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Lith, Pascal F. van; Betlem, Ben H.L.; Roffel, Brian

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A structured modeling approach for dynamic hybrid fuzzy-first principles models

Pascal F. van Lith*, Ben H.L. Betlem, Brian Roffel

Department of Chemical Technology, University of Twente, P.O.Box 217, 7500 AE Enschede, The Netherlands

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Abstract

Hybrid fuzzy-first principles models can be attractive if a complete physical model is difficult to derive. These hybrid models consist of a framework of dynamic mass and energy balances, supplemented with fuzzy submodels describing additional equations, such as mass transformation and transfer rates. In this paper, a structured approach for designing this type of model is presented. The modeling problem is reduced to several simpler problems, which are solved independently: hybrid model structure and subprocess determination, subprocess behavior estimation, identification and integration of the submodels to form the hybrid model. The hybrid model is interpretable and transparent. The approach is illustrated using data from a (simulated) fed-batch bioreactor.

Keywords: Process modeling; Hybrid modeling; Fuzzy logic; Identification; Optimization

1. Introduction

Dynamic process modeling in chemical engineering is often based on a combination of first principles and empirical relations. These models are interpretable, in the sense that, by analyzing the model, there is a physical understanding of the process behavior. Many process models, consisting of a framework of mass, component and energy balances describing the essential process accumulation, are available in a state-space representation. Within this framework, phenomena such as reaction rates or mass transfer can be described by static empirical relations. However, for many processes, empirical relations describing these phenomena are complex and may have limited validity.

Hybrid fuzzy-first principles models can be a useful alternative in these situations. By combining fuzzy logic submodels with a physical model framework, hybrid fuzzy-first principles models are obtained that combine a high level of interpretability with the ability to deal with complex behavior. Hybrid fuzzy-first principles models are especially suited to describe highly nonlinear behavior over a large operating domain. Examples are models of batch or fed-batch processes, cyclic processes or distributed parameter processes, such as plug flow reactors.

Combining black box techniques (e.g. neural networks) with physical equations is not new, however, until now, little research has been presented in which fuzzy logic is used in a similar context. This paper will demonstrate that, with respect to interpretability and transparency, fuzzy logic is a suitable technique that can be used in hybrid modeling. A structured procedure to construct hybrid fuzzy-first principles models from process data will be presented. This approach divides the modeling problem into smaller subproblems. The problems are solved independently and combined to form the overall hybrid model. The procedure will be discussed and illustrated using a (simulated) fed-batch bioreactor.

2. Model structure

In hybrid modeling a distinction can be made between a modular approach and a semiparametric approach. The latter approach can be further divided into a serial and a parallel approach [1].

In modular design approaches, several blocks of fuzzy logic submodels are combined to constitute the process model. The structure of the overall model is determined using prior knowledge, while every block calculates one specific variable or parameter.

In semiparametric modeling, a fuzzy logic submodel is placed in tandem with a physical model. The physical model structure is fixed and derived from first principles.

* Corresponding author. Fax: +31-53-489-3849.
E-mail address: p.f.vanlith@ct.utwente.nl (P.F. van Lith).

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Nomenclature

F(l/h)	Flow rate
IE_{val}	Integral error validation run
J	Goal function
K_x	Constant
L_σ	Lag where autocorrelation equals $2\sigma_z$
MIE	Mean integral error
P(g/l)	Product concentration
Q	Kalman filter process noise covariance matrix
R	Kalman filter error covariance matrix
$RMSE$	Root Mean Squared Error
S(g/l)	Substrate concentration
S_{f}(g/l)	Flow rate substrate concentration
X(g/l)	Biomass concentration
$Y_{p/s}$	Constant
$Y_{x/s}$	Constant
V(g/l)	Volume
e_P	Error signal in P
e_S	Error signal in S
e_X	Error signal in X
m_{xm}	Constant
$q_{\mathrm{p}}(\mathrm{h}^{-1})$	Product formation rate
$\alpha(\mathrm{h}^{-1})$	Growth rate
λ	Kalman filter stability border
μ_m	Constant
$\sigma(\mathrm{h}^{-1})$	Substrate consumption rate
$2\sigma_z$	Significance level autocorrelation

In the serial approach, fuzzy logic submodels calculate model variables which the physical part of the model requires. The input of these fuzzy submodels is provided by the physical part of the model. In the parallel approach, the outputs of the fuzzy logic block and the physical model are combined to determine the total model output. The model serves as a best estimate of the process. The fuzzy logic submodel is implemented such, that it is able to compensate for any discrepancy between the physical model output and process measurements.

If first principles models are preferred over black box models, it is proposed to leave the physical model structure intact as much as possible and only model those phenomena about which uncertainty exists (regarding model equations) with fuzzy submodels. The physical model structure is formed by dynamic mass and energy balances, while the fuzzy submodel(s) describe production rates, heat and mass transfer, equilibria, growth rates, etc. This way, hybrid fuzzy-first principles models are obtained which combine a high level of interpretability with the expectation of good extrapolating properties. Therefore, a serial semiparametric modeling approach is used. Thus in this work, hybrid models are defined as *a framework of dynamic mass and energy balances, supplemented with algebraic and fuzzy equations, formulated in state-space form.*

3. Modeling approach

Three main sources of information are generally available when constructing hybrid models. Physical understanding forms the basis of the model and is the result of fundamental research. The modeler has to acquire relevant first principles knowledge with respect to the modeling problem, that can be found in the general literature.

