Operating Regime Based Process Modeling and Identification

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ABSTRACT. This paper presents a non-linear modeling framework that supports model development "in between" empirical and mechanistic modeling. A model is composed of a number of local models valid in different operating regimes. The local models are combined by smooth interpolation into a complete global model. It is illustrated how different kinds of empirical and mechanistic knowledge and models can be combined with process data within this framework. Furthermore, we describe a flexible computer aided modeling tool that supports modeling within this framework. Simple but illustrative examples from chemical engineering are used to highlight the flexibility and power of the framework.

KEYWORDS. Process Modeling, Non-linear Dynamic Systems, System Identification, Heuristic Search Methods, Computer Aided Modeling.

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1 INTRODUCTION

In engineering, there are two fundamentally different philosophies that form the basis of modeling, namely the mechanistic and the empirical approach. A mechanistic model is derived mainly on the basis of a detailed understanding of the generic underlying mechanisms, or laws, that govern the system behavior. An empirical model, on the other hand, is derived mainly on the basis of the specific observed behavior of the system. Often, neither of these approaches is attractive. For example, if the system mechanisms are somewhat understood, but not so well that mechanistic model development is feasible, it is often not satisfactory to construct an empirical model, since it may be difficult to incorporate much of the available process knowledge in this approach, because engineering knowledge is incompatible with most empirical model representations.

This paper is an attempt to provide a framework that can support design of models on the basis of different kinds of knowledge and data. A typical situation is illustrated by Fig. 1, where the initial state of the model development is characterized by lack of both empirical process data and mechanistic process knowledge. With the empirical approach, one will collect more data, and end up in a state with more data and perhaps some improved mechanistic knowledge. With the mechanistic approach, on the other hand, one will end up with significantly improved mechanistic knowledge and perhaps some more data. The "in between" region and path corresponding to hybrid models, based on balanced amounts of empiricism and first principles, is often handled in an ad hoc manner, or avoided. A major reason for this may be that powerful frameworks and software tools for such problems are lacking. The purpose of the present paper is to discuss a framework that we believe is useful for solving such hybrid modeling problems, and to describe a software tool.

Recently, the hybrid modeling problem has been given considerable attention. One reason for this may be the interest and achievements in knowledge representation, non-linear empirical modeling and neural networks over the last decade, combined with the need for inexpensive, globally valid non-linear models of complex systems to be applied in intelligent controllers, diagnosis systems, and optimization based systems for design, scheduling, and supervisory control.

The interaction between the empirical and mechanistic approaches is widely discussed in the engineering and scientific literature. Through a series of work, e.g. (Box & Youle 1955, Box & Hunter 1965, Box & Draper 1987), the interplay between model purpose, experimentation, empirical models, and mechanistic models has been discussed in great detail. A more direct approach to hybrid modeling is the grey-box approach of Bohlin (1989), see also (Bohlin & Graebe 1994). Grey-box models are characterized by a structure that is mainly mechanistic, but augmented with stochastic elements, empirical relations and parameters that may not have a direct physical interpretation. In another approach, Lindskog & Ljung (1994) illustrates how simple mechanistic knowledge can be used to find adequate non-linearities in an input/output model. Thompson & Kramer (1994) proposed an approach where an a priori given mechanistic model is used as a starting point, and an empirical model based on a radial-basis function series expansion compensates for the mismatch between the prediction of the more or less inaccurate mechanistic model and the process data. Constraints on model behavior are taken into account, see also (Tulleken 1993). Another avenue to the hybrid modeling problem is described in (Psichogios & Ungar 1992) and (Aoyama & Venkatasubramanian 1993). A mechanistic model structure containing some unknown internal variables is supposed to be given. The unknown internal variables will typically be reaction rates or thermodynamic properties that depend in a complex manner on a number of other model variables. The idea is to use a neural network as an empirical model of these dependencies. Yet another possibility is fuzzy linguistic modeling, where empirical and qualitative knowledge is used to develop rules that describe the system behavior or mechanisms, e.g. (Zadeh 1973). Process data can also be used to identify the parameters and structure of such models (Takagi & Sugeno 1985, Sugeno & Kang 1988). The operating regime based modeling framework discussed in this paper is closely related to the model of Takagi & Sugeno (1985). The idea is as follows: a number of local models valid within different operating regimes are combined using an interpolation technique. The operating regimes can be constructed from modeling assumptions, process understanding, experimental conditions, or a search on the basis of process data. In (Takagi & Sugeno 1985, Johansen & Foss 1993*a*) the local models are empirical models, while in (Zhang, Visala, Halme & Linko 1994, Konstantinov & Yoshida 1989, Johansen & Foss 1993*b*) local semi-mechanistic models are used. As opposed to previous work on operating regime based models, the focus of the present work will be on the ability of the framework to include various forms of mechanistic and empirical knowledge, and in particular local mechanistic models. Moreover, a software tool for computer aided modeling in this framework is described. Related work includes (Banerjee, Arkun, Pearson & Ogunnaike 1995, Skeppstedt, Ljung & Millnert 1992).

Although the framework supports models that are either dynamic or static, continuous-time or discrete-time, distributed or lumped, or a mixture, we will describe the framework in the context of lumped continuous-time state-space models in the form

$$\dot{x} = f(x, u, \theta) \tag{1}$$

where f is a function of appropriate dimensions. The model variables are classified as follows: u is independent variables (inputs), x is dependent variables described by differential equations (states), θ is a time-invariant parameter vector.

The remainder of this paper is organized as follows: the operating regime based modeling framework is described in section 2, and aspects of computer aided modeling, including model structure identification, are discussed in section 3. Two simulation examples are included in section 4, and the paper ends with a discussion and some concluding remarks.

2 OPERATING REGIME BASED MODELING

Any model will have a limited range of validity. This may be given by the modeling assumptions for a mechanistic model, or by the experimental conditions under which the data or experience was collected for an empirical model. To emphasize this, a model that has a range of validity less than the desired range of validity will be called a *local model*, as opposed to a *global model* that will be valid in the full range of operation. In the present framework which is based on combining a number of local models, it is of particular importance to describe the region in which each local model is relevant, and we call such a region for an *operating regime*. The motivation behind this modeling approach is that global modeling is complicated because one will need to describe the interactions between a large number of phenomena that are relevant globally. Local modeling, on the other hand, is considerably simpler because locally there is a smaller number of phenomena to describe, and their interactions are simpler. Combining different local models using interpolation is usually straightforward, as we shall see, and the resulting model representation is transparent in the sense that it can be easily interpreted, and can easily absorb various kinds of process knowledge.

2.1 Model Representation

Assume that N local models corresponding to different operating regimes (indexed by i), are given in the following form

$$\dot{x} = f_i(x, u, \theta) \tag{2}$$

together with the conditions the models are assumed to be valid or relevant for. These conditions are characterized using variables $z = (z_1, ..., z_d)^T$ that are determined by the other variables in the model, i.e. $z = H(x, u)$. The choice of characteristic variables is highly problem dependent, and will be discussed in more detail in the next section, and in conjunction with the examples. Let Z be a set of operating points z that represents the full range of operation which the global model is required to cover. An operating regime Z_i can be viewed as a subset of Z, cf. Fig. 2a. Notice that the operating regimes will overlap and should be interpreted as sets with soft boundaries. A global model is now defined by the interpolation method

$$\dot{x} = \sum_{i=1}^{N} f_i(x, u, \theta) w_i(z) \tag{3}$$

where we have defined

$$w_i(z) = \frac{\rho_i(z)}{\sum_{j=1}^{N} \rho_j(z)}$$

and the smooth non-negative function $\rho_i(z)$ that characterizes the operating regime Z_i is called a local model validity function. We assume that for any $z \in Z$, $\sum_{j=1}^{N} \rho_j(z) > 0$. Hence, $w_i(z)$ is a normalized function as shown in Fig 2b, with the property $\sum_{i=1}^{N} w_i(z) = 1$ for all $z \in Z$. The local models are essentially interpolated in (3), and the relative weight w_i of each local model will be determined by the local model validity functions

$\rho_1, ..., \rho_N$. In particular, a local model that is not relevant at a given operating point, will have zero weight at that point in the interpolation. To avoid ill-posed computations (such as taking the square root of a negative number), the function f_i should not be evaluated when this model has zero weight. The local model validity functions are typically chosen as Gaussians or splines. It is our experience that the exact shapes and softness of these functions are of minor importance, as long as their locations and sizes are reasonably chosen.

Note that in principle there are no requirements to the internal structure of the local models, the only important issue is that it gives a satisfactory approximation for the operating conditions where it contributes to the global model. This implies that mechanistic and empirical local models may be mixed to form a global model. In (3) we have chosen to use the same superset of variables in all local models. Of course, each local model will only use the relevant subset of the variables. The motivation is the simplified notation, and the fact that dealing with all the variables simultaneously is required in the interpolation (3) anyway.

2.2 Operating Regimes

The design of operating regimes with corresponding local models is the key task with the proposed modeling framework. The operating regime Z_i is uniquely defined by its local model validity function $\rho_i(z)$. If the vector z has low dimension ($d \leq 2$), it is often possible to design suitable validity functions directly. In higher dimensions, design and visualization is more difficult, and it is useful to design a multi-variable local model validity function using mono-variable functions such as

$$\rho_i(z) = \prod_{j=1}^{d} \rho_{i,j}(z_j) \tag{4}$$

Often, there will be a large number of variables that are candidates for being used to characterize operating regimes, but experience shows that a small number is usually sufficient to achieve an acceptable model accuracy. When the process is highly complex and a large number of characteristic variables and operating regimes are needed, it is very helpful to use hierarchies as a multiresolution representation of the operating regimes. This improves the transparency of the model and simplifies visualization, design and analysis.

