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This report is part of the examination of the project work in the PhD course – Introduction to Anaerobic digestion model no 1, given at Lund University 2013.

Abstract

Co-digestion of sludge with external substrates at wastewater treatment plants is a common means to use residual wastes, utilise available capacity in the digester and boost biogas production. The Benchmark Simulation Model No. 2 (BSM2) is a platform for comparing plant-wide control strategies and includes among other things a model of the activated sludge process and the digester at a treatment plant. This report reviews the state of knowledge on possibilities and challenges to include co-digestion in the BSM2 model. The report also includes a survey of the hydrolysis coefficient for commonly used substrates at treatment plants in Sweden by using non-linear parameter estimation fitting models to Biomethane Potential (BMP) test data.

Since the ADM1-model is COD based the substrates have to be divided into state variables in terms of COD. All the methods available in literature involve some sort of COD analysis on the substrate, and the way to proceed would be different depending on the solids concentration of the substrate. It is recommended that each substrate is characterised individually and that the hydrolysis step is kept virtually separate for each of the substrates in the BSM2 model.

The study has found that the present hydrolysis coefficient in BSM2 (10 d^{-1}) needs to be updated and a more reasonable value is around 0.2 d^{-1} for mixed sludge. The coefficient for food waste is similar to that of mixed sludge.

Contents

Introduction

The objective for wastewater treatment plants (WWTPs) has traditionally been effluent water quality under the constraints of technical feasibility and cost. During recent years the scope has widened in a number of ways; the greenhouse gas emissions should be mitigated, the energy efficiency increased and resources recovered out of the wastewater. All of this puts focus on energy recovery with anaerobic digestion at WWTPs.

The international research community has developed several benchmark models describing wastewater treatment processes with the purpose to compare the performance of different control strategies in a unified framework. The Benchmark Simulation Model No. 2 (BSM2), described below, is a plant-wide model including digestion of sludge with the Anaerobic Digestion Model no. 1 (ADM1). In the light of the increased focus on digestion, it is important that this process is well described and allows common applications. One application that nowadays is common at WWTPs is anaerobic co-digestion (AcoD) of different organic wastes together with sewage sludge. This allows the WWTPs to use residual capacity in the digester to increase their biogas production and thereby increase the energy production in terms of power, heat or vehicle fuel. The current implementation of digestion in BSM2 has inadequacies and does not allow for addition of external substrates, i.e. AcoD.

The scope of this work is to investigate modelling of AcoD in a plant-wide context at WWTPs. The project aims to answer the following questions:

- what are the weak points of the digestion model in BSM2 and what alternatives are there to address those?
- what models are available for AcoD and which is preferable to use with BSM2?
- which methods are available for characterising substrates for modelling with ADM1 and which is most applicable for available data?
- which data is available to model different kinds of substrates?

Background

Description of BSM2

BSM2 is a model-based platform for developing, evaluating and analysing plant-wide control strategies for wastewater treatment plants (WWTPs). BSM2 is today the most accepted and widespread tool within the academic community for this purpose. It is developed within an IWA (International Water Association) task group on Benchmarking of Control Strategies for WWTPs, established in 2005 (see www.benchmarkwwtp.org), (Jeppsson *et al.*, 2007; Nopens *et al.*, 2010).

The BSM2 platform consists of six parts.

1. A standardised layout for the WWTP in question, see Figure 1. The activated sludge unit is a modified Ludzack-Ettinger configuration consisting of 5 tanks in series. Tanks 1 and 2 are anoxic, while tanks 3, 4 and 5 are aerobic. Tank 5 and tank 1 are linked by means of an internal recycle. The BSM2 plant further contains a primary and a secondary clarifier, a sludge thickener, an anaerobic digester (AD), a storage tank and a dewatering unit.
2. A complete setup of process models tracking organic matter (i.e. Chemical Oxygen Demand, COD) and nitrogen components through the different units of the plant. The activated sludge process is modelled with the Activated Sludge Model no. 1 (ASM1) model by Henze *et al.* (2000)

describing COD removal, nitrification, and denitrification by heterotrophic and autotrophic bacteria. The secondary clarifier is a one dimensional, 10-layer model proposed by Takács *et al.* (1991). The AD is modelled by the ADM1 model (Batstone *et al.*, 2002). The models for the remaining support processes of the plant can be found in Nopens *et al.* (2010).

3. A standardised dynamic influent for the full 609 days of simulation. The influent captures the characteristics of a real municipal wastewater with diurnal and weekly variations, rain and storm events and seasonal effects like temperature variation and holiday periods.
4. A set of actuators for control and sensors for monitoring the process. All actuators except the aeration system are considered ideal. A number of sensor classes have been defined from which a benchmark user selects the ones most appropriate. Noise level, time response, delay time, signal saturation levels and sampling time are sensor characteristics defined by the various classes.
5. A standardised simulation procedure. The plant is simulated for 609 days out of which the last 364 days are used for evaluation.
6. A set of evaluation measures of which the Effluent Quality Index and the Operational Cost Index are the two most important ones.

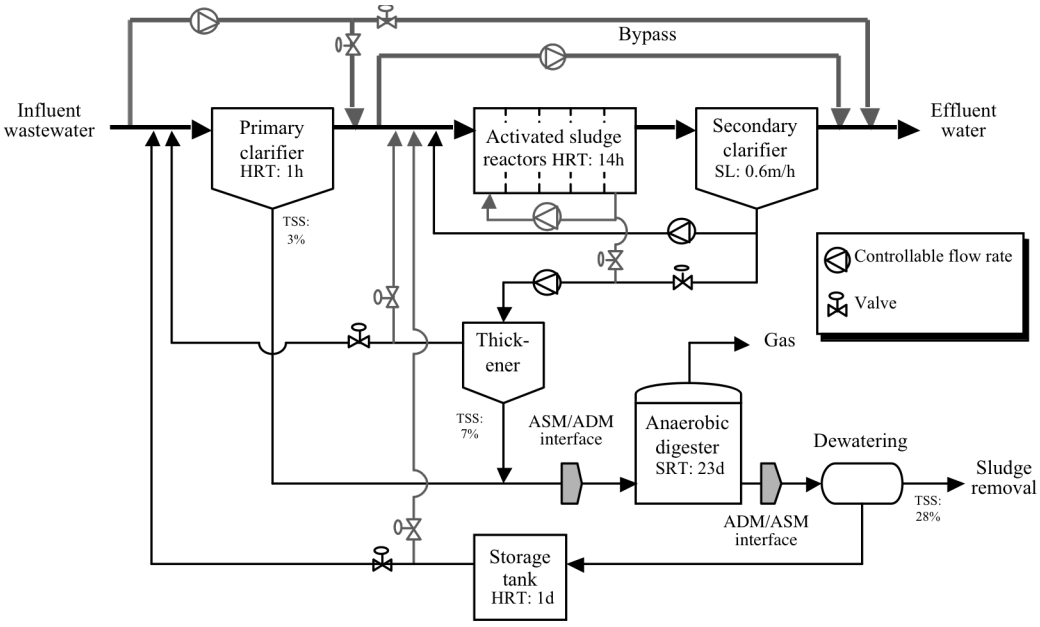

Figure 1 Principle plant layout for the WWTP in BSM2.

Digestion modelling in BSM2

The digester in BSM2 is a traditional CSTR with a volume of 3 700 m^3 (3 400 m^3 liquid volume). For the default operational strategy that gives a hydraulic retention time at about 23 days. Temperature compensation of model parameters are fully implemented according to Batstone *et al.* (2002) which means that the digester model could be operated from 0-60 °C without recalculation of parameter values. As default the AD operates at mesophilic temperature of 35 °C.

In the original ADM1 particulate substrate is fed to the digester model as particulate composite material (X_c). This acts as a pool for all composite organic material including dead biomass. The first process of ADM1 is the disintegration step, describing the breakdown of X_c into carbohydrates (X_{ch}), proteins (X_{pr}), lipids (X_{li}) and inerts (X_I). This step was included to model the extracellular, non-biological processes like

lysis and decomposition of complex materials. The disintegration is modelled with first order kinetics dividing X_c into X_{ch} (30 %), X_{pr} (30 %), X_{li} (30 %) and X_I (10 %). The second process of ADM1 is hydrolysis of X_{ch}, X_{pr} and X_{li} into small soluble compounds, i.e. monosaccarides (S_{su}), amino acids (S_{aa}) and long chain fatty acids (LFCA, S_{fa}). This is also modelled with first order kinetics with individual rate parameters. This model formulation has a few implications; one is that all material pooled into X_c will get the same stoichiometric composition with regards to X_{ch}, X_{pr}, X_{li} and X_I, dead biomass included, another one is that placing two reactions with first order kinetics next to each other means that the slower reaction will become rate limiting.

The implementation of ADM1 in BSM2 is consistent with the original ADM1 model description to a great extent. One significant exception is the degradation of particulate substrates in the AD. As described below an interface is needed to convert the ASM1 state variables into the corresponding ADM1 ditto. In the interface, all COD in the feed are converted directly into X_{ch}, X_{pr}, X_{li} and X_I rather than X_c. This allows for adapted composition depending on substrate and separates feed from dead biomass. The disintegration step is kept for dead biomass. However, since the disintegration step is rate limiting with the default ADM1 parameters the hydrolysis rates needs to be adjusted accordingly to get a realistic degradation rate. This adjustment is not done in the standard BSM2 parameterisation, leading to a too effective digestion process which overestimates capacity and gas production in the digester.