Process measurements are the most important source of information of a specific process. While first principles provide general information about the behavior of the process, process measurements are required to identify a suitable process model.

In addition to process measurements, human experience is an important source of information because it can be used to learn more about dependencies of relevant phenomena of the process and thus about the structure of the model. A human can, based on his or her experience, denote whether certain effects are important or negligible. Based on this information, the modeler can decide whether these effects have to be accounted for in the model. In addition, human experience can be used to design fuzzy relations which quantify the human experience. Since in modern plants most of the quantitative information is recorded, it is recommended to use this information instead of eliciting it from humans. This makes the hybrid modeling approach mostly data-driven, but it should be emphasized that using human experience to determine the model structure and dependencies is valuable and that it is worthwhile to investigate this knowledge when solving a hybrid modeling problem.

Most literature about modeling focuses mainly on the parameter identification step. Relatively little is written on how to design a specific strategy for model development. This section will present such a strategy, based on the approaches presented in [2,3]. The two different approaches are integrated and adapted for hybrid fuzzy-first principles models.

The modeling approach is shown in Fig. 1. The approach consists of several sequential steps, performed independently of each other. Other research on hybrid modeling promotes a global approach [4,5]. A global approach is usually based on training the black box relations within the hybrid model using error feedback. The advantage of this approach is that it can reduce the number of steps that have to be taken during model development. The disadvantage is that one is easily inclined to only judge overall model fit, irregardless of the complexity and number of fuzzy relations. This is detrimental to model transparency. The advantage of

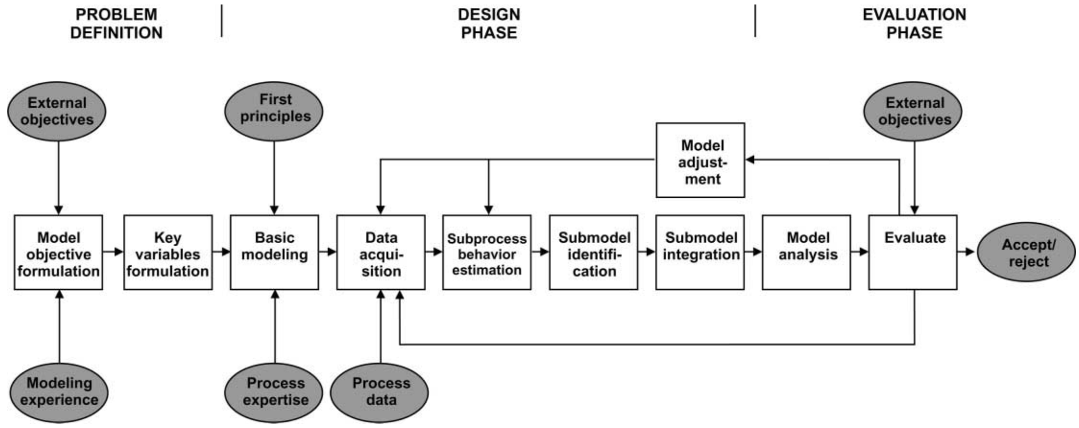

Fig. 1. Hybrid modeling approach.

independent steps is that the modeling problem is reduced to several smaller and simpler problems. The solutions of these problems are then combined to form the overall model.

The approach consists of three phases. In the first phase, the problem is defined, based on external objectives (the application of the model) and modeling experience. The result is the formulation of key variables of the process which the model needs to describe.

The design phase follows the problem definition phase. In this phase, the model is built. The design phase consists of 4 steps. In the first three steps the modeling problem is reduced to simpler problems, which are subsequently solved. The fourth step integrates the solutions of these steps.

During *basic modeling*, the model structure is designed using first principles and process expertise. In this step, a physical framework is designed that describes the key variables and the mathematical dependencies for non-linear model parameters. Additional variables are also determined. In addition, the parameters that will be described by fuzzy logic are listed. The next step is to determine the behavior of the subprocesses that are described by these parameters. If this behavior is available, the fuzzy models can be identified. If the behavior cannot be measured, estimation techniques can be used. This way, the modeling problem is reduced to several *subprocess behavior estimation* problems. The aim is to deal with these problems independently. Data for the estimation is obtained in the *data acquisition* step. The estimates are used in the *submodel identification* step to build submodels. These submodels are subsequently *integrated* to form the hybrid model, which involves connecting the submodels and optimization of the hybrid model performance.

In the evaluation phase, finally, model performance and properties are analyzed and evaluated with respect to the external objectives. If performance and properties are satisfactory, the model is accepted. Model adjustment may be necessary if this is not the case.