For example, consider a set of linearized differential equations describing the mass- and energy balances of a chemical reactor. Such a model would clearly be a local model, since it is well known that chemical reactors usually exhibit strongly non-linear behavior. Different regimes may be characterized by variables like temperature and flow-rate, since the behavior of the reactor in relation to the linearized dynamic model will be different at high and low temperature, because the reaction rate is usually highly temperature dependent. Likewise, the flow-rate will influence the holdup-time, mixing, and flow patterns, and thereby the dynamic behavior. In addition, there may be different operating regimes because a different set of chemical reactions may dominate under different conditions, often characterized by temperature, composition, or presence of catalysts. Although this example is simple, it illustrates two important points: First, the operating regimes and local models structures are closely bound up with each other. For example, if the local linear models in the example are replaced by non-linear models where the reaction rate constants are replaced by suitable Arrhenius-type terms, then each local model would be valid over a much wider, possibly global, temperature range. Hence, the number of operating regimes can usually be reduced at the cost of increasing the complexity of the local models, and of course also at the cost of the increased process knowledge that suggested the introduction of the Arrhenius-type terms in the local models. Second, the example illustrates that the process knowledge used for decomposition into operating regimes may be quite elementary and qualitative, like knowledge of conditions under which different chemical reactions dominate, and the knowledge that the reaction rates depend strongly on temperature. Supplementary knowledge, like "The reaction rate will be approximately doubled if the temperature increases by 10 K" will be sufficient to decide roughly on how to design regimes along the temperature axis.

When a rough decomposition into regimes is designed, one must make a choice on how much the local model validity functions should overlap, and how soft they should be. The main motivation for using a smooth interpolation of the local models is that the system usually has some smoothness properties, i.e. the phenomena or behavior change smoothly as the operating point changes. However, one may occasionally come across processes that are non-smooth, in the sense that they exhibit abrupt changes in dynamics, for example phase transition or flow pattern changes (Hilhorst 1992, Söderman, Top & Strömberg 1993). Hence, the optimal degree of overlap and softness will depend on the modeling problem. On the other hand, we have also experienced that a rough choice will often give a close-to-optimal result. An important factor that may influence the choice of overlap is that a large overlap may lead to decreased transparency of the model. The reason for this is essentially that an increased overlap will give increased interdependencies between the local models. If the parameters of the local models are fitted using empirical data, a large overlap implies that the same data will be relevant for a significant number of regimes. This may lead to local models that cannot be interpreted as local approximations to the system, since the parameters of some local models may be highly influenced by remote data points in addition to the parameters of other local models (Murray-Smith & Johansen 1995).

So far, we have only discussed regimes that are characterized by model variables. Sometimes, one may choose to characterize regimes directly on the basis of time (e.g. batch processes or periodic systems), and sometimes on the basis of spatial variables (in distributed models). Although these extensions are straightforward, they will not be discussed in the present paper.

2.3 Local Models

The operating regime based modeling framework allows integration of different types of local models. We have already mentioned the possibility of using both mechanistic and empirical local models.

Consider first local mechanistic state-space models

$$\dot{x} = f_i(x, u, q, \theta)$$

where q is a vector of internal variables that depend algebraically on other model variables in an unknown way. If there are no such unknown internal variables q, the model is already on the form (2). On the other hand, we suggest to use a set of simple generic *local* empirical models to describe q, for example a linear model

$$q = h_i(x,u,\theta) = \theta_{i,1} + \theta_{i,2}^T x + \theta_{i,3}^T u$$

or simply a constant model

$$q = h_i(x,u,\theta) = \theta_{i,1}$$

where the parameter vectors $\theta_{i,1}, \theta_{i,2}$, and $\theta_{i,3}$ are sub-vectors of θ. This leads to a set of semi-mechanistic local models

$$\dot{x} = f(x,u,h_i(x,u,\theta),\theta) \tag{5}$$

which are on the form (2), since $h_i(x,u,\theta)$ has a known structure. The regime Z_i in which this model is valid, is expected to be a subset of the full range of operation, simply because the functional structure chosen for $h_i(x,u,\theta)$ is expected to be simpler than the "true function". In general, the region in which $h_i(x,u,\theta)$ is a good approximation to the unknown function will determine the region in which the local model (5) is a good approximation to the system. Notice that these two regions will in general not be equal. Also notice that simple h_i-functions such as those suggested above will approximate any q locally, provided q is a continuous function of its arguments. Hence, we may conclude that an incomplete mechanistic model in many cases can be transformed to a set of local models of the form (2). Furthermore, the conditions under which such a model is valid under will usually be given as explicit restrictions on some variables, or as assumptions about the relevance of different phenomena. These last assumptions can be translated into explicit restrictions on the variables in many cases.

Some qualitative knowledge can also quite easily be represented as local state-space models. For example, a typical qualitative statement about a biochemical process could be "If the temperature is too high, or the pH is too high or low, then the amount of live micro-organisms will quickly decrease towards zero". A possible local model for the operating regime where the "temperature is too high, or the pH is too high or low" is $\dot{x} = -\frac{1}{\tau}x$, where x is the amount of live micro-organisms, and τ is a small time constant. More complex and complete examples of this can be found in (Jian 1993, Takagi & Sugeno 1985, Sugeno & Yasukawa 1993) that describe qualitative models developed on the basis of operator experiences. Of course, one can also find examples of qualitative knowledge that can not be written in the form (2).

2.4 Model Development Procedures

One simple modeling procedure is the following: the first step is to choose the variables z used to characterize the operating regimes, and then find the operating regimes that describe the validity of any a priori available local model(s), and identify which regions of the full range of operation are not covered sufficiently well using the a priori available models. Then the task is to decompose this region further into operating regimes and select parameterized local model structures for these regimes. These new local model structures may be empirical, mechanistic, or a mixture. Finally, the unknown local model parameters are identified using empirical data. Notice that the choice of operating regimes and local model structures should not be decoupled, as the complexity and validity of the local model structures should be taken into account when decomposing into operating regimes.

3 Computer Aided Modeling

The operating regime based modeling framework contains extensive flexibility, where different levels and kinds of mechanistic and empirical process knowledge and data can be utilized. During model development, the engineer can play with different local model structures, different decompositions into regimes, interpolation parameters for the local models, different parameter sets, and model validation procedures. To support the modeling, we have developed a flexible computer aided modeling tool, which at one extreme can function as an automatic (i.e. data-driven) empirical modeling algorithm, and at the other extreme is only a graphical user interface for developing operating regime based models "by hand". The most interesting application area for this tool, however, lies in between these extremes, as an interactive modeling tool. We believe such flexibility is important, since neither the fully automatic nor the manual approach can take full advantage of the modeling framework by themselves.

The software tool is called ORBIT, an acronym for Operating Regime Based modeling and Identification Toolbox (Johansen 1995). ORBIT is implemented in MATLAB, taking advantage of the available functions for data pre-processing, simulation, and numerical computation in general. The software is not restricted to any particular model representation, but can effectively deal with continuous-time or discrete-time models, input/output or state-space models, and lumped or distributed model representations. A small library of generic operating regime based model representations is available. It includes local MIMO ARX models to build NARX models, and multivariable non-linear regression models based on local linear multivariable linear regression models. Other model representations must be implemented as MATLAB functions.

The ORBIT architecture is illustrated by the dataflow diagram in Figure 3. The core modules are the Operating Regimes Manipulation Module, and the Model Parameters Manipulation Module. Another important module is the Model Validation Module, which includes the possibility of comparing different models by simulation and statistical estimates of the prediction performance. Developed models are made available as SIMULINK blocks.

3.1 Operating Regimes Manipulation Module

In ORBIT, the operating regimes are represented as hypercubes with soft boundaries. An arbitrary number of such regimes can be placed at arbitrary locations in the operating space. When the operating regimes are characterized by two variables, the regimes can be visualized as rectangles, see Figure 4a. Figure 4b shows a general way of visualizing the operating regime. The projections (soft shadows) of the soft hypercube onto the individual axes corresponding to the characteristic variables $z_1, ..., z_d$ are visualized. The toolbox includes a point-and-click type graphical user interface for manipulation of the operating regimes. The number, size, locations and softness of the operating regimes can easily be tuned, the user can select between different local model structures on a menu for each operating regime, and characterizing variables can be added or removed. Moreover, an algorithm for structure identification using process data is available. It is based on a heuristic search algorithm that searches the set of model structures, or a specified subset thereof, for the model structure that minimizes a selected objective criterion, see Figure 5. Notice that in each regime, there may in addition be several local model structure candidates and integer model parameters to choose among. The possible objective criteria are statistical criteria that estimate the expected prediction performance of the model on the basis of process data. These include advanced structure selection criteria such as the Final Prediction Error (FPE) criterion (Akaike 1969), Cross-Validation (Stoica, Eykhoff, Janssen & Söderström 1986), and Generalized Cross Validation (GCV) (Craven & Wahba 1979) that allow parameter identification data to be recycled. Notice that such criteria favor parsimonious model structures rather than under- or over-parameterized model structures. Not only will this algorithm determine the regime locations, sizes and corresponding local model structures, but it will also determine the number of regimes. An in-depth discussion of this algorithm and its properties can be found in (Johansen & Foss 1995). In the literature, there exists other structure identification algorithms that can be used to identify model structures based on local models (Jordan & Jacobs 1994, Murray-Smith & Gollee 1994, Jones & co-workers 1991, Yoshinari, Pedrycz & Hirota 1993, Yager & Filev 1993, Nakamori & Ryoke 1994). In general, these are automatic modeling algorithms based on more complex parameterization of the operating regimes. Consequently, they do not have the same flexibility to incorporate process knowledge, and the models may be considerably more difficult to interpret for high-dimensional problems.