Literature study

Methods for characterisation of substrates for modelling with ADM1

One of the most important aspects for a successful modelling project is characterisation and fractionation of the substrate feed. Characterisation means both to map the physiochemical properties of the substrates to the about 20 state variables of the ADM1 model; and to identify the substrate-related biological parameters of the model. Since the ADM1 was first published in 2002 a number of approaches have been presented on characterisation.

Physiochemical

Several schemes have been presented on how to characterise the substrate with standard physical and chemical (phys-chem) analysis methods (Souza *et al.*, 2013; Angelidaki *et al.*, 2009; Galí *et al.*, 2009; Lübken *et al.*, 2007). Common analyses include, total solids (TS), volatile solids (VS), total Kjeldahl nitrogen (TKN), total ammonia nitrogen (TAN), volatile fatty acids (VFAs), total alkalinity (ALK), pH and total and soluble chemical oxygen demand (COD). In some publications (Jimenez *et al.*, 2013; Girault *et al.*, 2012; Galí *et al.*, 2009; Lübken *et al.*, 2007) these parameters are complemented with one or more analyses for carbohydrates, proteins and lipids. To address the issue of biodegradability it is also common to do biomethane potential (BMP) tests, which also gives information on hydrolysis rates, see below.

Anaerobic respirometry

In order to assess the biological availability of the substrate, BMP tests are widely used (Souza *et al.*, 2013; Angelidaki *et al.*, 2009; Galí *et al.*, 2009). These are also used to characterise substrates for modelling with ADM1. Girault *et al.* (2012) presented a method called Anaerobic Respirometry. They perform a BMP test but plot methane production rate against time and deduce fractions with different availability for biological degradation from the curve. In combination with some phys-chem analyses they characterise both the applicable state variables and the substrate dependent model parameters. The phys-chem analyses are TS, VS, TKN, TAN, VFA and COD. They also analysed lipid content with Soxhlet extraction.

Elemental analysis
The phys-chem analyses can be complemented with information about the elemental composition of substances, e.g. for C, H, O, N and P (Kleemebezem and Van Loosdrecht, 2006). An elemental analysis also ads valuable information (Batstone, 2013).

Model interfacing
In the special case where two models are coupled as in BSM2 with the digester feed coming from the ASM1 model, the feed is characterised in detail in the form of state variables of another model. In this case only conversion / interfacing to ADM1 is needed, see section on interfacing below. For other, external, substrates a combination of phys-chem methods and interfacing has been published by Zaher *et al.* (2009). In their method they characterise the substrate with the following 11 analyses: particulate COD, soluble COD without VFA, VFA, total organic carbon, total inorganic carbon, total organic nitrogen, TAN, organic phosphorous, ortho-phosphorous, ALK and fixed solids. These results acts as input to a transformer model based on the continuity based interfacing method (CBIM) described below.

Interfacing ADM1 with ASM-type models and external substrates

Being a plant-wide model the BSM2 comprises a number of different sub models. Connecting different models raises a number of issues, where the most critical one is to connect models with different sets of state variables. That is the case between several of the models in BSM2 but the most significant differences are between ASM1 and ADM1, see Table 1 for a list of the state variables of ASM1 and ADM1. There are two different approaches to address this problem; i) the supermodel approach, putting up one large model for both (or all) subsystems with a uniform set of state variables, or ii) the interfacing approach, defining the conversion from the state variables of one model into the states of another. The latter allows the usage of established and well-known models and is used in BSM2. The interfaces ASM1 to ADM1 and back to ASM1 are described by Nopens *et al.* (2009).

In literature, two different principles for setting up a model interface are found, continuity-based interface methodology (CBIM) (Volcke *et al.*, 2006) and what we call knowledge based interfaces (Nopens *et al.*, 2009). Both preserve continuity but have a different way to define the explicit mapping of the states.

Knowledge based interfaces

In this approach available information and expert knowledge about the incoming substrate are used to characterise the substrate in terms of ADM1 state variables. The method will be explained and exemplified with the Modified Copp interface by Nopens *et al.* (2009).

The Modified Copp interface was developed for interfacing the sludges arising in the waterline of the BSM2 WWTP with the ADM1 digester model. In the waterline, basically all models are based on the state variables of ASM1. As can be seen in Table 1 there are, apart from the difference in count, a number of principal differences in how the states are defined,

- In ASM1 nitrogen is modelled as separate states, whereas in ADM1 the nitrogen is associated with the COD.
- The COD in ASM1 is categorised as particulate or non-particulate and biodegradable and non-biodegradable. In ADM1 it is separated in a number of defined compounds, like carbohydrates, lipids, proteins, etc. all having different characteristics.
- pH is not modelled in ASM1 while it is in ADM1.
- Following the different handling of pH, the charge balance has major differences between the models.

Table 1 State variables or ASM1 and ADM1 respectively.

ADM1		ASM1	
Variable	**Description**	**Variable**	**Description**
Xc	Composite	S_I	Soluble inerts
X_{ch}	Carbohydrates	S_S	Readly biodegradables
X_{pr}	Proteins	X_I	Particulate inerts
X_{li}	Lipids	X_S	Slowly biodegradables
X_I	Particulate inerts	$X_{B,H}$	Heterotrophic biomass
S_I	Soluble inerts	$X_{B,A}$	Autotrophic biomass
S_{su}	Monosacharides	X_P	Particulate by-products from biomass decay
S_{aa}	Amino acids	S_O	Oxygen
S_{fa}	Total LCFA	S_{NO}	Nitrate and nitrite nitrogen
S_{va}	Total valerate	S_{NH}	Ammonium and ammonia nitrogen
S_{bu}	Total butyrate	S_{ND}	Soluble biodegradable organic nitrogen
S_{pro}	Total propionate	X_{ND}	Particulate biodegradable organic nitrogen
S_{ac}	Total acetate	S_{ALK}	Alkalinity
S_{h2}	Hydrogen	T	Temperature
S_{ch4}	Methane		
S_{IC}	Inorganic carbon		
S_{IN}	Inorganic nitrogen		
X_{su-h2}	Biomass (7 pcs.)		
S_{cat}	Cations		
S_{an}	Anions		
pH	pH		
T	Temperature		
$P_{gas,i}$	Partial pressure of gas		
P_{gas}	Total gas pressure		

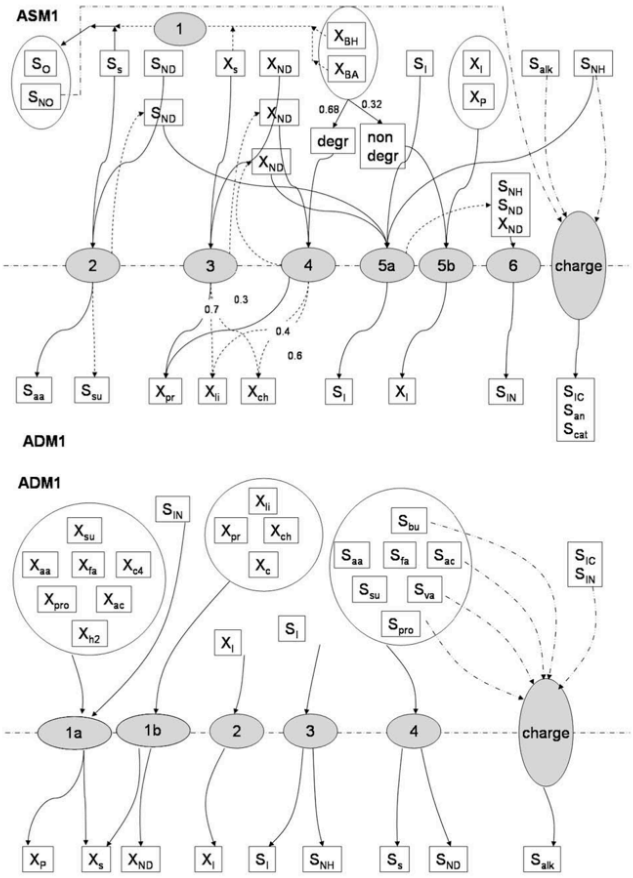

Figure 2 Approach for the interface between ASM1 and ADM1 in BSM2. The scheme shows how ASM1 states are mapped into their ADM 1 counterpart and back. Figure from Nopens *et al.* (2010).

In the case with ASM1 to ADM1, the ASM1 states provide a detailed characterisation of the digester feed. This gives a possibility to put up a rule-based method to convert them to the appropriate ADM1 counterpart. The principle scheme for the interface is shown in Figure 2.

Continuity-based interfaces

The continuity-based interfacing method (Volcke *et al.*, 2006) gives a more mechanistic approach to interfacing models with different sets of state variables. The method is based on fractioning substances in their elements, i.e. C, H, O, N, P, charge and COD and defining the conversion with composition and Petersen matrices, which are familiar to modellers.