The remainder of this paper will focus on the design phase of the modeling approach. This will be demonstrated using a simple model of a fed-batch penicillin fermentation process, described in detail in [1]. Although actual operation and behavior of these kind of processes are more complex than suggested by this model, its simple nature is useful for illustration purposes and procedure development. The bioreactor model will be used to simulate the actual process. Noise is added to the simulation results. A hybrid model for the simulated process will be developed based on these results. The hybrid model that will be developed will, therefore, not be the solution to a specific modeling problem, but will serve as an illustration and a basis for discussion, an approach also followed by other researchers [6].

4. Basic modeling

To illustrate the modeling approach, the objective of the hybrid model for the bioreactor will be to describe the product concentration P during a fed-batch run based on a model that describes the key processes taking place. The result is that a basic representation of the interaction between substrate, biomass and product will be obtained.

The following assumptions are made. The duration of a one fed-batch operation cycle is approximately 200 h. The feed flow rate and the substrate concentration in the feed may vary between process runs within known ranges. Measurements are available for the biomass concentration X, the substrate concentration S, the product concentration P and the volume V. The sampling interval for these measurements is 1 h. Measurements of several different runs are available (see Table 1). In addition, the feed substrate concentration S_f and the flow rate F are known.

A first principles framework describing X, S, P and V can be set up. Following common practice in bioprocess modeling, the accumulation balances describing these

Table 1
Initial conditions for batch runs

Batch No.	X (g/l)	S (g/l)	P (g/l)	V (l)	F (l/h)	S_f (g/l)
ID1	5.0	0.5	0.0	20.0	0.110	525
ID2	5.0	0.5	0.0	20.0	0.132	525
ID3	5.0	0.5	0.0	20.0	0.154	525
ID4	5.0	0.5	0.0	20.0	0.176	525
ID5	5.0	0.5	0.0	20.0	0.198	525
ID6	5.0	0.5	0.0	20.0	0.220	525
ID7	7.5	0.5	0.0	20.0	0.110	525
ID8	10.0	0.5	0.0	20.0	0.110	525
ID9	12.5	0.5	0.0	20.0	0.110	525
ID10	15.0	0.5	0.0	20.0	0.110	525
ID11	17.5	0.5	0.0	20.0	0.110	525
ID12	20.0	0.5	0.0	20.0	0.110	525
ID13	22.5	0.5	0.0	20.0	0.110	525
ID14	25.0	0.5	0.0	20.0	0.110	525
ID15	27.5	0.5	0.0	20.0	0.110	525
ID16	30.0	0.5	0.0	20.0	0.110	525
VAL1	8.25	1.0	0.0	20.0	0.165	525

states will account for overall growth, consumption and production rates. Described are the net growth rate α, the product formation rate q_p and the substrate consumption rate σ, which depends on the growth rate according to a Monod equation, the product formation rate and a maintenance energy factor. Relationships for α and q_p are assumed to be unknown. Structural dependencies for these rates are assumed to be known; they both depend on S and X. Therefore, fuzzy models will be developed.

The resulting model is similar to the reference model described in [1]. Since the goal of this paper is not a detailed discussion on parameter identification in ordinary state-space models, further design steps will focus on the fuzzy submodels and their integration within the physical framework. Information about the framework is directly taken from the literature and assumed to be known. This concerns model parameters and additional empirical equations. As a result of the sequential modeling approach, common identification techniques can be applied to determine parameters within the non-fuzzy parts of the model and reference is made to well-known texts such as [7,8].

The structure of the hybrid model is as follows:

$$\frac{dX}{dt} = X\left(\alpha - \frac{F}{V}\right) \tag{1}$$

$$\frac{dS}{dt} = -\sigma X + (S_f - S)\frac{F}{V} \tag{2}$$

$$\frac{dP}{dt} = q_p X - P\left(\frac{F}{V} + K\right) \tag{3}$$

$$\frac{dV}{dt} = F \tag{4}$$

$$\sigma = \frac{\mu_m S}{Y_{x/s}(K_x X + 10)} + \frac{q_p}{Y_{p/s}} + \frac{m_{xm} X}{X + 10} \tag{5}$$

$$\alpha = f_{\text{fuzzy}}(S, X) \tag{6}$$

$$q_p = f_{\text{fuzzy}}(S, X) \tag{7}$$

where μ_m, $Y_{x/s}$, K_x, $Y_{p/s}$ and m_{xm} are constants.

5. Subprocess behavior estimation

Most fuzzy identification algorithms require input–output data. Since no measurements of α and q_p are available, some other means of obtaining information about these rates needs to be employed. These rates are nonlinear and time varying. One could use simple PI-feedback control techniques [9] or state estimation approaches such as Kalman filtering to obtain parameter estimates. An extended Kalman filter was designed and two additional state equations were introduced; one for α and one for q_p. The derivatives are set equal to zero, assuming constant rates. The filter subsequently adjusts the initial estimates of the rates in order to obtain the desired time varying behavior. The new state vector for the system was formulated as:

$$x = \begin{bmatrix} X \\ S \\ P \\ V \\ \alpha \\ q_p \end{bmatrix} \tag{8}$$

Tuning of the filter was done by setting the measurement error covariance matrix R and the process noise covariance matrix Q. Filter settings are shown in Table 2 and results are given in Table 3. Filter performance is judged by evaluating the stability criterion discussed in [10], which results in a stability border λ. This border can achieve a maximum value of 1/2 and the filter is more stable for smaller values. Furthermore, the autocorrelation in the filter innovation is analyzed. An indication for good tuning is that the filter innovation is uncorrelated. The 95% significance level for the autocorrelation in the innovation, $2\sigma_z$, was calculated in order to determine the lag at which the autocorrelation is equal to the significance level (L_σ) [11]. The smaller the lag, the smaller the autocorrelation, which indicates good tuning. Table 3 indicates stable performance and