3.2 Model Parameters Manipulation Module

The local model parameters can also be manipulated using a point-and-click user interface, see Figure 6. This interface supports identification of parameters using process data, it allows the user to set any parameter values explicitly and define bounds on the parameter to be taken into account during parameter identification. Various algorithms are available, including variations over least squares and prediction error methods (Söderström & Stoica 1988) based on multi-step predictors, and a locally weighted least squares algorithm where the parameters of the individual local models are fitted using local weighting of the data (Murray-Smith & Johansen 1995). Any parameter can be set to local or global, meaning that its value is different or the same in the different operating regimes, respectively. Also, integer parameters such as dynamic model order parameters can be manipulated with the functions in this module.

4 SIMULATION EXAMPLES

4.1 Example 1: A pH-neutralization tank

Consider a pH-neutralization tank, where there are three influent streams and one effluent stream:

- Influent acid stream Q_1 (HNO_3)
- Influent buffer stream Q_2 ($NaHCO_3$)
- Influent base stream Q_3 ($NaOH$ and traces of $NaHCO_3$)
- Effluent stream Q_4

For our simulation study we use the experimentally verified model of Hall & Seborg (1989) to simulate the system, see Appendix A. We will develop a hybrid model that is a combination of a simple mechanistic model and a simple input/output model. The data used for model identification are shown in Fig. 7a, while the data used for validating the model are shown in Fig. 7b. Both data sequences are noise-free, and the sampling interval is 15 s. Clearly, the validation data cover a significantly wider operating range than the identification data, which is typical for many applications.

4.1.1 A simple mechanistic model

Let us first consider a very simple model of the tank, based on neglecting the buffer in the model. Consequently, the only reaction considered in this model is

$$H_2O \rightleftarrows OH^- + H^+$$

A reaction invariant is $W = [H^+] - [OH^-]$, and an implicit equation for $[H^+]$ is

$$W = [H^+] - K_w/[H^+] \tag{6}$$

The mass balances are

$$A\dot{h} = Q_1 + Q_3 - c\sqrt{h - h_0} \tag{7}$$

$$hA\dot{W} = Q_1(W_1 - W) + Q_3(W_3 - W) \tag{8}$$

This model is validated against the validation data by a simulation shown in Fig. 8a. We observe that the model is accurate for high and low pH values, but inaccurate for intermediate values of pH, where the buffer is important. In fact, this model is a reasonable model of almost any neutralization process at high and low pH values. Of course, what is high and low in this context will depend on the particular process.

4.1.2 An ARX model

Next, the ARX model

$$pH(t+1) = 7.06 + 0.78(pH(t) - 7) + 0.10(Q_3(t) - 15) \tag{9}$$

is identified using the least squares method and the identification data. A simulation of the model on the validation data is shown in Fig. 8b. The prediction error is clearly smallest for intermediate pH values, while the predictions are completely wrong for large pH values. An NARX model based on two or three local ARX models gives better fit for intermediate pH values, but even less convincing predictions when extrapolated to regimes with a large or small pH value.

4.1.3 A Hybrid Model

Finally, consider the case when we develop a model on the basis of a mixture of local ARX model structures and a simplified local mechanistic model. The hybrid model is a discrete-time model, and the operating regimes are characterized by $z = \text{pH}$. The continuous-time mechanistic local model is integrated numerically over the 15 s sampling interval (unit time-step of the ARX model). Upon transition from a regime where the ARX model is applied to a regime where the mechanistic model is being applied, an initial state for the mechanistic model must be provided. This is a general problem related to the fact that the local model state spaces are different. It is possible to compute the model state W directly from (6) and the pH value. The model consists of three local models:

1. The first local model is simply the differential equation (8) combined with the algebraic equation (6), used to predict the pH value when the process is operating at low or high values at pH.
2. The second local model is the ARX model (9), used to predict the pH value at intermediate pH values.
3. The third "local" model is the differential equation for the level (7), which is valid under all operating conditions.

The model is chosen as a combination of local mechanistic models in the regimes where there are no data, and local empirical models in regimes that contain sufficiently large amounts of data. The hybrid model is able to fit the data well, as an empirical model, and provides reliable extrapolation, as a mechanistic model. The relative weight in the interpolation is shown in Fig. 9, and a simulation of the model on the validation data is shown in Fig. 8c. We see that the prediction accuracy has improved significantly for most operating conditions, but we also see that there exists room for improvement by fine-tuning the regimes and local model validity functions.

4.2 Example 2: A biochemical reactor

Consider a batch biochemical reactor, where the fermentation of glucose to gluconic acid by the micro-organism *Pseudomonas ovalis* takes place. The main overall reaction mechanism is described by

$$\begin{aligned}
\text{Cells} + \text{Glucose} + O_2 &\stackrel{\mu}{\to} \text{More Cells} \\
\text{Glucose} + O_2 &\stackrel{\sigma}{\to} \text{Gluconolactone} \\
\text{Gluconolactone} + H_2O &\stackrel{k_p}{\to} \text{Gluconic Acid}
\end{aligned}$$

The first reaction is the reproduction of cells (χ), using the substrate glucose (s) and oxygen (c). The second reaction is the production of gluconolactone (l), again using glucose and oxygen. This reaction is enzyme-catalyzed by the cells, while the last reaction forms the final product, gluconic acid (p). A set of mass balances for this reactor can be found using knowledge of the reaction mechanism, stoichiometry, and oxygen uptake mechanism (Ghose & Ghosh 1976)

$$
\begin{array}{rcl}
\dot{\chi} & = & \mu\chi \\
\dot{l} & = & \sigma\chi - \frac{1}{Y_{l|p}} k_p l \\
\dot{p} & = & k_p l \\
\dot{s} & = & -\frac{1}{Y_{s|\chi}}\mu\chi - \frac{1}{Y_{l|\chi}}\sigma\chi \\
\dot{c} & = & k_l a(c^\star - c) - \frac{1}{Y_1}\mu\chi - \frac{1}{Y_2}\sigma\chi
\end{array}
\tag{10}
$$

The internal variables μ, σ and k_p are reaction rates for the three reactions, $c^\star$ is the maximum dissolved oxygen concentration, and $k_l a$ is a mass transfer coefficient that describes the uptake of oxygen. The yield coefficients $Y_1, Y_2, Y_{l|p}, Y_{l|\chi}$, and $Y_{s|\chi}$ are determined by the stoichiometry. The model is not complete unless expressions for the internal variables and parameters mentioned above are known. Without more process knowledge, one may use empirical relations of the form

$$
\begin{array}{rcl}
\mu & = & \mu(c, s) \\
k_p & = & k_p(c, s) \\
\sigma & = & \sigma(c, s) \\
c^\star & = & \text{constant} \\
k_l a & = & \text{constant}
\end{array}
\tag{11}
$$

The dependence on variables like temperature, pH, and agitation speed is ignored in this example, but can be included in the same way. Let us now consider how the modeling problem can be solved using the operating regime based modeling framework, when it is assumed that some process data are available. In our simulation example, we have generated data from 100 simulated 10 hour batches, sampling all five states every 0.5 hour, which gives a total of 2000 points. The different batches start from different (random) initial states $\chi(0)$ and $s(0)$. The simulator uses the model (10) with the experimentally verified reaction rate equations and parameters found in (Ghose & Ghosh 1976). Small amounts of "measurement noise" and "disturbances" were added to the data. On the basis of (10) and (11), we apply local semi-mechanistic models based on local empirical approximations

$$
\begin{array}{rcl}
\mu_i(c, s) & = & \theta_{i,1} + \theta_{i,2}c + \theta_{i,3}s \\
k_{p_i}(c, s) & = & \theta_{i,4} \\
\sigma_i(c, s) & = & \theta_{i,5} + \theta_{i,6}c + \theta_{i,7}s
\end{array}
$$

where the unknown local model parameters $\theta_{i,1}, ..., \theta_{i,7}$ correspond to local model i. The variable k_p is approximated locally by a constant, while σ and μ are approximated locally by linear functions. The reason for this difference is that it is expected that k_p will show considerably less variation than the other two variables. In addition, the model consists of two unknown global parameters

$$
\begin{array}{rcl}
c^\star & = & \theta_{0,1} \\
k_l a & = & \theta_{0,2}
\end{array}
$$

The model is found with the aid of the structure identification algorithm described in (Johansen & Foss 1995), using the FPE criterion (Akaike 1969). The algorithm identifies four regimes, cf. Fig. 10. The trajectory in this figure corresponds to a typical batch, projected into the two-dimensional subspace of the state-space defined by c and s. The prediction performance of the model on a typical batch (with initial conditions not included in the identification data) is depicted in Fig. 11, from which we see that the model has captured the major non-linear effects. Since the reaction rates appear linearly in the model equations, we are able to study the identified kinetic model directly, because

$$\begin{aligned}
\hat{\mu}(c,s) &= \sum_{i=1}^{4} \hat{\mu}_i(c,s) w_i(c,s) \\
\hat{k}_p(c,s) &= \sum_{i=1}^{4} \hat{k}_{p_i}(c,s) w_i(c,s) \\
\hat{\sigma}(c,s) &= \sum_{i=1}^{4} \hat{\sigma}_i(c,s) w_i(c,s)
\end{aligned}$$

These functions are illustrated in Fig. 12, which also contains the "true kinetic model" used in the simulator. Comparing the identified functions with the "true ones" clearly shows that the identified model is a close approximation to the "true model" in the regimes that are densely populated with process data, while there may be some mismatch elsewhere, cf. Fig. 10. The hybrid model may be a useful intermediate step in the search of a mechanistic model.