Four steps can describe the CBIM.

1. *Formulation of elemental mass fractions and charge density.*
   Elemental mass fractions for all state variables are formulated assuming a molecular formula of C, H, O, N and P adding up to 1. Also charge density and COD content are identified for each state variable.
2. *Set-up of composition matrices.*
   The composition matrix summarises the composition of all state variables for all the models in the interface. The elemental mass fractions from step 1 are multiplied by the specific mass of the component in order to get mass units in the matrix.
3. *Definition of transformation matrices.*
   The transformation matrix comprises the transformation processes of the state variables of the origin model into the ones of the target model. The user defines separate stoichiometric conversion factors and puts them up in a Petersen matrix. The matrix is based on COD-mass, and continuity for all substances and elements must be preserved.
4. *Transformation equations.*
   In the last step the stoichiometric coefficients in the Petersen matrix are complemented with rate coefficients for each transformation. This preserves continuity in each time-step and assures conversion in the right direction, i.e. that the flux is really from the origin to the target model.

Modelling substrate addition and degradation of particulate material

The characterisation of substrates results in individual composition and degradation kinetics for each substrate. From a modelling point of view it has to be considered how to keep this separated though the disintegration and/or hydrolysis steps of ADM1. In the original model there is only one set of X_c, X_{ch}, X_{pr}, X_{li} and X_I with corresponding disintegration and hydrolysis rates. If the substrates were to be combined in the model prior to the feed the composition could be kept correct but it would be impossible to apply different degradation rates. In literature there are a few examples on how to address this using the ADM1 with modifications.

The simplest approach is to do the characterisation of substrate on the actual feed mix. Derbal *et al.* (2009) uses the standard procedure from Batstone *et al.* (2002) to get the stoichiometric composition of X_c, i.e. fractions of X_c for X_{ch}, X_{pr}, X_{li} and X_I. Then the disintegration rate parameter is calibrated using BMP tests and modelling. This is successful in terms of model prediction but leads to a very inflexible model since the substrate mix cannot be varied without repeating the characterisation process.

Esposito *et al.* (2008) models AcoD of sewage sludge and organic fraction of municipal solid waste (OFMSW). For the purpose they use the ADM1 but propose a number of modifications. For the degradation of particulate organic matter they use the standard formulation of ADM1 with disintegration and hydrolysis for all substrates and dead biomass. In order to separate the different streams they use multiple pools of composite material i.e. X_{c1} , X_{c2}, etc. see Figure 3. Moreover, they use different disintegration kinetics for the different X_cs. In the paper, a lot of focus is put on describing a more complex, surface-

based, disintegration kinetics for more complex substrates like OFMSW. The hydrolysis is then kept to be the same, and not rate limiting, as in ADM1. Galí *et al.* (2009) uses a similar approach as Esposito *et al.* (2008), but uses first order kinetics for all tested substrates, pig manure, apple, orange, pear, sunflower, glycerol and rape. The digester feed will then be mixed to one stream that consists of several X_cs and the parameter set up of stoichiometric compositions of X_c.

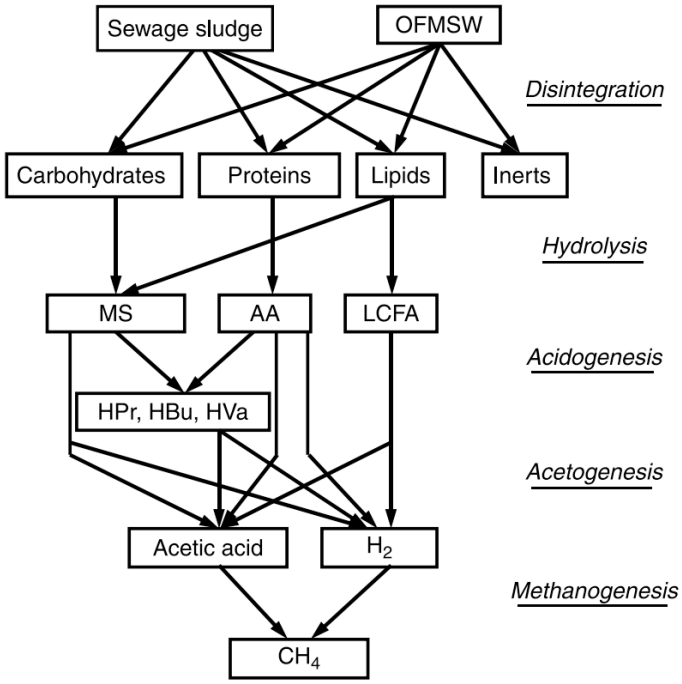

Figure 3 Schematic representation of the model of Esposito *et al.* (2008).

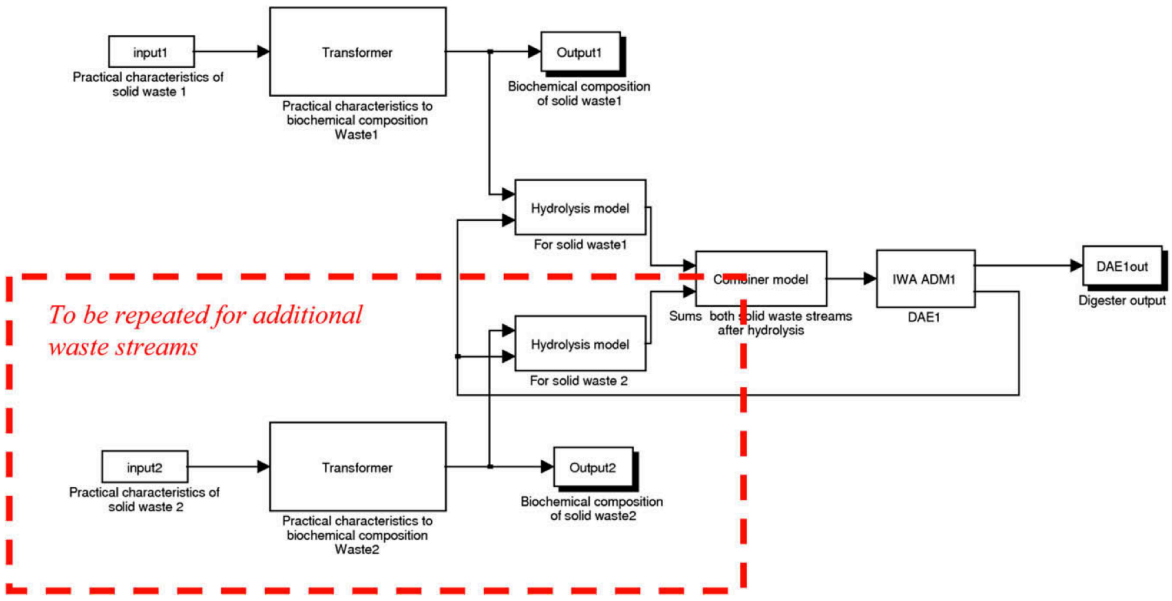

Figure 4 The model GISCOD in Matlab/Simulink. Figure from Zaher *et al.* (2009).

The most general and flexible method, known to the authors, for applying AcoD with ADM1 is presented by Zaher *et al.* (2009) in the GISCOD model. Unlike the above examples the GISCOD uses the formulation of BSM2 with feeding particulate substrate as X_{ch}, X_{pr}, X_{li} and X_I, and using X_c only for biomass decay. To keep the hydrolysis for different substrates apart the GISCOD model separates the hydrolysis model from the remaining processes of ADM1, see Figure 4. This makes the model easy to expand for arbitrary number of substrates.

Suggested implementation in BSM2

As described in the literature review, when implementing AcoD in a plant-wide fashion some issues needs to be addressed: *i)* can sewage sludge be handled the same way as without AcoD? *ii)* which method is preferred to characterise the substrate? *iii)* how to interface the additional substrates? and *iv)* how to separate the different substrates in terms of degradation (disintegration and/or hydrolysis) in the digestion model?

For the specific case of AcoD in the BSM2 platform these issues are discussed below.

Treatment of sewage sludge

The current strategy with one knowledge-based interface handling both primary and secondary sludge and making use of the detailed information about those in form of ASM1 states is very good. However, it is a fact that the AD in BSM2 is too effective due to the discarded disintegration step and still the high hydrolysis rate of 10 d^{-1}. This needs to be addressed and the most reasonable solution is to update the hydrolysis rate to the overall degradation rate determined from BMP tests.

