DYNAMIC PROCESS MODELING USING FUZZY SUBMODELS

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Abstract: This article discusses a new modular design approach for hybrid models consisting of a dynamic framework augmented with static fuzzy sub-models. As the framework is physically based, the models have a dynamic behaviour that corresponds well with the original process. Their fit to process data assures good steady state behaviour and corrects the dynamic behaviour for assumptions and simplifications. The hybrid model design is illustrated for three dynamically different processes: an ideally mixed, a distributed and a chained process.

Keywords: dynamic modelling, fuzzy modelling, distributed-parameter systems, lumped parameter systems, polymer reactor, pulp digester, batch distillation column.

1. INTRODUCTION

Dynamic modelling for optimisation requires models that describe the essential dynamic characteristics of the process under study well over a large operating range. The success of data driven approaches may be limited in an industrial environment where the process is subject to control and measurements are difficult to obtain, while development of a first principles model may be time consuming. In such cases hybrid models may be attractive. The term *hybrid* is used here to denote the combination of white-box and black-box modelling.

Hybrid modelling has received a growing interest since the early 1990's. Most of the research concerns artificial neural networks, which are used to augment the first principles physical model structures. Most notably are the publications by Psichogios and Ungar (1992) and Thompson and Kramer (1994). Some applications in which fuzzy logic is used, have been reported (eg: Babuška *et al.*, 1996; Johansen and Foss, 1997). Most literature concerning hybrid modelling focuses on the parameter identification. Usually, the black box relationships are trained 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. However, the disadvantage is that only the overall model fit is considered, regardless of the complexity and number of fuzzy relationships. This is detrimental to model transparency.

The proposed modular design approach consists of two ideas: (1) partitioning of the problem into dynamic and static transparent sub-problems which can be solved independently of each other and (2) phasing of the modelling procedure into sequential steps (Van Lith *et al.*, 2002). The hybrid model consists of a dynamic framework of mass and energy balances, supplemented with static sub-models. The dynamic framework is not structured according separated input-output relationships, to maintain the interacting relationships between the balances. This makes the model more suitable for optimisation in all variables. The sub-models describe the additional equations, such as mass transformation and transfer rates. Usually, these are static relations and therefore only steady state data is necessary for identification. Fuzzy sub-models are used, because they are able to describe non-linear relationships over a large operating range.

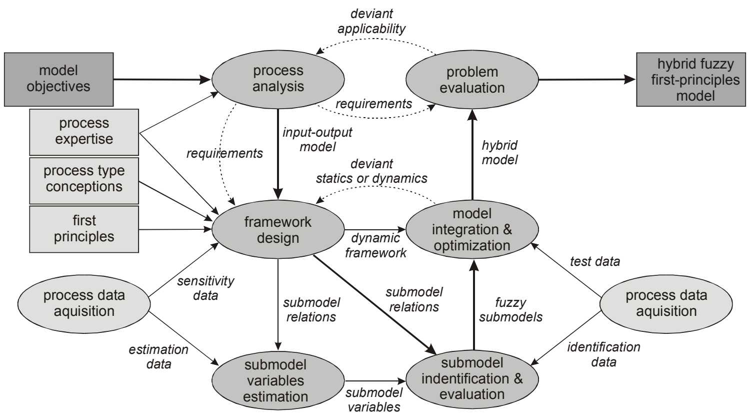

Fig. 1. Steps for development of a hybrid model.

Separation between dynamics and statics is essential. An unrealistic multi-parameter model may closely fit the data but may be quite unreliable for predictions in untried situations. The advantage of independent design steps is that the modelling problem is reduced to several smaller and simpler problems and the result is more transparent. After solving these sub-problems, the framework and sub-models are integrated to form the overall model. In this contribution processes with different dynamics are worked out.

2. DESIGN METHODOLOGY

Four main sources of information are available ranging from general to specific process information: first principles, process unit conceptions, specific expertise and measurements. Physical understanding is based on basic concepts such as balances, equilibria and driving forces as well as on application concepts considering their coherence in processes. Experience is an important source of information in order to judge whether phenomena are relevant or negligible. Process data offer specific information about a process. Hybrid models enables to construct tailored process models for a required operating range, using as much information as is available.

For the development of the hybrid models, a structured modelling approach will be used. Six sequential steps are indicated in Fig. 1: process analysis, four model-design steps and finally an evaluation. From top to bottom, the level of detail increases from analysis, global design to detailed design. Analysis has its counterpart in problem evaluation, global design in model integration and detailed design in identification of the detailed models. In the process analysis phase, the model objective, model quality requirements, level of detail and the domain range are defined. In this phase also an environmental model defining the inputs and outputs will be produced. In the final evaluation phase these listed requirements have to be checked.