Table 2
Kalman filter settings

Diag(Q)	[0.0001,0.0001,0.0001,0.0001,0.0045,0.009]
Diag(R)	[0.2,0.01,0.03,0.2]

Table 3
Kalman filter performance

λ	0.49
L_σ for S	1
L_σ for X	3
L_σ for P	5

limited autocorrelation, which indicates that the filter is tuned correctly.

6. Submodel identification

Since the fuzzy models are based on input-output data, Sugeno fuzzy models are more appropriate than linguistic (Mamdani) fuzzy models. Sugeno models are less complex than Mamdani models (with respect to the number of rules and data processing). They can be viewed upon as a collection of local linear models. Research efforts in the field of identification of these fuzzy models has been enormous, as is the number of algorithms. They vary from manual design, tree search methods [12] to an abundance of combinations of soft computing algorithms. It is unfeasible to present a thorough evaluation of the different techniques. However, three different approaches representing three different classes of identification algorithms were applied in order to be able to give some guidance with regard to building hybrid models. They are fuzzy clustering, genetic algorithms and neuro-fuzzy methods.

6.1. Identification techniques

The basic idea behind fuzzy clustering is to divide a set of objects into self-similar groups (clusters). Clustering methods are usually based on assumptions about the geometry of the clusters that need to be determined, which include spheres, lines, hyperplanes, ellipsoids etc. A useful overview of different techniques can be found in [13]. In this work, Gustafson-Kessel (GK) clustering [14] is applied in combination with a structure optimization procedure. A detailed description of the clustering technique is given in [15].

Genetic algorithms (GAs) are well known for their optimization capabilities. Following basic Darwinistic propagation, the method is based on a "survival of the fittest" principle, in which only the solution candidates with the best desirable properties (e.g. smallest error) from a "population" will survive. The candidates that will survive are selected by evaluating their fitness value through the fitness function (similar to the objective function in more traditional optimization algorithms).

Many applications of developing fuzzy systems with GAs have been reported [16]. Using GAs to set up a fuzzy system involves coding the problem into "chromosomes" and setting up a fitness function. Since Sugeno models are used, the consequent part of the fuzzy model can be calculated using a least squares approach, if the premise part is available [17]. Therefore, a hybrid identification approach is used: only the premise part of the fuzzy model is coded into chromosomes and optimized by the GA. In each iteration, the consequent parts of all candidates are calculated using the least squares approach, after which the fitness function is calculated. Since the local models in the consequent part of each rule are least squares optimal, no rule structure optimization is necessary. Optimization of the number of rules involves a more elaborate approach and significantly increases the search space.

The third and final algorithm comes from the field of neuro-fuzzy methods, in which a combination of fuzzy logic and artificial neural networks is used. The fuzzy inference system is implemented in the framework of these adaptive networks. Examples of approaches covering both linguistic and Sugeno models can be found in [18,19]. The algorithm used here is the well-known ANFIS approach [20], which also uses a hybrid approach; the premise part is interpreted as a neural net, while the consequent part is calculated using a least squares approach. Training is executed using standard backpropagation algorithms.

6.2. Analysis

To compare the approaches, these three methods were used to identify a fuzzy model for α as a function of S and X. The input–output data was prepared by performing data reduction in order to obtain a data set in which the data features are evenly distributed in the input domain. This was done to improve the least squares calculation that is used in the algorithms. Specific settings for the identification techniques are shown in Tables 4–6 and model performance is given in Table 7. With respect to modeling errors, all techniques give acceptable results. It is, therefore, more interesting to compare the methods with respect to their application and model structure results.

Fuzzy clustering requires less a priori structure information than the GA and ANFIS. The latter two methods need a pre-determined rule base structure and membership functions to initialize parameter identification, whereas the clustering approach determines the number of rules automatically. The results are therefore less sensitive to initialization. ANFIS uses an initial model

Table 4
Clustering settings

No. of initial clusters	5
No. of clusters after convergence	3
Cluster merging threshold	0.5
Clustering termination criterion	0.01

Table 5
Genetic algorithm settings

No. of membership functions on S	2
No. of membership functions on X	2
No. of rules	4, fully dependent
Population size	77
No. of generations	77
Criterion	Tournament
Crossover probability (1 point)	0.77
Mutation probability	0.0077

Table 6
ANFIS settings

No. of membership functions on S	2
No. of membership functions on X	2
No. of rules	4, fully dependent
No. of training epochs	1000
Initial learning rate	0.01
Learning rate decrease rate	0.9
Learning rate increase rate	1.1

Table 7
Identification results

Algorithm	RMSE
Clustering	0.0083
GA	0.0083
ANFIS	0.0071

as a starting point for further optimization. Such an initial model may be difficult to set up if no prior information is available. Furthermore, experimental results have shown what can be anticipated: the identified model is closely related to the initial model with respect to premise part parameters. This makes ANFIS sensitive to choices made before identification. With the GA, information about the structure of the model also has to be provided (in terms of the rule base and corresponding membership functions) in advance. The GA searches for a solution in a much larger search space than the back-propagation algorithm and determines starting points for the search itself, which makes it not very sensitive to initial parameter values. Not the initial values of the parameters affect the result, but the specified search space does. The restrictions that ANFIS and the GA have do not apply to fuzzy clustering, which takes the data as a starting-point and derives the model from it.