Moreover, the identified kinetic model suggests a possible interpretation of the four regimes. It is evident that neither oxygen nor glucose is rate-limiting in the initial phase of the batch corresponding to Regimes 1 and 2, cf. Fig. 10, where it is the biomass concentration alone that limits the reaction rates. On the other hand, oxygen is rate-limiting through Regime 3, and at the end of this regime and through Regime 4, glucose is rate-limiting. Hence, the identified model is transparent and easy to interpret qualitatively. It should be mentioned that a similar approach was taken in (Psichogios & Ungar 1992, Aoyama & Venkatasubramanian 1993), where the kinetic model was represented by a neural network. Of course, the general properties of such models are quite similar to the properties of the one presented here.

4.3 Discussion

Both examples clearly illustrate the power of the operating regime based modeling framework: in addition to a sequence with process data, only rather rough and elementary process knowledge is applied. In the examples in this paper we have focused on local mechanistic models, and the combined use of local mechanistic and empirical models, since to the authors' knowledge, these cases have not previously been discussed in the literature in detail, with the exception of (Konstantinov & Yoshida 1989, Zhang et al. 1994). On the other hand, there are several example (both simulated and experimental) of operating regime based models using local empirical models, typically local linear regression or local ARX models. These include river flow modeling (Sugeno & Kang 1988), multi-layer incinerator modeling and control (Sugeno & Kang 1986, Nakamori, Suzuki & Yamanaka 1992), simulated fermentation reactor modeling and control (cf. Example 2) (Johansen & Foss 1995, Foss, Johansen & Sørensen 1995), a converter in a steel-making process (Takagi & Sugeno 1985), in chemometrics (Næs & Isaksson 1991, Næs 1991), and biomedical applications (Gollee, Hunt, de N. Donaldson, Jarvis & Kwende 1994).

5 Discussion

5.1 Assets

The motivation for introducing the operating regime based framework is its ability to absorb a variety of process knowledge in a transparent and flexible manner. This has been illustrated by the examples, where various types of knowledge is introduced through the choice of the operating regimes, the local model validity functions and the structure of the local models, as well as the local model parameters.

From an industrial point of view, it is important that the model representation is transparent, i.e. compatible with the engineer's understanding of the system. The high transparency of the operating regime based modeling framework is related to the possibility of interpreting the operating regimes in terms of either physical phenomena or system behaviors. Moreover, it is related to our ability to interpret the simpler local models individually. We claim that the operating regime paradigm corresponds closely to the approach engineers commonly take in problem solving. This is appealing, since the framework may support effective communication about the process between people with different backgrounds.

Model accuracy requirements may vary according to operating conditions. The reason for this is that the pay-back on the use of model-based applications, e.g. model-based control, may differ at different operating conditions. The modeling framework supports variations in accuracy by simply varying the accuracy of the local models or the granularity of the operating regime decomposition.

Typically, the knowledge one has about a process will change with time, as experience increases, new phenomena are discovered, and more process data becomes available. Sometimes, such new knowledge is connected to particular operating conditions. If this is the case, the present framework supports simple maintenance of the model, as one may only need to change one local model, or one may choose to decompose one operating regime into two or more sub-regimes. In any case, the remaining local models can be left unchanged. In a sense, this modeling approach can be though of as modular, where the modules are the different local models and corresponding operating regimes. It is also appealing that one can for example start out with a linear model, which can subsequently be refined until a non-linear model of the desired accuracy is obtained.

Since some knowledge about the validity (or relevance) of each local model is implicit in this modeling framework, it is often possible to determine operating conditions under which the system is not sufficiently well understood. Hence, experiment design support is directly available in the form of hints on the operating conditions under which experiments should be conducted in order to improve the model. In addition, standard experiment design tools can be applied (Box & Draper 1987).

5.2 Relationship to Fuzzy Modeling

An operating regime Z_i can be viewed as a fuzzy subset of Z, with membership function $\mu_{Z_i}(z) = \rho_i(z)$. Then each local model can be represented as a rule

$$\text{IF } z \in Z_i \text{ THEN } \qquad \dot{x} = f_i(x, u, \theta)$$

The interpolation method is equivalent to a fuzzy inference mechanism, and the model can be looked upon as a fuzzy model as defined by Takagi & Sugeno (1985), and the theory of fuzzy sets can be used to construct local model validity functions.

For example, if a fuzzy set Z_i is defined by

$$z \text{ IS } Z_i \quad = \quad (z_1 \text{ IS LARGE}) \text{ AND } (z_3 \text{ IS NOT INCREASING})$$

this would give, by the use of the most common intersection and complement operators on fuzzy sets, a membership function like

$$\mu_{Z_i}(z) \quad = \quad \min\left(\mu_{z_{1,\text{large}}}(z_1), 1 - \mu_{z_{3,\text{incr}}}(\dot{z}_3)\right)$$

where $\mu_{z_{1,\text{large}}}(z_1)$ is the mono-variable membership function for the fuzzy subset where "z_1 is large" and $\mu_{z_{3,\text{incr}}}(\dot{z}_3)$ is the membership function that represent the fuzzy subset where "z_3 is increasing".

We would like to stress that fuzzy sets is only one way of interpreting the operating regimes and modeling framework based on multiple local models. We have chosen to suppress this interpretation in the presentation, because it is unnecessary. It does not contribute with any fundamentally new aspects to the framework, and we fear it may be confusing to those who are not familiar with fuzzy set theory.

5.3 Open problems

Although our results so far have been promising, there remain several open questions that need to be answered: First, most examples of models based on local models are quite simple. There may therefore be problems related to the application of the framework on high-dimensional and highly complex problems. In particular, it may be difficult or impossible to find a small number of variables to characterize the operating regimes. This situation is unfortunate, because of the possibly large number of local models (curse of dimensionality) and the resulting loss of transparency of the model and modeling framework. An interesting approach to the identification of good characterizing variables appears to be an analysis of the correlation structure and collinearities in the process data (Sugeno & Kang 1986, Nakamori et al. 1992).

There are fundamental problems associated with the interpolation of local state-space models. Consider a system that, during a particular time interval, undergoes a transition from one operating regime to another, and assume that the two corresponding local models use a different set of variables, for example have different state spaces. The obvious question that arises is "What is the correct 'initial' state of the local model associated with the regime just entered?" In some cases there exists an obvious answer to this question. For example, if known mappings between the two state spaces exists, then the state information can be transfered between the local models. Unfortunately, there are situations when no such simple answer exists. A solution to the problem can be to model the irrelevant states in each local model as random walk processes (Johansen & Foss 1993*b*). If these states are observable globally, or at least in a sufficiently large neighborhood of the relevant operating regimes, an extended Kalman-filter or observer, e.g. (Söderström & Stoica 1988), can be used to track these states and provide an initial value upon entering the regime, provided the system output is known. Example 1 illustrates a simple application of this approach, but a detailed investigation is still missing. Another solution is to introduce constraints that ensures consistency between different state-space representations (Barton & Pantelides 1994). In the pH neutralization example in section 4.1, the algebraic equation (6) is essentially a constraint that links pH and the state W.

6 CONCLUDING REMARKS

The modeling framework discussed in this paper is intended to support the design of non-linear models. While linear modeling is often sufficient for many control or optimization problems, non-linear modeling may be of interest when the process is operating within a wide range of operating conditions, for example batch processes, during startup and shutdown, during product shifts, and other exceptional operating conditions.

Fig. 1 illustrates the authors' view on when the proposed modeling framework is useful. The conditions are characterized by moderate amounts of both process knowledge and data, as opposed to the mechanistic modeling approach which requires good process knowledge, and the empirical modeling approach that requires large amounts of informative process data. With the operating regime based modeling approach, the process knowledge required for operating regime decomposition can be of a rather qualitative nature. Moreover, the modeling framework provides an alternative that may give transparent, accurate, and reliable models at reasonably low cost.

Appendix A

Here we describe the model developed by Hall & Seborg (1989). It is based on the assumptions of perfect mixing, constant density, fast reactions and completely soluble ions. Only the following chemical reactions are modeled

$$
\begin{aligned}
H_2O &\rightleftarrows OH^- + H^+ \\
H_2CO_3 &\rightleftarrows HCO_3^- + H^+ \\
HCO_3^- &\rightleftarrows CO_3^{2-} + H^+
\end{aligned}
$$

because HNO_3 is a strong acid and NaOH is a strong base. Chemical reaction invariants for the process are (Gustafsson & Waller 1983)

$$W_a = [H^+] - [OH^-] - [HCO_3^-] - 2[CO_3^{2-}]$$

$$W_b = [H_2CO_3] + [HCO_3^-] + [CO_3^{2-}]$$

Using the equilibrium equations $K_{a1} = [HCO_3^-][H^+][H_2CO_3]^{-1}$, $K_{a2} = [CO_3^{2-}][H^+][HCO_3^-]^{-1}$, and $K_w = [H^+][OH^-]$, an implicit equation for $[H^+]$ is found

$$W_a = [H^+] - \frac{K_w}{[H^+]} - W_b \frac{K_{a1}/[H^+] + 2K_{a1}K_{a2}/[H^+]^2}{1 + K_{a1}/[H^+] + K_{a1}K_{a2}/[H^+]^2}$$

Solving this equation for $[H^+]$, we can find pH $= -\log_{10}[H^+]$. A total mass balance of the tank gives

$$A\dot{h} = Q_1 + Q_2 + Q_3 - c\sqrt{h - h_0}$$

where c is a valve constant, A is the tank cross-section area, h is the freely varying tank level, and h_0 the vertical distance from the bottom of the tank to the outlet. Component balances give

$$\begin{aligned} hA\dot{W}_a &= Q_1(W_{a1} - W_a) + Q_2(W_{a2} - W_a) + Q_3(W_{a3} - W_a) \\ hA\dot{W}_b &= Q_1(W_{b1} - W_b) + Q_2(W_{b2} - W_b) + Q_3(W_{b3} - W_b) \end{aligned}$$

where W_{ai} and W_{bi} are chemical reaction invariants of the i-th stream. The variables are defined in Table 1.