Characterising and fractionating substrates

The reviewed methods have different approaches to characterise and fractionate substrates but some common elements exist. Since the ADM1 model is COD-based the substrate has to be fractionated into the different state variables in units of COD. Different phys-chem or biological approaches exist to find the fractions, but all make use of at least the total COD and often also the soluble COD for this purpose. This is problematic since it is well known that it is hard to make a representative and correct COD analysis of particularly solid substrates as e.g. OFMSW, fat, oil and grease (FOG) or industrial solid waste. None of the reviewed methods can fully exclude the COD analysis; and therefor the authors cannot give any conclusive recommendation on choice of method valid for all kind of substrates. However, some guidance depending on substrate can be provided:

- For liquid and fairly easily degradable substrates that are well mixed where a total and soluble COD analysis is possible the method by Zaher *et al.* (2009) is easy to apply. With a number of phys-chem analyses a completely automated method is provided where the analysis result is fed to a spreadsheet from which an automated fractionation is made based on the CBIM.
- For solid substrates where extensive phys-chem analyses are not applicable different versions of BMP tests provide a useful alternative. The method by Girault *et al.* (2012) uses degradation tests to assess the COD fractions with different degradations rates in a substrate. This saves a lot of measurements but still for example VFA and lipid content analyses are needed. Moreover, the total COD value is used to fractionate particulate and soluble parts between X_{ch}, X_{pr} and X_{li} respectively S_{su}, S_{aa} and S_{fa}. In all methods the total COD is also needed to account for the inert parts of COD, X_I and S_I.

Interfacing substrates

If the applied characterisation method provides a full description of the substrate in ADM1 state variables no interface is needed for the external substrate. Then, the ASM1 to ADM1 interface is used only for sludge feed and the additional substrate is fed separately to the AD model.

Implementation and separating hydrolysis

To keep the flexibility in the model, it is suggested that each substrate is characterised independently and that the substrates are kept separate through the hydrolysis step in ADM1. Since the current BSM2 implementation for good reasons has excluded the disintegration step for the feed, it is advised to keep this formulation when adding AcoD. Altogether, that means that the model has to be extended with individual states (X_{ch}, X_{pr} and X_{li}) and hydrolysis reactions for each substrate. This separation could be achieved similar to Derbal *et al.* (2009) or Esposito *et al.* (2008) with adding these additional reactions etc. directly into the model. However, this is rather inflexible since the user has to reprogram the model each time the number of substrates is changed. The method by Zaher *et al.* (2009), Figure 4, where the hydrolysis is separated virtually from the remaining ADM1 processes provides a more general and flexible solution to this.

Modelling study

When modelling several substrates with the GISCOD model the separate hydrolysis coefficients for each substrate are required inputs to the model. Also, as mentioned above, the present BSM2 model is not updated with a realistic degradation rate leading to an over estimation of capacity.

In order to improve the knowledge about substrates commonly used in digesters at treatment plants in Sweden, this part of the study involves non-linear parameter estimation to estimate the *first-order hydrolysis coefficient* (*k.hyd*, d^{-1}) and the *ultimate methane yield* (*Pf*, $mlCH_4/gVS$) from BMP data provided by treatment plants and universities in Sweden.

Non-linear parameter estimation

In a static model the model output (*y*) at a given time (*t*) is a function of model parameters ( ) in the following way:

$$y = f(\theta, t)$$

To estimate the model parameters of the model given access to measurement data a classical Frequentist's approach to model estimation can be used. In this approach the true values of are treated as fixed values, while the estimators ($\hat{\theta}$) are treated as belonging to a distribution.

Measurements are uncertain, which will cause the estimators to be uncertain. The error of the parameter estimation will propagate to the model output. Parameters can be estimated through minimising a cost function *S(t,)*:

$$\hat{\theta} = argmin(S(t, \theta))$$

If the model is linear in the parameters, linear least squares can be used. Linear least squares can be solved by performing a fixed number of operations and no initial values are needed. If the model is non-linear in the parameters, non-linear parameter estimation should be used. In non-linear parameter estimation the solution is found in an iterative manner, and an initial guess is required. To obtain the solution to the non-linear optimisation problem, a minimisation algorithm is needed, such as the interior-point or the simplex methods, and the problem is solved numerically.

The quality of the estimate can be calculated from the covariance matrix of the estimators, given by:

$$COV(\hat{\theta}) = s^2(J' * J)^{-1} \quad \text{where} \quad J = \frac{\partial y}{\partial \theta}$$

where s^2 is the unbiased estimate of the standard deviation (^{2}) of the estimators and *J* is the Jacobian of the model outputs with respect to the model parameters. From the theory of linear regression, the expres-

sion for the approximate confidence interval of the estimation of the parameters when the number of measurements is large becomes:

$$\theta_{1-\alpha} = \hat{\theta} \pm t_{n-p}^{\alpha/2} \sqrt{diag(COV(\hat{\theta}))}$$

where $t_{n-p}^{\alpha/2}$ is the percentile of the Student's t-distribution, *n* is the number of measurements and *p* is the number of parameters. If the number of measurements is small – as in some of the data sets in this study – the estimate of the standard deviation of the estimators will be less good. The covariance matrix of the model predications, *COV*(*y*), can be calculated from the covariance matrix of the estimators, assuming linear error propagation:

$$COV(y) = J * COV(\hat{\theta}) * J^T$$

The confidence interval of the model output is given by:

$$y_{1-\alpha} = y \pm t_{n-p}^{\alpha/2} \sqrt{diag(COV(y))}$$

For more reading on the theory behind non-linear regression see e.g. Seber and Wild (1989).

Cost functions

There are different alternatives of cost functions in linear and non-linear parameter estimation. The cost function will be a measure of the discrepancy between the model output and the measurement data. The most commonly used cost function in parameter estimation is the *sum of squared error* (SSE). Another alternative is to minimise the *sum of absolute errors* (SAE), see Table 2.

The *least squares* estimate is equivalent to using SSE as a cost function. Using the least squares approach in the cost function will be equivalent to the Maximum Likelihood Estimate if the errors are normally distributed. Using SAE as the cost function is referred to as *least absolute deviation*. This method will be equivalent to the Maximum Likelihood Estimate if the errors belong to a Laplace distribution.

The benefit from using least absolute deviation is that the results are more robust towards outliers in the data. But compared to using least squares, least absolute deviation can result in several minima and the solution can be unstable.

Table 2. Cost functions used for non-linear parameter estimation. *n* is the number of data points, *y* is the model output and *yd* is the measurement data.

Name	Abbreviation	Equation
Sum of squared error	SSE	$\sum_n (y - yd)^2$
Sum of absolute error	SAE	$\sum_n \lvert y - yd \rvert$

Method

Measurement data

To obtain an estimate of the values of *khyd* and *Pf* for different substrates, 26 datasets were collected from universities and wastewater treatment plants in Sweden. The datasets are described in Table 3. Mixed sludge is a combination of primary and secondary sludge. Data was provided from Lund University, the course exercise on parameter estimation, Uppsala Vatten, Stockholm Vatten, Käppalaförbundet, Växjö kommun, Tekniska Verken and Linnéuniversitetet. The average result of triplicates was used.

Models for parameter estimation

The models used to estimate *khyd* and *Pf* are presented in Table 4.

Method for non-linear parameter estimation

The modelling in the project has been made in MATLAB® (version R2012b, MathWorks). BMP test data was read into MATLAB and the data was used to fit Models 1 and 2 to the data. The fitting was based on non-linear optimisation, where the objective function was a function of the residuals between model output and measurement data. Least squares and least absolute deviation were used (Table 2). The uncertainty analysis was made based on source code provided by Technical University of Denmark (DTU) (Sin, Gernaey, & Lantz, 2009). An example of the shape of Model 1 and Model 2 for *Pf* = 400 $mlCH_4/gVS$ and *khyd*= 0.35 d^{-1} is found in Figure 5.

Table 3. Datasets with BMP data used in the modelling study.

No.	Name	Description	Data points	Days
1	Inoculum 1	Inoculum	470	20
2	Biosludge 1	Secondary sludge	9	41
3	Biosludge 2	Secondary sludge	9	28
4	Biosludge 3	Secondary sludge, with enzyme addition	9	28
5	Mixed sludge 1	Mixed sludge	9	28
6	Mixed sludge 2	Mixed sludge, with enzyme addition	9	28
7	Mixed sludge 3	Mixed sludge	10	35
8	Mixed sludge 4	Mixed sludge	9	40
9	Mixed sludge 5	Mixed sludge	14	26
10	Mixed sludge 6	Mixed sludge	16599	35
11	Mixed sludge 8	Mixed sludge	67	66
12	Mixed sludge 9	Mixed sludge and KemiCond® sludge	35	34
13	Mixed sludge 10	Mixed sludge and KemiCond® sludge	35	34
14	Mixed sludge 11	Mixed sludge and KemiCond® sludge	55	54
15	Mixed sludge 12	Mixed sludge and KemiCond® sludge	49	48
16	Mixed sludge 13	Mixed sludge	7	28
17	Mixed sludge 14	Mixed sludge and food waste	7	28
18	Mixed sludge 15	Mixed sludge and food waste	7	28
19	Mixed sludge 16	Mixed sludge	7	45
20	Mixed sludge 17	Mixed sludge	10	56
21	Food waste 1	Food waste	12	35
22	Food waste 2	Food waste (paper bag household)	11	49
23	Food waste 3	Food waste (kitchen grinder)	7	34
24	FOG 1	Fat in liquid form (from households)	11	49
25	FOG 2	Fat in solid form (from households)	11	49
26	Vegetable waste 1	Waste from vegetable market	10	35

Table 4. Models used for non-linear parameter estimation.