By definition, input–output fuzzy clustering gives the most flexible model structure. Each cluster is represented by a rule in the rule base. Each cluster can be described independently from the other clusters, which makes the rules *independent*. Common rule base design usually starts with partitioning the input variables with membership functions and defining rules by combining them. The same membership functions can be present in several rules, which makes the rules *dependent*. Many rule bases designed without any prior knowledge contain all possible combinations of input membership functions. Dependent rules will be orthogonal, which makes the model less flexible. The drawback of independent rules is the increase in the number of membership functions, and thus the number of model parameters. Fig. 2 illustrates the difference between independent (a) and dependent (b,c) rules. The contour plot shows the location of the rules in the input space. The dots indicate the measurements. In Fig. 2(b) and (c), the rules are designed by making all possible combinations of the two membership functions that are defined on each of the input variables. Changing the membership function on S for rule 2 will also affect rule 4. In Fig. 2(a), each rule is defined by unique membership functions.

The input–output data for the growth and production rate are not distributed over the complete input space of the system. Normal operation of the reactor causes S and X to be limited to a certain part of the input space, as shown in Fig. 2. A fuzzy model with independent rules will be able to cope with this data much better, because the rules of these models will be able to describe working areas within the part where data is present, without influencing other rules.

The advantage of fuzzy clustering is that it focuses on the data and derives a fuzzy model with independent rules. To obtain the same result with the GA or with ANFIS, prior knowledge has to be provided about the

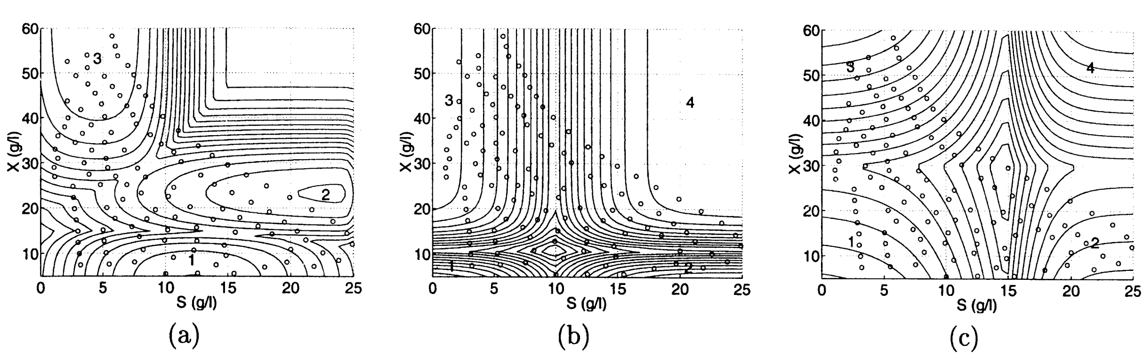

Fig. 2. Contour plots of degree of fire (DOF) of the fuzzy models for α identified with clustering (a), the GA (b) and ANFIS (c). Dots indicate input data.

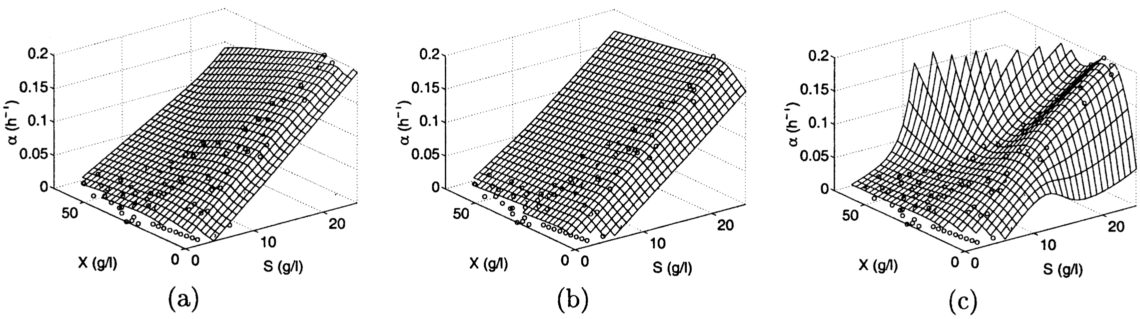

Fig. 3. Fuzzy models for α identified with clustering (a), the GA (b) and ANFIS (c). Dots indicate input–output data.

structure and initial location of the rules. This may be cumbersome for high dimensional systems. If this prior knowledge is not provided, rules may be present that have no meaning and that can complicate optimization. This is illustrated in Fig. 3. A initial model without prior knowledge about the data and a fully dependent rule base was optimized using ANFIS. Although the overall result is good for the part where data is present, rule 4 in the area with high S and X is not desirable [Fig. 3(c)] since no data is available in this area.