Acknowledgments

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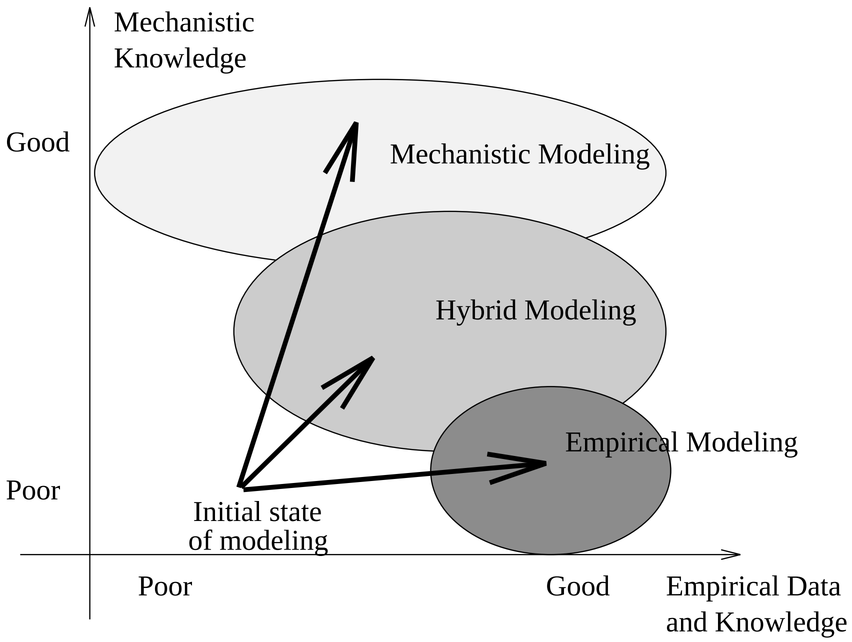


Figure 1: The figure illustrates different approaches to modeling.

Table 1: Symbols, constants and variables used in models.

Symbol	Variable	Nominal value
A	Tank area	207 cm^2
h	Tank level	14 cm
h_0	Tank outlet level	5 cm
Q_1	Acid flow-rate	16.6 ml/s
Q_2	Buffer flow-rate	0.55 ml/s
Q_3	Base flow-rate	15.6 ml/s
$[HNO_3]_1$	Acid concentration in acid stream	0.003 mol/l
$[NaHCO_3]_3$	Buffer concentration in base stream	0.00005 mol/l
$[NaOH]_3$	Base concentration in base stream	0.003 mol/l
$[NaHCO_3]_2$	Buffer concentration in buffer stream	0.03 mol/l
c	Valve constant	8 $ml/s\sqrt{cm}$
pK_{a1}	$-\log_{10} K_{a1}$	6.35
pK_{a2}	$-\log_{10} K_{a2}$	10.33
pK_w	$-\log_{10} K_w$	14.00
W_{a1}	$[HNO_3]_1$	0.003 mol/l
W_{a2}	$-[NaHCO_3]_2$	-0.03 mol/l
W_{a3}	$-[NaHCO_3]_3 - [NaOH]_3$	-0.00305 mol/l
W_{b1}		0
W_{b2}	$[NaHCO_3]_2$	0.03 mol/l
W_{b3}	$[NaHCO_3]_3$	0.00005 mol/l
W_1	$[HNO_3]_1$	0.003 mol/l
W_2		0
W_3	$-[NaOH]_3$	-0.003 mol/l

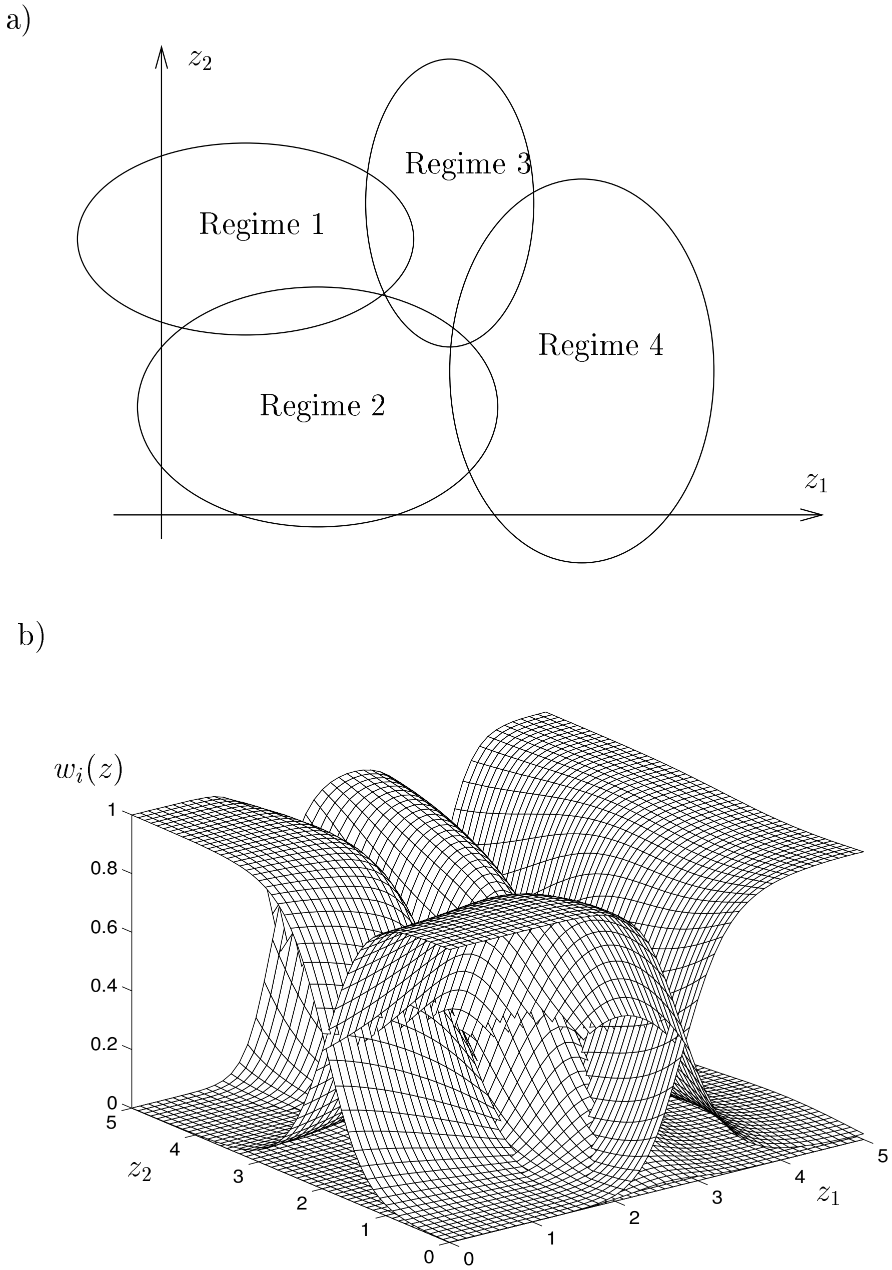


Figure 2: a) Example of four operating regimes characterized by two variables z_1 and z_2, and b) corresponding interpolation functions $w_i(z)$.

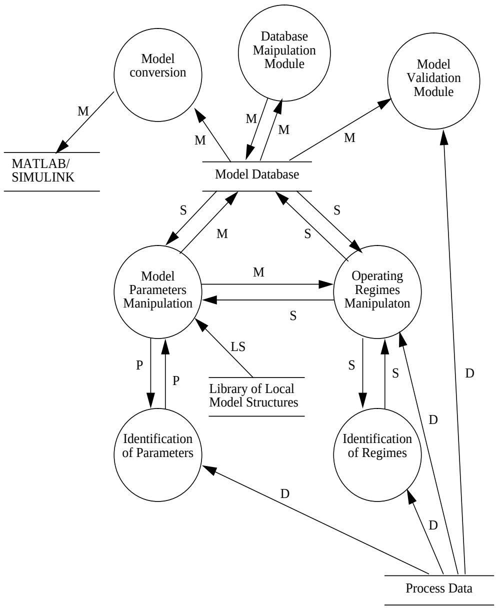
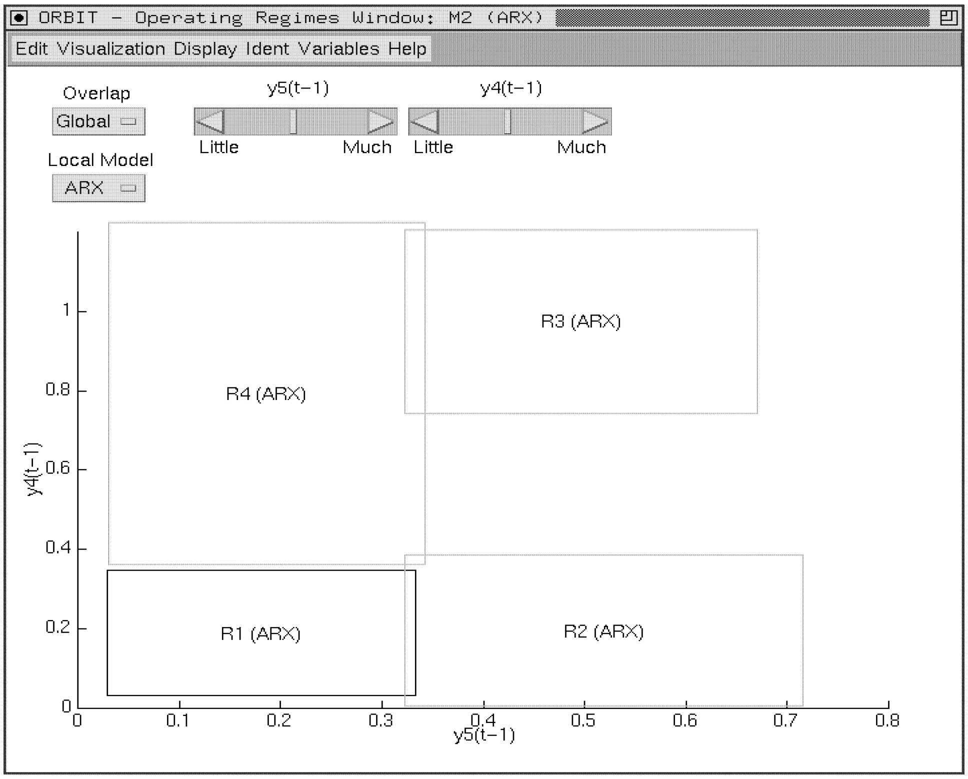