Name	Reference	Equation	Comment
Model 1 Monod-type model	Koch *et al.* (2009)	$V = \frac{Pf k_{hyd} t}{1 + k_{hyd} t}$	Assuming reactor is fully mixed, the volume is constant and the hydrolysis is the rate-limiting step and of first-order. In Koch *et al.* (2009), *Pf* is referred to as F_0G
Model 2 First-order model	Angelidaki *et al.* (2009) Donoso-Bravo *et al.* (2010) Jensen *et al.* (2011)	$V = Pf(1 - e^{-khyd*t})$	The model is derived from the first-order differential equation for growth: $\frac{dS}{dt} = -k_{hyd}S$. *khyd* is the inverse of the time constant of the model

V is the specific methane production ($mlCH_4/gVS$) and t is time (d).

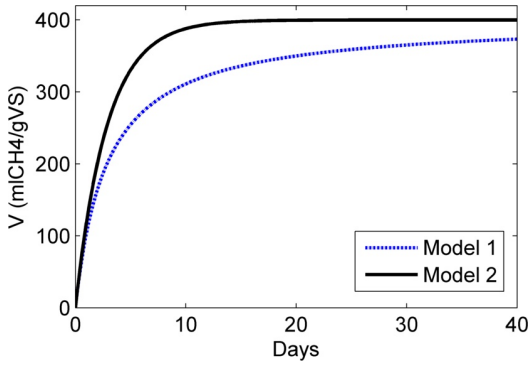

Figure 5 The dynamics of Model 1 (Monod-type model) and Model 2 (first-order model).

MATLAB has several functions for mathematical optimisation. In this study the optimization problems are non-linear. To solve these types of problems there are several solvers available. The solvers make use of different algorithms to minimise the cost function given constraints on the variables to minimise. In this study, the optimisation problem is unconstrained. *fminsearch* with the Nelder-Mead simplex direct search was used (MATLAB Documentation).

The starting guess of *khyd* is 0.2 d^{-1} and on *Pf* the maximum measured gas production.

Results and discussion

The results from estimating the parameters *khyd* and *Pf* from BMP data with Model 2 are found in Table 6 and Table 5 presents a summary of the results based on each type of substrate. An example of model output with confidence intervals with a good and with a poor fit is shown in Figure 6. The full results of the model output are found in appendix A.

Model 1 results in an estimate of *khyd* which is higher than the Model 2 estimate in all but six occasions for SSE and four occasions for SAE. The estimate of *Pf* is always higher for Model 1 compared to Model 2. SAE results in larger confidence intervals on the parameters than SSE.

Model 2 has a better fit to the parameters (measured as either SSE or SSA) for a majority of the BMP tests. When the fit is better the confidence intervals on the parameters are smaller. There are several examples where the confidence interval for *khyd* is twice as large for Model 1 than for Model 2. In seven occasions Model 1 leads to a better fit than Model 2. Tests number 11-15 are included in this group. These five tests were performed in the same lab and with a continuous measurement of the methane concentration.

The tests with a lag in gas production (test 3-6, test 24-25) are not possible to fit well to either of the models since the models do not handle time lags.

There is not a large difference between the size of the confidence intervals resulting from using SSE or SAE as a cost function in the parameter estimation. The confidence intervals are most of the time smaller for the case of SSE. The most important factor which decides the size of the confidence interval is the sample size. For large sample sizes the t-distribution percentile will be smaller than for small sample sizes. This is why the confidence intervals for the automatic BMP tests with many samples (i.e. test 1, test 10-15) are smaller than from the manual tests. Another reason for the better fit with the automatic measurements is that the samples are smoother with fewer outliers. Still, the results from the manual sampling is believed to be qualified enough to be used with a good result in ADM1.

The parameter estimation is relatively non-sensitive to the starting guess of the parameters. A change in starting guess of *khyd* of +100 % or a change in starting guess of *Pf* of ± 20 % do not impact the results.

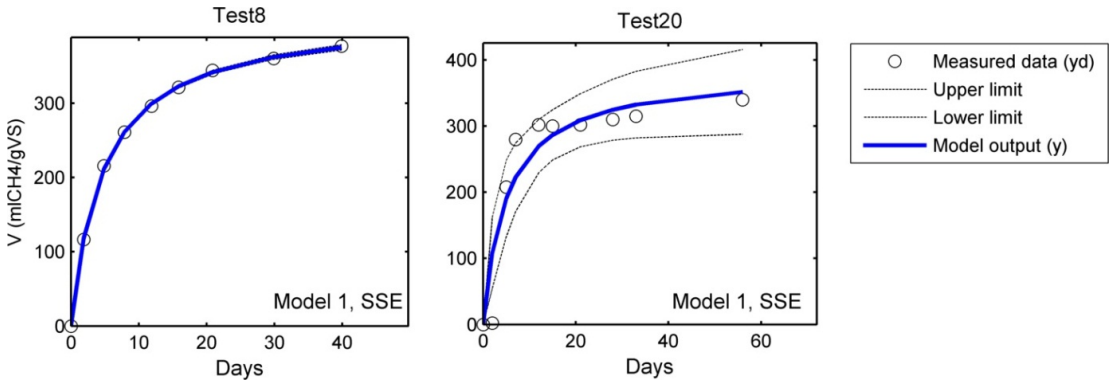

Figure 6 Example of a good model fit (left, SSE/n= 4.7) and a less good model fit (right, SSE/n= 1689). Limits showing the calculated confidence intervals

The correlation coefficient between *khyd* and *Pf* is given in Table 6. The correlation takes an average value of -0.9 for Model 1 and -0.7 for Model 2. Since the value of the coefficient is high the parameters are correlated with each other and it is therefore important to estimate both parameters together. The lower correlation between the parameters in Model 2 explains the smaller confidence intervals for this model.

Using the Frequentist's approach to uncertainty estimation is known to underestimate the uncertainty of the model predictions (Omlin & Reichert, 1999). An alternative method is to use the Bayesian approach for uncertainty estimation which is better at estimating the uncertainty in over parametrised models. For the purpose of this project the Frequentist's method was judged to be sufficient to use.

There is an assumption of uncorrelated random errors in the measurement data. If there are many measurements the errors will probably be autocorrelated which in the method used here will result in an underestimate of the confidence interval in the model output, see test 10. A possible improvement could be to re-sample the datsets where the errors are autocorrelated. Re-sampling is made through using a sample technique to reduce the number of samples from the test data, thereby reducing the number of samples and also the cross-correlation of the error signal with itself.

Table 5. Summary of parameter estimation for the different categories of substrates (Model 2, SSE).

	Khyd **(d^{-1})**			***Pf*** **($mlCH_4/gVS$)**		
	Min	**Max**	**Median**	**Min**	**Max**	**Median**
Secondary sludge	0.04	0.11	0.08	315	378	327
Mixed sludge	0.09	0.55	0.20	45	407	324
Food waste	0.15	0.18	0.17	348	598	422
Fat, oil and grease	0.06	0.10	-	676	1010	-

Table 6 Parameter estimation from Model 2, using SSE as a cost function. The 95 % confidence interval of the parameters is included.

		Model 2, cost function: SSE			
No.	**Name**	***Khyd*** **(d^{-1})**	***Pf*** **($mlCH_4/gVS$)**	**Covariance**	**SSE/n**
1	Inoculum 1	0.26 ± 0.006	66.1 ± 0.4	-0.76	6.1
2	Secondary sludge 1	0.11 ± 0.017	314.8 ± 16.6	-0.80	65
3	Secondary sludge 2	0.04 ± 0.024	378.2 ± 155	-0.98	114
4	Secondary sludge 3	0.08 ± 0.022	326.6 ± 45.1	-0.91	91
5	Mixed sludge 1	0.11 ± 0.042	330.7 ± 60.9	-0.87	314
6	Mixed sludge 2	0.14 ± 0.05	406.9 ± 65.2	-0.83	554
7	Mixed sludge 3	0.21 ± 0.036	371.6 ± 16.1	-0.64	154
8	Mixed sludge 4	0.17 ± 0.034	358.6 ± 19.3	-0.70	147
9	Mixed sludge 5	0.55 ± 0.069	321.5 ± 11.7	-0.61	130
10	Mixed sludge 6	0.42 ± 0.002	304.5 ± 0.4	-0.71	222
11	Mixed sludge 8	0.09 ± 0.005	47 ± 0.6	-0.68	2.6
12	Mixed sludge 9	0.28 ± 0.02	45.4 ± 0.6	-0.53	1.6
13	Mixed sludge 10	0.2 ± 0.014	51 ± 0.8	-0.64	2.2
14	Mixed sludge 11	0.19 ± 0.014	80.4 ± 1	-0.51	9.0
15	Mixed sludge 12	0.2 ± 0.016	71.4 ± 1	-0.52	6.5
16	Mixed sludge 13	0.35 ± 0.142	264.6 ± 19.8	-0.62	139
17	Mixed sludge 14	0.31 ± 0.064	344.5 ± 14.7	-0.65	70
18	Mixed sludge 15	0.34 ± 0.087	340.1 ± 16.5	-0.63	95
19	Mixed sludge 16	0.2 ± 0.092	357.3 ± 40.1	-0.60	508
20	Mixed sludge 17	0.18 ± 0.1	325.7 ± 46.8	-0.64	1266
21	Food waste 1	0.18 ± 0.037	597.9 ± 32.9	-0.73	644
22	Food waste 2	0.17 ± 0.026	348.4 ± 13.1	-0.60	129
23	Food waste 3	0.15 ± 0.039	422 ± 30.2	-0.70	218
24	FOG 1	0.06 ± 0.03	1009.8 ± 195	-0.88	6398
25	FOG 2	0.1 ± 0.037	676.3 ± 82.5	-0.75	2795
26	Vegetable waste 1	0.38 ± 0.099	353.8 ± 16	-0.50	215

Conclusions

This report has investigated the different aspects of AcoD in a plant-wide WWTP model. The three main issues to address are characterisation of the substrate for fractionation of COD, estimation of substrate related biological parameters (i.e. *khyd* and *Pf*) and implementation of multiple substrates in ADM1.