As with all black box techniques, care has to be taken in extrapolating the fuzzy models. Fig. 3(c) shows an example of extrapolation properties that seriously will impair hybrid model results. Post-processing of the identification results can improve this by assuming linear behavior when extrapolating, which often is the best assumption that can be made. Since TS models are a collection of local linear models, evaluating rules located at the edge of the input space and adjusting membership functions when necessary will ensure this.

In summary, one can state that the advantage of submodel identification over global identification is that one can easily pinpoint undesirable behavior in the submodel and eliminate it. This keeps the overall process model also interpretable and transparent.

7. Submodel integration

Since the general structure of the hybrid model is a framework of accumulation balances accompanied with algebraic fuzzy relations, integration of the physical and fuzzy parts is straightforward.

With respect to the fuzzy models, two sources of error may result in unacceptable hybrid model performance. First of all, estimates are made in order to obtain input–output data. Estimation errors will manifest themselves through the fuzzy model in the hybrid model. Secondly, the fuzzy models are fit to input–output data. Errors resulting from fuzzy model identification can also cause hybrid model errors. Since the hybrid models are dynamical and usually are simulated as a "free run" (numerically and in an autoregressive manner), small errors are integrated which eventually can result in large offset.

If hybrid model performance is unacceptable, it can be improved by manipulating the fuzzy parts of the hybrid model. This means optimizing fuzzy model parameters with respect to the hybrid model output. The problem can be formulated as follows.

The number of parameters that has to be optimized is quite large. One rule of the fuzzy model for α, for example, contains about 10 parameters, depending on the type of membership function that is used. Due to the "curse of dimensionality" this number increases exponentially for systems with higher dimensions. The optimization algorithm has to be able to deal with large sets of parameters.

During optimization, it is proposed to account for the *meaning* of the parameters of the fuzzy model. In TS models, the premise part parameters determine the working areas of the local linear models. These should be changed only marginal, since they provide the interpretability and transparency of the model. An optimization algorithm has to be selected that can deal with this. In addition, constraints for the premise part parameters should be introduced. These constraints can put limitations on the level of fuzziness of the sets and their location in the input domain. The constraints can be determined from the fuzzy model and heuristic knowledge.

Research in the area of optimization of fuzzy models is extensive and it is infeasible to present a complete overview. For optimization based on input-output data, techniques range from fine tuning membership functions (for example [21,22]) to gradient based techniques or neuro fuzzy approaches to evolutionary optimization (genetic algorithms, for example [23–25]). The optimization of black box relations in hybrid models mainly involves gradient based methods [1,4] and evolutionary optimization [5]. The advantage of gradient based approaches is that the initial fuzzy models are used as a starting point. This way, transparency is maintained.

The optimization algorithm described in [26,27] was found to be suitable for the problem. This approach transforms large parameter problems into a two dimensional quadratic approximation for a certain "trust region" by using a preconditioned conjugate gradient approach. This quadratic problem is subsequently solved. Box constraints are incorporated by "reflecting" the search path when it encounters a bound. The algorithm is available commercially.

For the objective function, a simple approach was found to be the most effective. Since the goal is to improve performance of the hybrid model, all relevant states should be incorporated in the objective function. They also should have equal importance. The errors were therefore normalized. The objective function is defined as:

$$J = \frac{1}{2}\|e_S + e_X + e_P\|_2^2 = \frac{1}{2}\sum_{k=1}^{M\cdot N}\left(e_{S,k} + e_{X,k} + e_{P,k}\right)^2 \tag{9}$$

in which e_S, e_X and e_P are normalized error signals, defined as:

$$e_{S,k} = \left|\frac{S_{ij} - \hat{S}_{ij}}{\bar{S}_j}\right| \text{ with } k = i\cdot j \tag{10}$$

$$e_{X,k} = \left|\frac{X_{ij} - \hat{X}_{ij}}{\bar{X}_j}\right| \text{ with } k = i\cdot j \tag{11}$$

$$e_{P,k} = \left|\frac{P_{ij} - \hat{P}_{ij}}{\bar{P}_j}\right| \text{ with } k = i\cdot j \tag{12}$$

with index i indicating the time step and index j indicating the fed-batch run. M indicates the number of samples per run and N denotes the number of runs. $\hat{S}$ indicates model estimates for S and $\bar{S}$ indicates the average value of S for a run, with similar definitions for X and P.

Fuzzy models for α and q_p were identified with fuzzy clustering. The estimates for α and q_p contain errors. Consequently, the hybrid model does not perform well. The optimization algorithm was used to optimize the internal parameters of the fuzzy models of α and q_p simultaneously for the identification batch runs shown in Table 1. Table 8 shows the number of parameters for the two models. No bounds were imposed on the consequent parameters; the bounds for the premise part parameters were the initial values $\pm 10\%$. Table 9 shows an overview of the optimization results, in which MIE denotes the mean integral error after optimization and IE_{val} denotes the integral error for validation experiment VAL1. The validation run is shown in Fig. 4.