Figure 3: Overall dataflow diagram for ORBIT. S is model structure, P is model parameters, M=(S,P) is models, LS is local model structure, and D is process data.



ORBIT - Operating Regimes Window: M2 (ARX)
Edit Visualization Display Ident Variables Help
Overlap
Global
y5(t−1)
Little
Much
y4(t−1)
Little
Much
Local Model
ARX
R4 (ARX)
R3 (ARX)
R1 (ARX)
R2 (ARX)
y4(t−1)
y5(t−1)
0
0.2
0.4
0.6
0.8
1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8

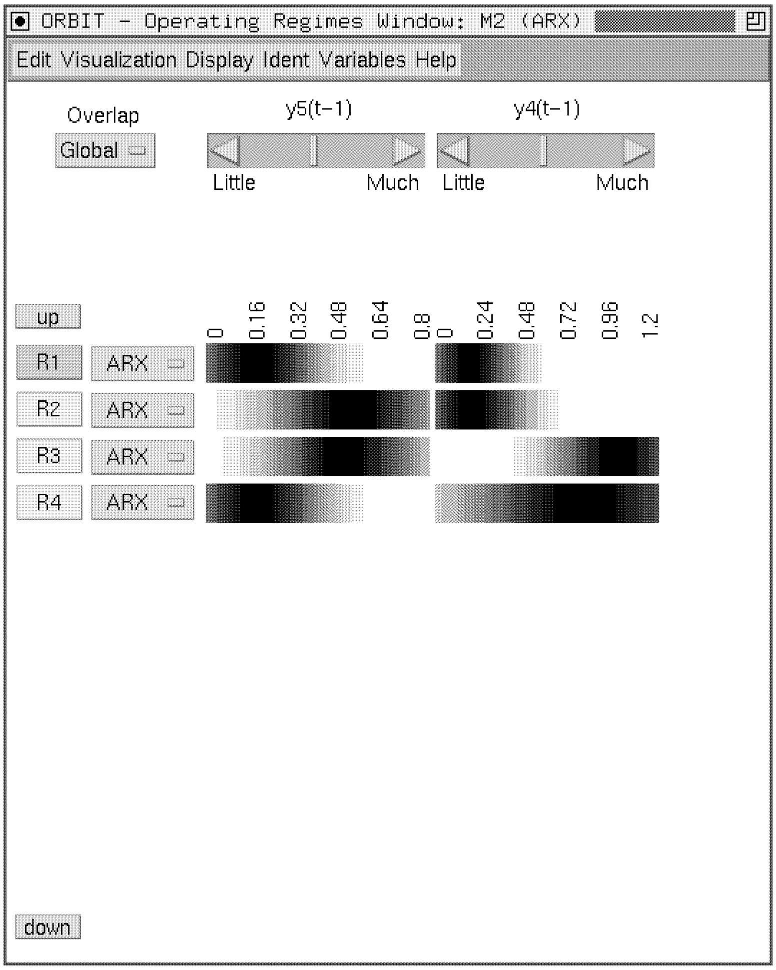


Figure 4: The Operating Regimes Window is the user interface to the Operating Regimes Manipulation Module in ORBIT.

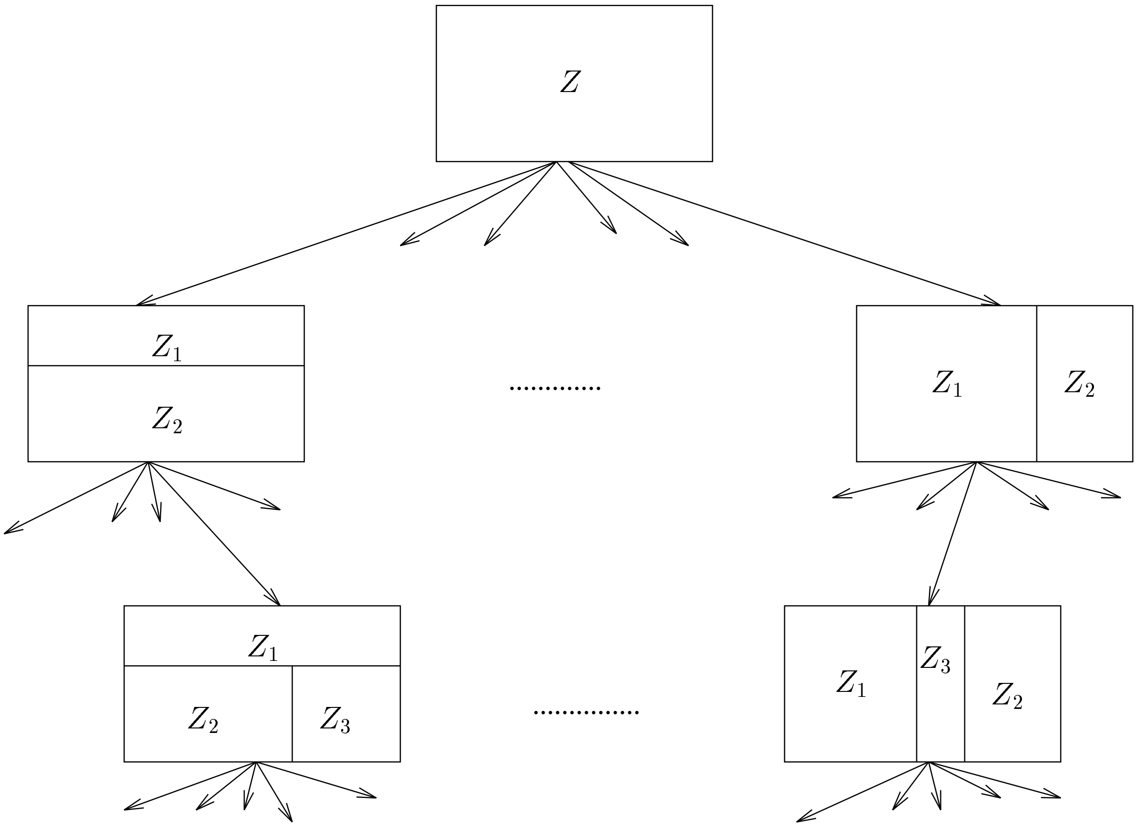


Figure 5: The set of possible operating regime decompositions defines a tree of model structures.

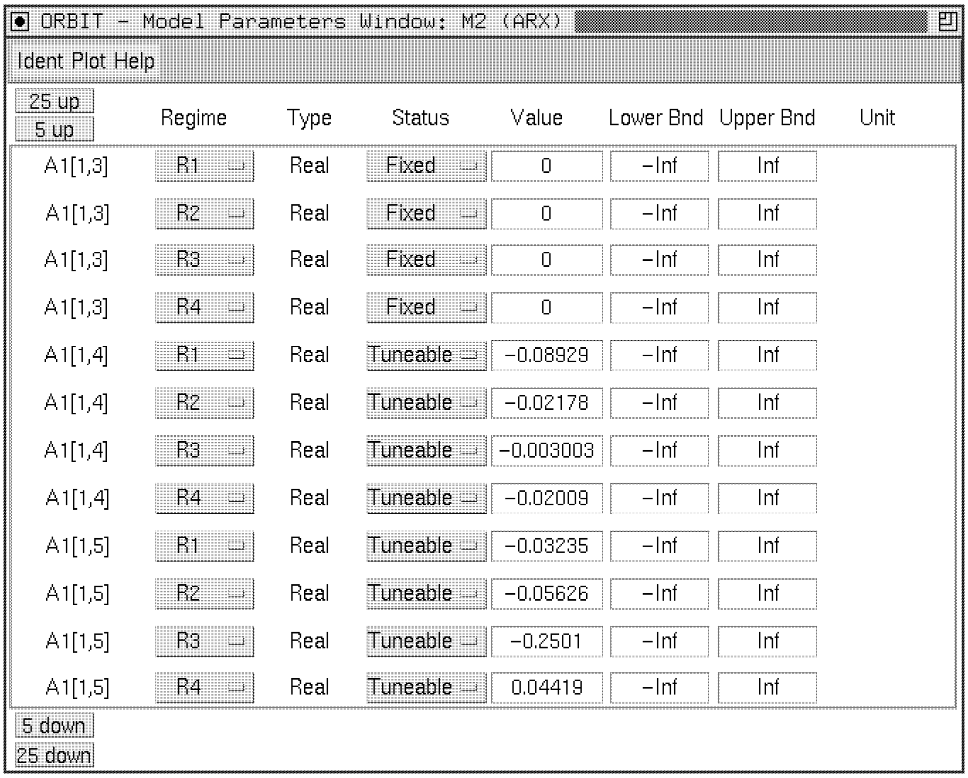


Figure 6: The Model Parameters Window is the user interface to the Model Parameters Manipulation Module in ORBIT.