Characterisation and fractionation of COD

No generally applicable method for characterising the substrates exists. For substrates where representative sampling and common phys-chem analyses are possible the CBIM based method in the GISCOD model is flexible and easy to apply. For solid and inhomogenous substrates where reliable measurements cannot be expected for some analyses (e.g. COD) methods such as anaerobic respirometry based on traditional degradation tests provide a better alternative.

Estimating the hydrolysis coefficient of substrates

Non-linear parameter estimation has been used to estimate the first-order hydrolysis coefficient *khyd* and the ultimate methane yield *Pf* from BMP test data. The study can conclude that:

- The recommended method to estimate the hydrolysis coefficient from BMP tests is to use a first-order model (Model 2) and use the sum of squared error (SSE) in the optimisation algorithm;
- The Monod-type model (Model 1) proved to fit better to data from continuous measurements of methane;
- The smoother the BMP curve and the more samples in the test, the smaller the confidence interval of the estimated gas production;
- The value of *khyd* for mixed sludge from treatment plants is on average 0.2 d^{-1}.

Anaerobic co-digestion in ADM1 and BSM2

To provide maximum flexibility and favour easy implementation it is concluded that:

- Each substrate should be charactericed separately and mixed into the feed;
- The disintegration step for the feed substrate of ADM1 should be excluded and one hydrolysis expression is fitted to describe the overall degradation of particulate material;
- The hydrolysis process should be virtually separated from the remaining steps of ADM1 for easy adjustment of the number of substrates.

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Appendix A. Results from modelling study

Table A-1 Parameter estimation from Models 1 and 2, using SSE as a cost function. The 95 % confidence interval of the parameters is included.

		Model 1, cost function: SSE				Model 2, cost function: SSE			
No.	**Name**	**khyd**	**Pf**	**Covariance**	**SSE/n**	**khyd**	**Pf**	**Covariance**	**SSE/n**
1	Inoculum 1	0.29 ± 0.005	79.7 ± 0.4	-0.92	1.2	0.26 ± 0.006	66.1 ± 0.4	-0.76	6.1
2	Secondary sludge 1	0.12 ± 0.029	387.2 ± 31.5	-0.92	67	0.11 ± 0.017	314.8 ± 16.6	-0.80	65
3	Secondary sludge 2	0.02 ± 0.019	634.9 ± 353	-0.99	125	0.04 ± 0.024	378.2 ± 155	-0.98	114
4	Secondary sludge 3	0.06 ± 0.023	467.8 ± 93.8	-0.96	96	0.08 ± 0.022	326.6 ± 45.1	-0.91	91
5	Mixed sludge 1	0.09 ± 0.051	452.7 ± 125	-0.94	339	0.11 ± 0.042	330.7 ± 60.9	-0.87	314
6	Mixed sludge 2	0.12 ± 0.07	537.2 ± 139	-0.92	689	0.14 ± 0.05	406.9 ± 65.2	-0.83	554
7	Mixed sludge 3	0.27 ± 0.068	426 ± 25	-0.85	133	0.21 ± 0.036	371.6 ± 16.1	-0.64	154
8	Mixed sludge 4	0.21 ± 0.011	420.4 ± 5.9	-0.87	5.0	0.17 ± 0.034	358.6 ± 19.3	-0.70	147
9	Mixed sludge 5	0.67 ± 0.142	363.9 ± 19.7	-0.78	177	0.55 ± 0.069	321.5 ± 11.7	-0.61	130
10	Mixed sludge 6	0.51 ± 0.005	342.6 ± 1.0	-0.81	585	0.42 ± 0.002	304.5 ± 0.4	-0.71	222
11	Mixed sludge 8	0.11 ± 0.004	55.2 ± 0.4	-0.89	0.3	0.09 ± 0.005	47 ± 0.6	-0.68	2.6
12	Mixed sludge 9	0.41 ± 0.022	50.5 ± 0.5	-0.83	0.3	0.28 ± 0.02	45.4 ± 0.6	-0.53	1.6
13	Mixed sludge 10	0.26 ± 0.011	59 ± 0.5	-0.88	0.3	0.2 ± 0.014	51 ± 0.8	-0.64	2.2
14	Mixed sludge 11	0.28 ± 0.005	89.3 ± 0.3	-0.83	0.2	0.19 ± 0.014	80.4 ± 1	-0.51	9.0
15	Mixed sludge 12	0.3 ± 0.005	79.3 ± 0.2	-0.83	0.1	0.2 ± 0.016	71.4 ± 1	-0.52	6.5
16	Mixed sludge 13	0.7 ± 0.832	284.2 ± 44.8	-0.87	248	0.35 ± 0.142	264.6 ± 19.8	-0.62	139
17	Mixed sludge 14	0.51 ± 0.295	380.3 ± 36.9	-0.88	143	0.31 ± 0.064	344.5 ± 14.7	-0.65	70
18	Mixed sludge 15	0.64 ± 0.546	368.3 ± 45.1	-0.87	241	0.34 ± 0.087	340.1 ± 16.5	-0.63	95
19	Mixed sludge 16	0.25 ± 0.165	409 ± 61.6	-0.83	448	0.2 ± 0.092	357.3 ± 40.1	-0.60	508
20	Mixed sludge 17	0.2 ± 0.191	383.7 ± 94.4	-0.85	1690	0.18 ± 0.1	325.7 ± 46.8	-0.64	1266
21	Food waste 1	0.21 ± 0.108	713.8 ± 99.6	-0.90	1672	0.18 ± 0.037	597.9 ± 32.9	-0.73	644
22	Food waste 2	0.21 ± 0.087	400.9 ± 39.3	-0.83	417	0.17 ± 0.026	348.4 ± 13.1	-0.60	129
23	Food waste 3	0.17 ± 0.113	508.4 ± 95.2	-0.90	569	0.15 ± 0.039	422 ± 30.2	-0.70	218
24	FOG 1	0.05 ± 0.04	1414.3 ± 508	-0.96	8290	0.06 ± 0.03	1009.8 ± 195	-0.88	6398
25	FOG 2	0.09 ± 0.066	859.7 ± 213	-0.91	4334	0.1 ± 0.037	676.3 ± 82.5	-0.75	2795
26	Vegetable waste 1	0.59 ± 0.101	386.9 ± 10.8	-0.77	45	0.38 ± 0.099	353.8 ± 16	-0.50	215

Table A-2. Parameter estimation from Models 1 and 2, using SAE as a cost function. The 95 % confidence interval of the parameters is included.