Fig. 5 shows the fuzzy models after optimization. The adjustments to the fuzzy models have improved hybrid model performance significantly. Since bounds were imposed on the premise part parameters, most adjustments were made to the consequent part of the fuzzy models. The resulting model for q_p shows a minimum as a function of the substrate concentration, something that might be difficult to explain.

The optimization results can be explained by investigating the sensitivity of the states for changes in the parameters. The sensitivity functions [28] were numerically solved for each run and results are given in Fig. 6.

Table 8
Number of internal fuzzy model parameters

Model	No. of premise part	No. of consequent part	No. of constraints
α	24	9	24
q_p	24	9	24

Table 9
Optimization results

	Before optimization		After optimization	
State	MIE	IE_{val}	MIE	IE_{val}
S	102.31	66.05	20.82	21.47
X	803.84	525.90	85.55	106.63
P	310.08	230.26	52.76	47.97

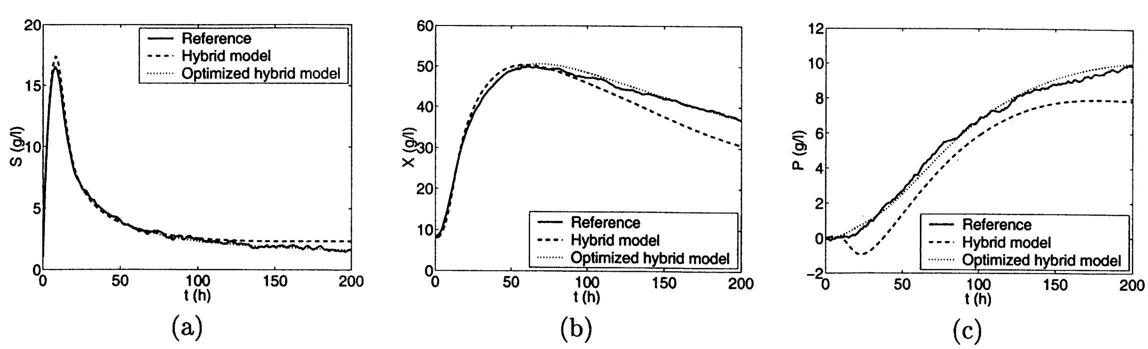

Fig. 4. Hybrid model results for S (a), X (b) and P (c).