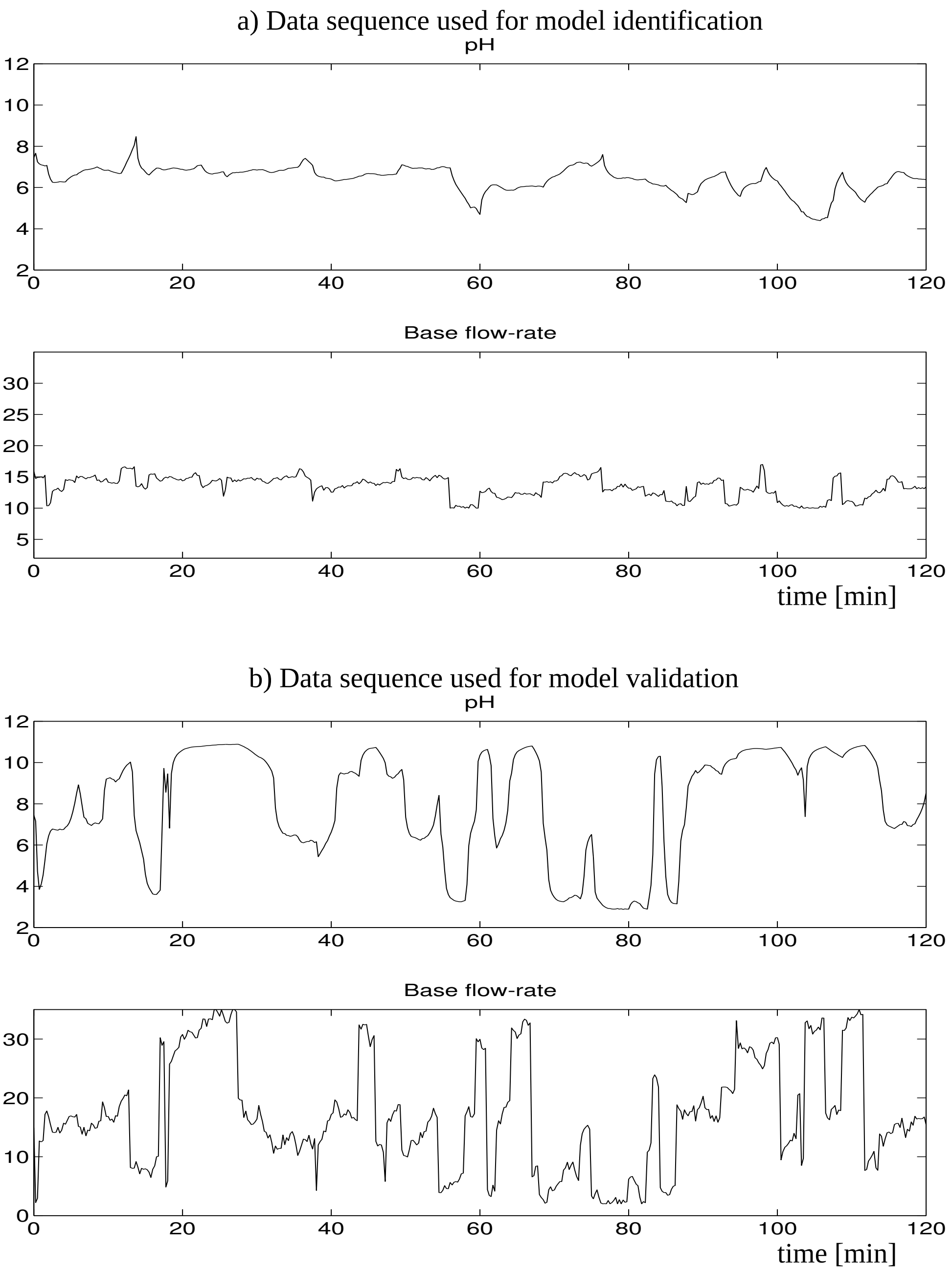


Figure 7: Simulated data sequences.

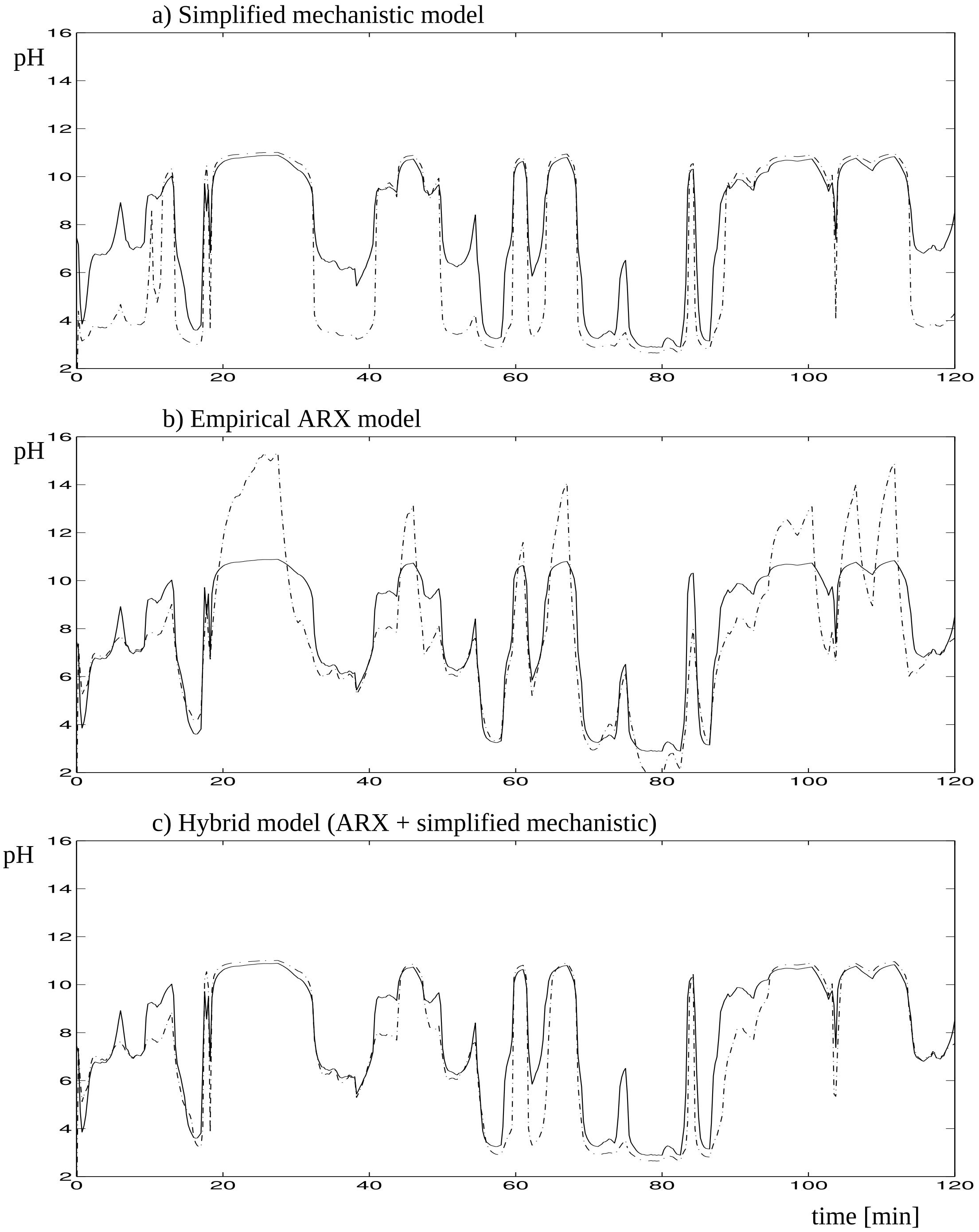


Figure 8: Simulations on the validation data using the three identified models. Solid curves (—) are the system, while dashed-dotted curves (− · − · −) are predictions.

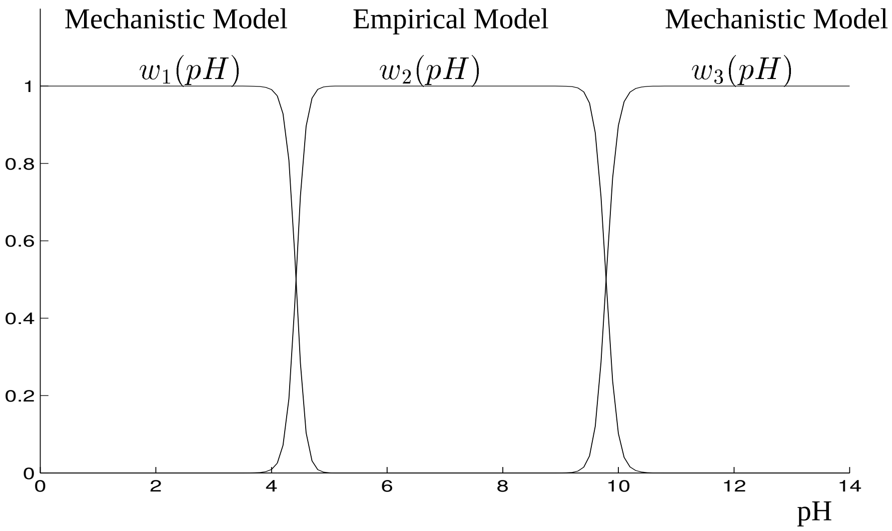


Figure 9: Interpolation functions for the hybrid model.