		Model 1, cost function: SAE				Model 2, cost function: SAE			
No.	**Name**	**khyd**	**Pf**	**Covariance**	**SAE/n**	**khyd**	**Pf**	**Covariance**	**SAE/n**
1	Inoculum 1	0.27 ± 0.005	81.3 ± 0.4	-0.92	0.8	0.24 ± 0.006	66.8 ± 0.4	-0.78	2.0
2	Secondary sludge 1	0.14 ± 0.04	372.4 ± 33.3	-0.91	5.6	0.1 ± 0.017	317.6 ± 17.2	-0.81	3.9
3	Secondary sludge 2	0.02 ± 0.021	675.7 ± 476	-0.99	8.7	0.04 ± 0.027	398.4 ± 211	-0.98	8.4
4	Secondary sludge 3	0.06 ± 0.024	461.1 ± 91.5	-0.96	6.5	0.08 ± 0.022	334.4 ± 50	-0.92	6.7
5	Mixed sludge 1	0.11 ± 0.062	428.1 ± 114	-0.93	13.7	0.11 ± 0.041	337.6 ± 63.1	-0.87	13.1
6	Mixed sludge 2	0.16 ± 0.1	490.9 ± 126	-0.90	17.7	0.14 ± 0.051	408.1 ± 64.5	-0.82	16.9
7	Mixed sludge 3	0.27 ± 0.067	428.9 ± 25.4	-0.85	8.5	0.2 ± 0.035	375.5 ± 17.6	-0.66	9.8
8	Mixed sludge 4	0.2 ± 0.012	423.5 ± 6.7	-0.87	1.7	0.17 ± 0.035	354.6 ± 20.5	-0.70	9.7
9	Mixed sludge 5	0.79 ± 0.189	354.7 ± 20.8	-0.77	8.0	0.58 ± 0.083	313 ± 12.6	-0.60	9.0
10	Mixed sludge 6	0.62 ± 0.006	328 ± 1.0	-0.80	20.9	0.46 ± 0.002	300.8 ± 0.5	-0.71	11.4
11	Mixed sludge 8	0.11 ± 0.004	55.4 ± 0.4	-0.89	0.4	0.09 ± 0.005	47.1 ± 0.6	-0.69	1.3
12	Mixed sludge 9	0.46 ± 0.031	49.9 ± 0.5	-0.82	0.5	0.25 ± 0.02	45.6 ± 0.7	-0.56	0.8
13	Mixed sludge 10	0.26 ± 0.011	58.7 ± 0.5	-0.88	0.4	0.19 ± 0.014	51 ± 0.8	-0.66	1.0
14	Mixed sludge 11	0.28 ± 0.006	89 ± 0.3	-0.83	0.4	0.16 ± 0.013	80.9 ± 1.2	-0.55	2.4
15	Mixed sludge 12	0.3 ± 0.005	79.4 ± 0.2	-0.83	0.3	0.18 ± 0.015	71.5 ± 1.1	-0.55	2.0
16	Mixed sludge 13	0.66 ± 0.815	279.6 ± 48	-0.87	10.7	0.36 ± 0.157	260.2 ± 20.4	-0.61	8.2
17	Mixed sludge 14	0.54 ± 0.338	373.2 ± 37.8	-0.88	7.4	0.32 ± 0.077	338.8 ± 16	-0.64	6.1
18	Mixed sludge 15	0.75 ± 0.743	357.5 ± 45.5	-0.87	11.1	0.34 ± 0.097	335.4 ± 17.6	-0.62	6.2
19	Mixed sludge 16	0.24 ± 0.159	417.2 ± 63.7	-0.83	14.0	0.17 ± 0.081	371.3 ± 45.8	-0.63	16.1
20	Mixed sludge 17	0.27 ± 0.289	362.1 ± 85.6	-0.83	23.0	0.22 ± 0.132	315.3 ± 45.4	-0.60	19.5
21	Food waste 1	0.21 ± 0.115	698.5 ± 101.5	-0.90	33.4	0.19 ± 0.041	584.6 ± 34.5	-0.73	19.9
22	Food waste 2	0.29 ± 0.153	385.8 ± 41.7	-0.80	15.5	0.18 ± 0.031	352.6 ± 14.5	-0.59	9.3
23	Food waste 3	0.16 ± 0.108	511.4 ± 100	-0.90	17.1	0.14 ± 0.039	424.5 ± 33.2	-0.72	10.1
24	FOG 1	0.05 ± 0.04	1401 ± 499	-0.95	74.6	0.06 ± 0.033	966.4 ± 191	-0.87	63.8
25	FOG 2	0.11 ± 0.081	812.2 ± 191	-0.90	55.0	0.12 ± 0.054	654.4 ± 81.4	-0.68	39.7
26	Vegetable waste 1	0.59 ± 0.102	388 ± 10.9	-0.77	5.0	0.35 ± 0.091	355.9 ± 16.7	-0.52	9.1

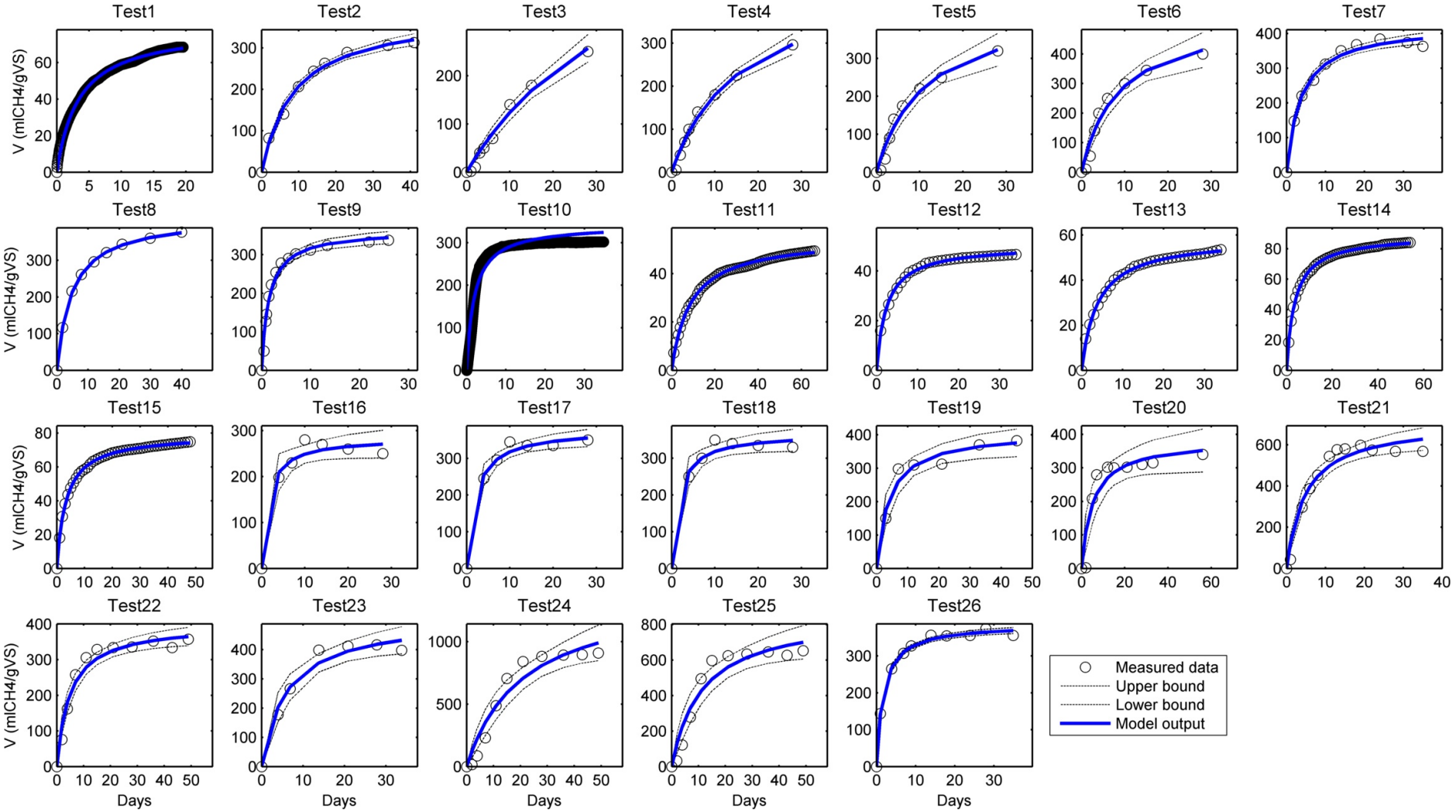

Figure A1 Results of model fitting with Model 1 and cost function SSE.