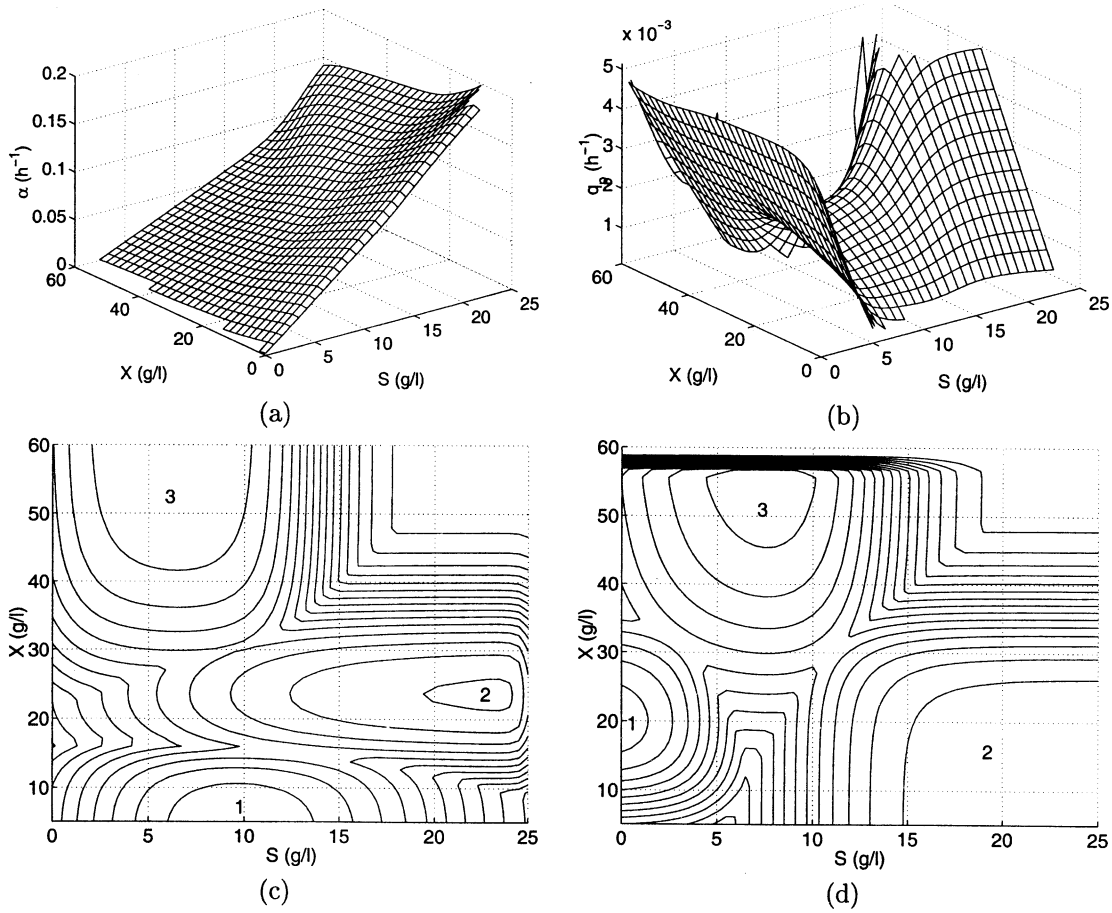

Fig. 5. Fuzzy models for α (a) and q_p (b) and corresponding rule locations (c and d).

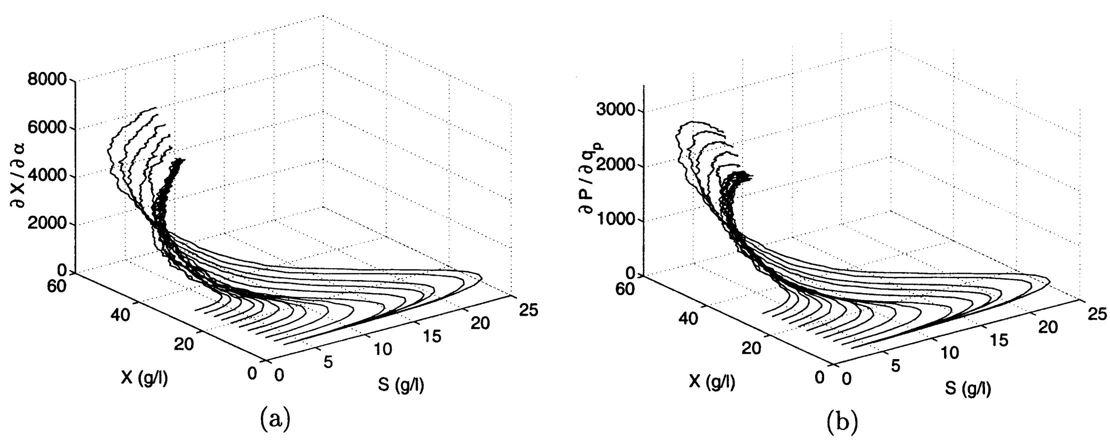

Fig. 6. Sensitivity functions for X with respect to α (a) and P with respect to q_p (b).

It can be seen P is relatively insensitive to changes in q_p for rule 2 of the fuzzy model. This is confirmed by manual adjustment of the consequent parameters of this rule and simulating the hybrid model. Due to the use of gradient information, the optimization algorithm "focuses" on areas where sensitivity is relatively large. In the case of q_p, the sensitivity is relatively large for rule 3. The main improvements of the performance of the hybrid model are achieved by the optimization of parameters of this rule. A similar explanation can be given for the fuzzy model of α.

Incorporating sensitivity functions into the objective function as proposed in [4] was also investigated. Incorporating sensitivity functions introduces the relative importance of errors in different model states with respect to one model parameter (in this case α or q_p). The optimization results were comparable with the results obtained with Eq. (9). The gradient information that the optimization algorithm uses indicates the importance of these parameters (and thus of the parameters of the fuzzy model) with respect to the states. Therefore, the contribution of incorporating the sensitivity functions explicitly is limited.

The sensitivity equations could be used to reduce the size of the optimization problem in advance by leaving out optimization of parameters with limited sensitivity. It should be noted, however, that the analysis above was done after the results were obtained and that optimization results may be negatively affected if the complete model is not included in the optimization.

Whether behavior as illustrated by the model of q_p should be accepted depends on the objectives of the modeler. The overall hybrid model performance is good. If, however, according to the modeler's judgement, the fuzzy relationship in a certain working area is unrealistic, it could be rejected. It should be noted that fuzzy logic is still a black box technique and that care should be taken in associating a physical meaning with the results.

8. Conclusions

A hybrid fuzzy-first principles model of a (simulated) fed-batch bioreactor has been designed. This model consists of a framework of dynamical mass balances, supplemented with one algebraic and two fuzzy equations. The model was developed using a sequential modeling approach. For the identification of the fuzzy models, fuzzy clustering was preferred over genetic algorithms and ANFIS. The clustering approach derived the fuzzy model without the need to make a priori assumptions about model structure or parameters.

After integration of the first-principles and fuzzy parts, hybrid model performance could be improved by optimizing the fuzzy model parameters. To accomplish this, a large parameter optimization approach was used. Optimization improved model performance significantly. A posteriori analysis of the fuzzy models showed the relative importance of the fuzzy rules, which assisted in the interpretation of the fuzzy model.

The combination of first principles with fuzzy logic results in dynamical process models that have a relatively high level of interpretability. In addition, the use of fuzzy logic provides flexibility in describing the process without making detailed assumptions about the nonlinear behavior. This makes the use of hybrid fuzzy-first principles models suitable in situations where transparency is valued, but where physical models are difficult to derive.

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