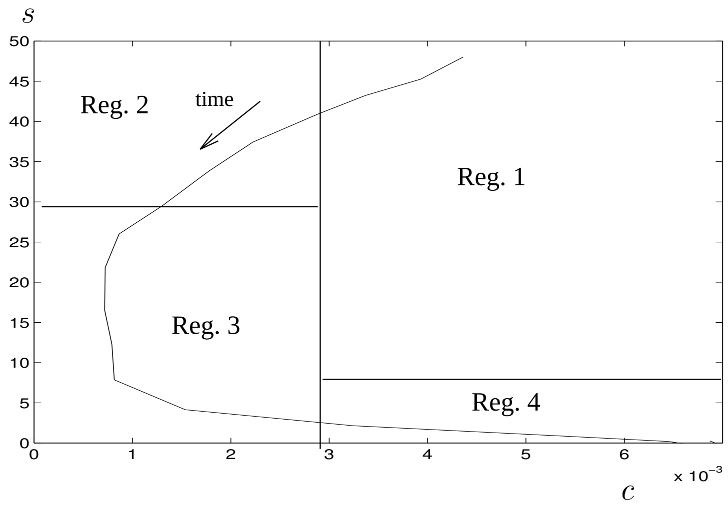


Figure 10: The identified decomposition into four regimes in the fermentor simulation example.

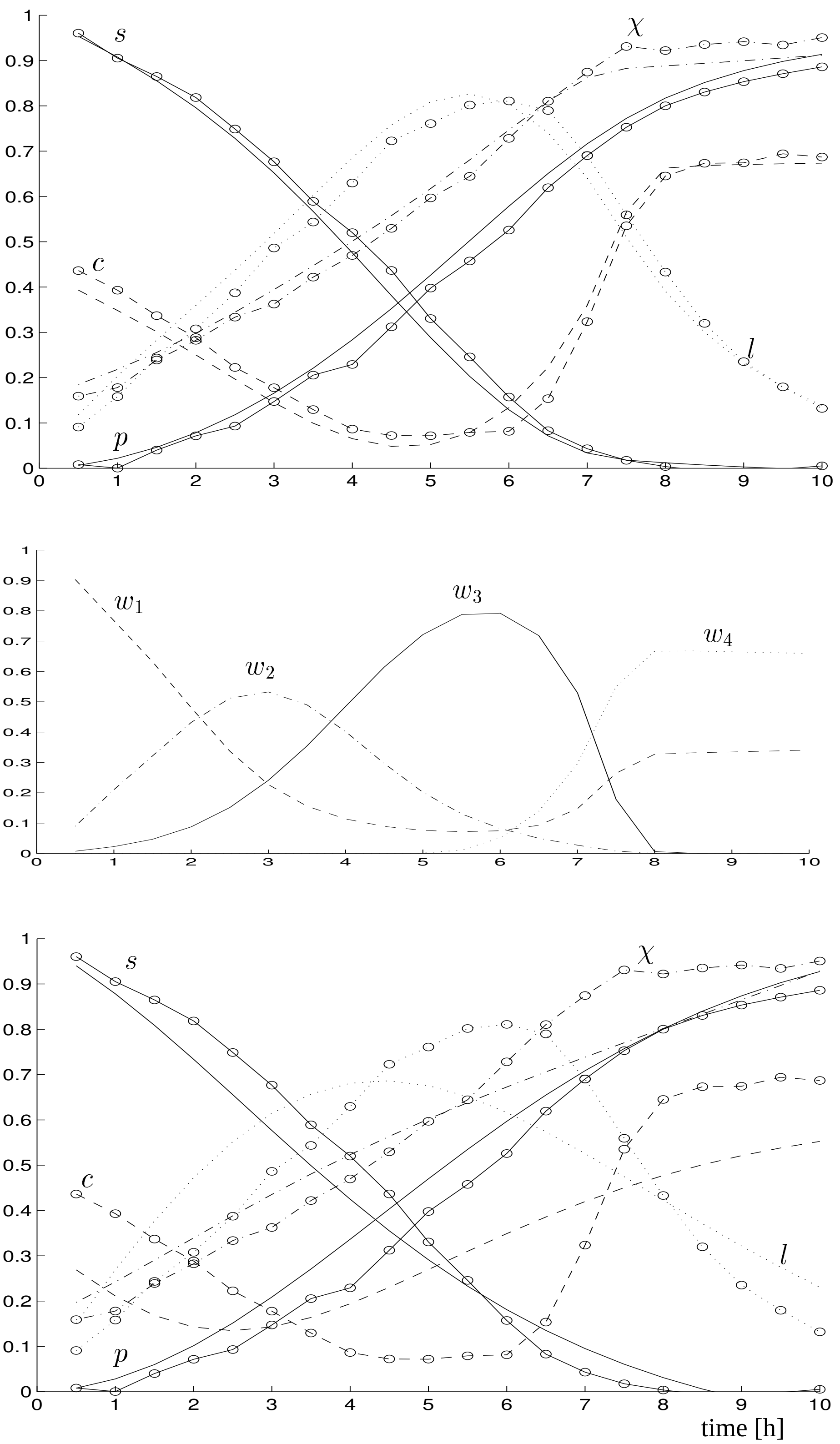


Figure 11: Top: Curves with circles are generated by the simulated system, while the others curves are simulations of the identified model with four operating regimes. All variables are normalized. Middle: The relative weight of the various local models in the interpolation. Bottom: A simulation with an identified model with only one operating regime (for the purpose of comparison).

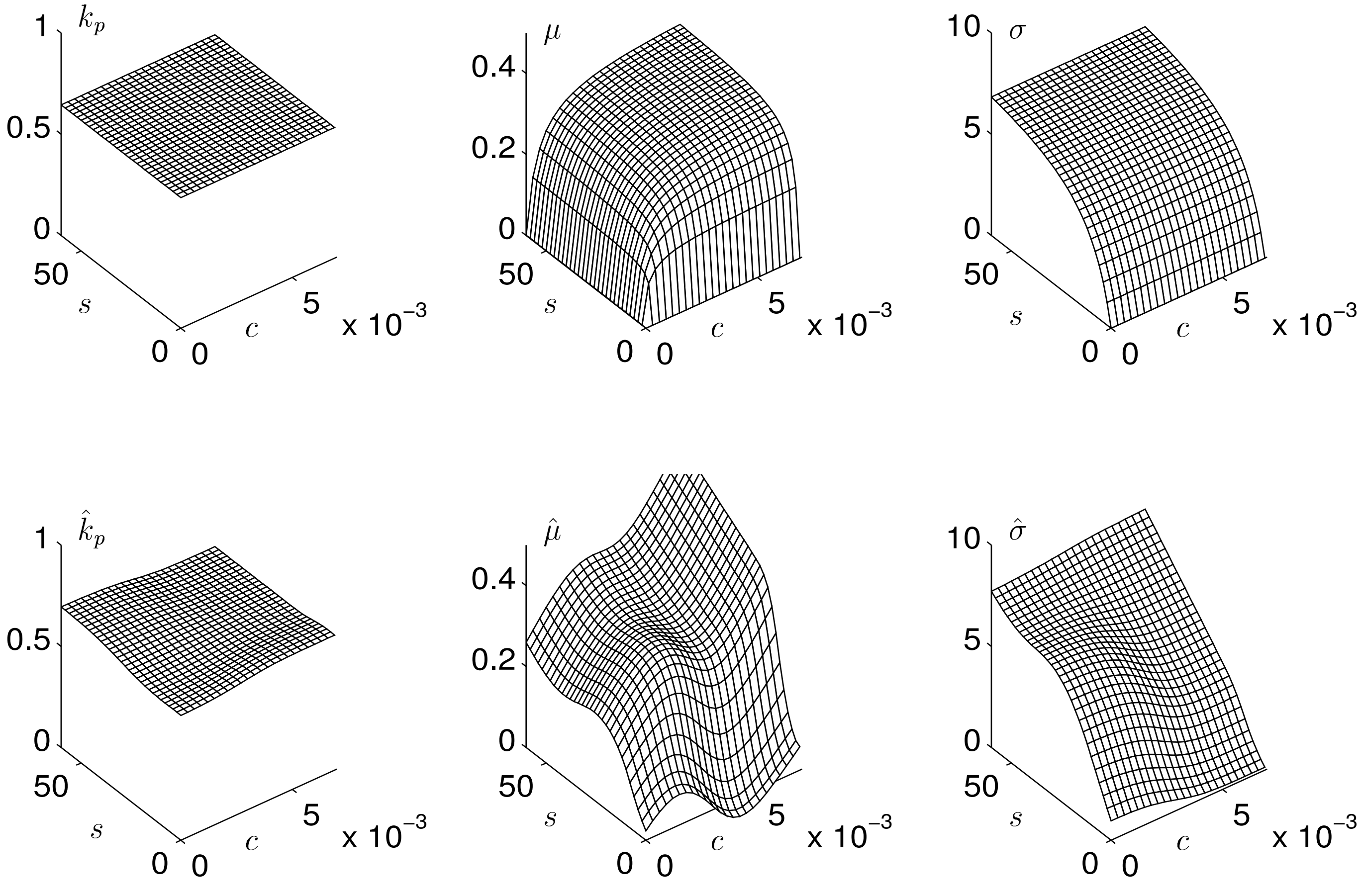


Figure 12: Top: The true kinetic model used in simulator. Bottom: Identified kinetic model.