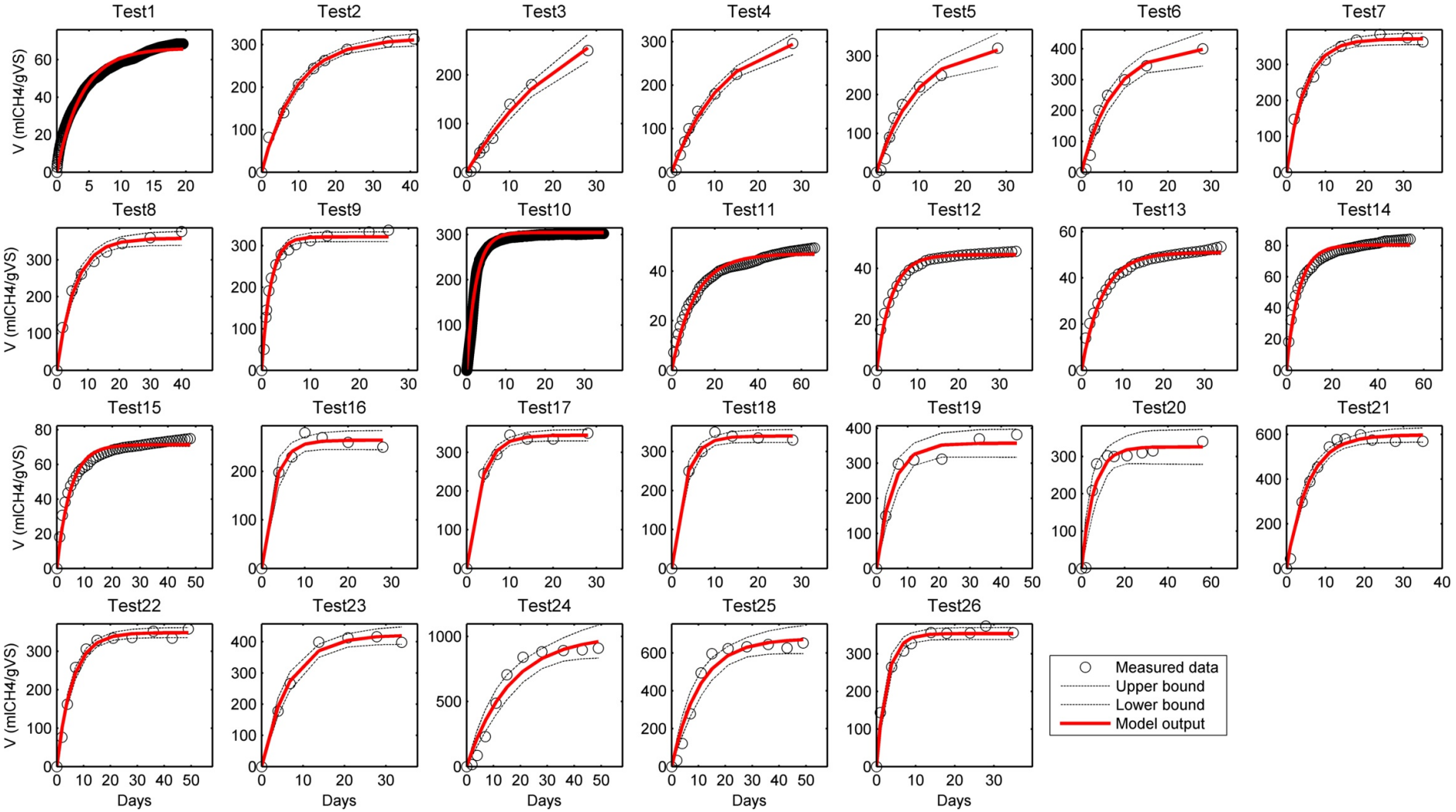

Figure A-2 Results of model fitting with Model 2 and cost function SSE.

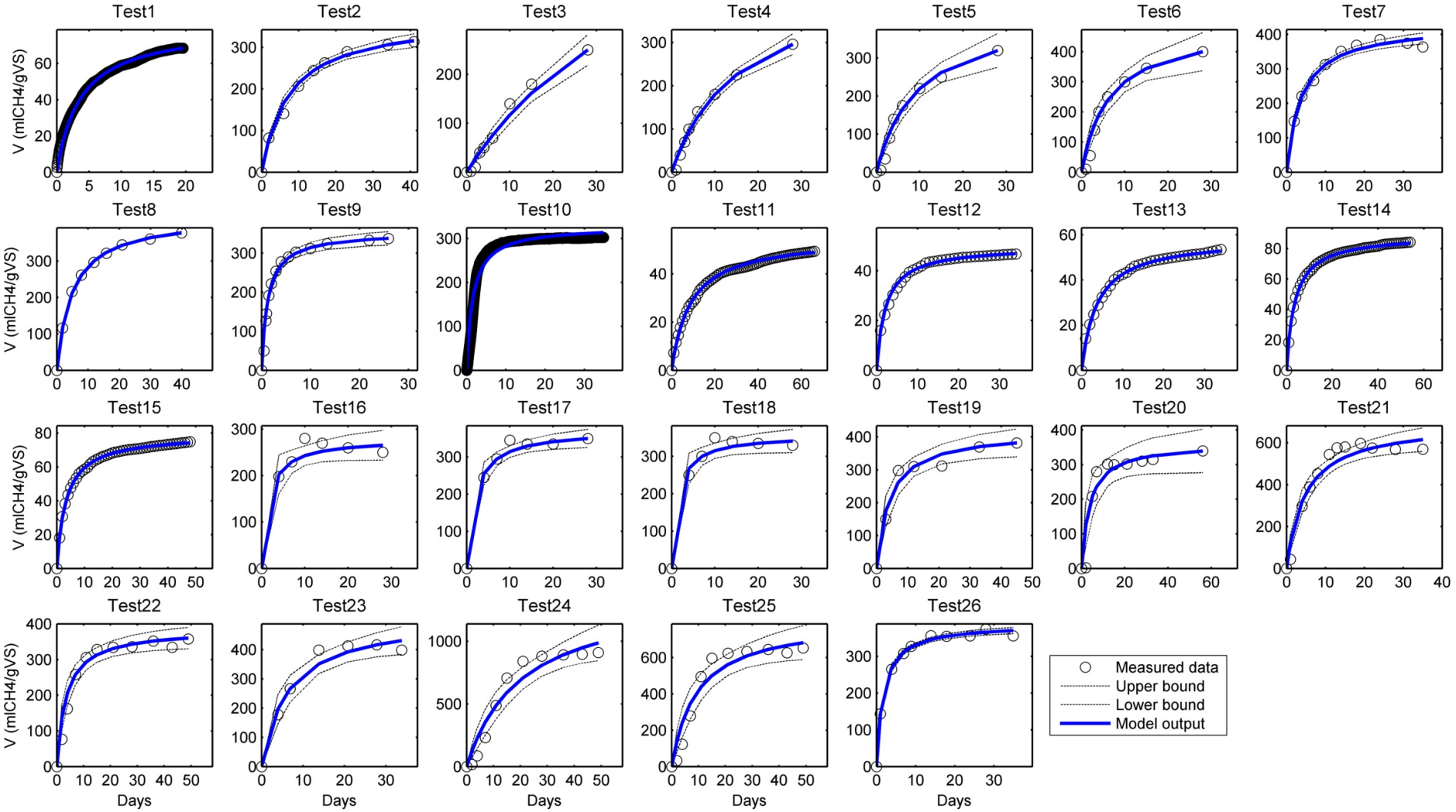

Figure A-3 Results of model fitting with Model 1 and cost function SAE.

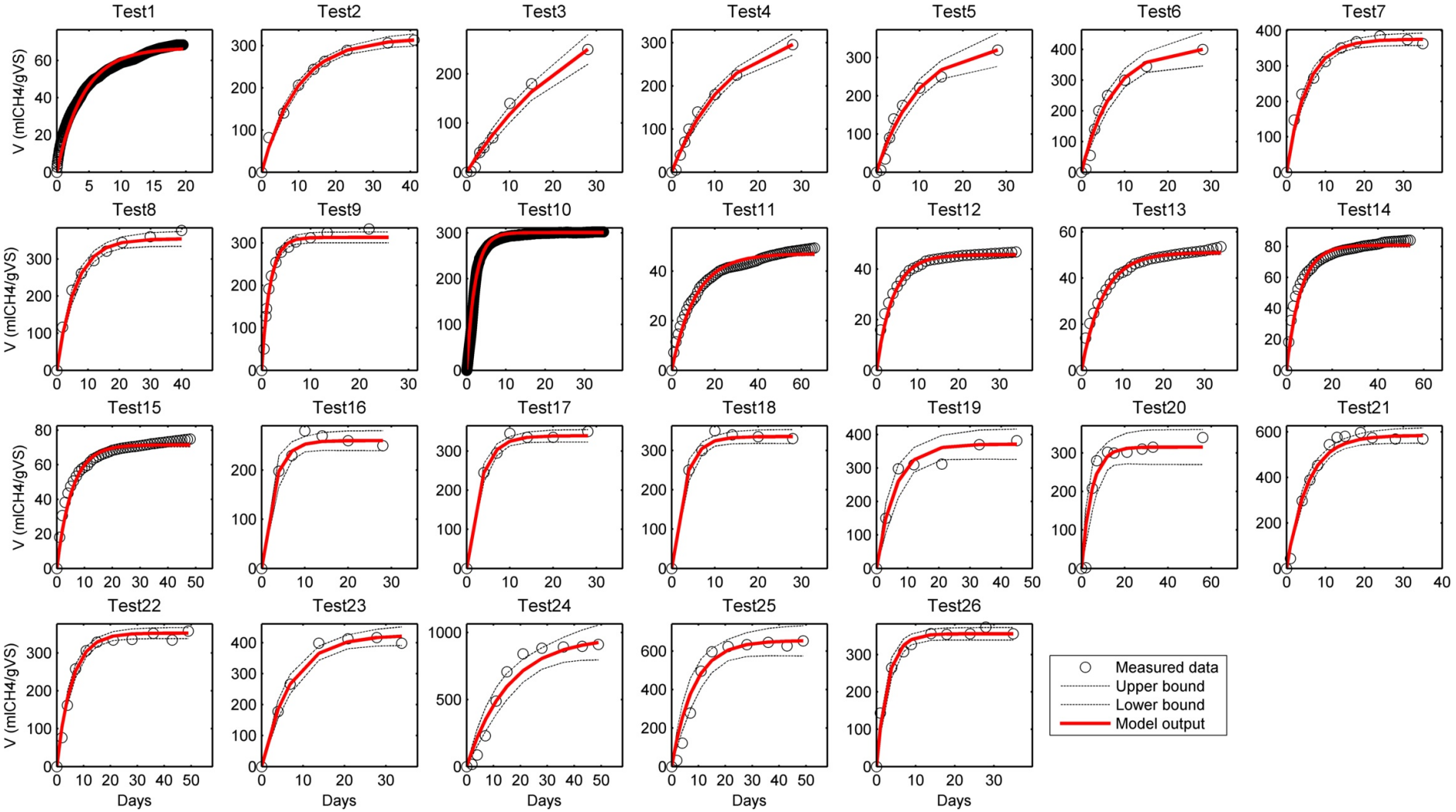

Figure A-4 Results of model fitting with Model 2 and cost function SAE.