During the framework design, first-principles, process-type conceptions and process expertise are compiled to create a physical dynamic framework (Fig. 2) consisting of accumulation balances, known relationships as well as sub-models for the unknown relationships. This can be considered as the global design of the hybrid model. First, the key variables and the characteristic phenomena are distinguished. The key variables are the state variables or variables derived from the states. For the unknown parameters, such as reaction rates, diffusion coefficients and growth rates, fuzzy-logic based sub-models are used. In principle these are static models. Possibly, dynamics can be incorporated by using an ARX-structure. The sub-models describe the parameters as a function of the state and control variables. However, the independent variables are not always easy to define. On which state and to what extent, a certain parameter depends, can be determined by a sensitivity analysis. Finally, the sub-models and the structure of the framework can be defined. The framework structure can be represented by a data flow diagram (DFD), as will be shown for the three process examples. In the next phase the sub-models are designed. This is done in three steps: estimation of the sub-model inputs and outputs, modelling of all individual sub-models and combining them according to the framework. To identify the behaviour of the sub-models, sufficient measurements have to be obtained. The data needs to be equally distributed over a sufficiently large domain in the input space, so that all operating conditions are equally covered. Usually, the fuzzy relationships are static, and no additional dynamic data is required. This means that a limited number of

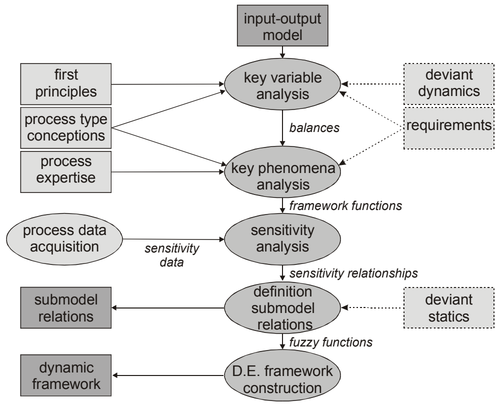

Fig. 2. Steps in framework design phase

experiments is sufficient; only steady state measurements of the process operated under different conditions need to be obtained. Since the sub-model inputs and outputs often cannot be measured directly, the modelling problem is reduced to several sub-process behaviour estimation problems. For the estimation several techniques are available, such as: PI-estimation or Kalman-filtering. For the examples, PI-estimation has been applied (van Lith *et al.*, 2001).

Fuzzy clustering provides a good way to identify the fuzzy sub-models (de Bruin and Roffel, 1996). It is an unsupervised learning algorithm and requires little a-priori model structure information. The method used is the Gustafson-Kessel clustering algorithm, which is very flexible in describing complex systems and insensitive to scaling of the data or initialisation. It is iteratively used together with Modified Compatible Cluster Merging, to merge compatible clusters that show a certain degree of conformity. The iteration is necessary because the number of clusters in the Gustafson-Kessel clustering algorithm needs to be determined beforehand, which is not always possible. The method derives a fuzzy model with independent rules directly from the data, which results in models that are not likely to show anomalous extrapolation behaviour.

Takagi Sugeno Kang (TSK) type fuzzy models are used. In TSK models, the antecedent part is similar to other fuzzy models, while the consequent part of each rule consists of a linear equation. This type of fuzzy models can be interpreted as a collection of local linear sub-models and is suitable to describe highly non-linear relationships. In addition, the model structure is simple and transparent.

The different sub-models are integrated within the framework to form the hybrid model, which describes the earlier defined environmental model as appropriately as possible. Since there may be interactions caused by this integration, an optimisation of the hybrid model may be necessary. Also errors from sub-process estimation or sub-model identification can manifest themselves in the hybrid model. In this phase, process measurements are used to weigh the sub-models in such a way that an optimal result with respect to the hybrid model output will be obtained. With TSK models, the premise part parameters determine only the operating range for which the local linear models are valid. The consequence parameters have the largest impact on the model performance. Optimisation with a gradient-based method has the advantage that it takes the initial fuzzy sub-models as a starting point and hence maintain the transparency of the model.

The next step is to analyse the hybrid model in order to determine whether the quality requirements are met. The hybrid model will be analysed with respect to steady-state and dynamic performance separately. A distinction is made between model validation within (interpolation) and outside (extrapolation) the operating area. A convenient way of visualizing interpolation and extrapolation properties is a parity plot (calculated against measured parameter values) or an error plot as a function of an independent variable. The dynamic performance can be evaluated by applying a varying input signal to the process.

3. DIFFERENT PROCESS TYPES

In this section hybrid modelling have been worked out for different types of processes: an ideally mixed, a distributed and a chained process. An overview of the approaches are listed in Table 1. The hybrid models of polymer reactor and pulp digester are derived from existing detailed simulation models. The hybrid model design and the evaluation are based on training and validation data sets derived from these simulations. The hybrid model for the batch distillation has been developed from process measurements. Table 2 shows some characteristics of the fuzzy sub-model results.

3.1 Ideally mixed process: polymer reactor

The example of the ideally mixed process is a liquid phase polymer reactor. The states of the reactor are the fraction of the monomer (x_m), hydrogen (x_{H2}), activated catalyst ($x_{c,a}$), and non-activated catalyst ($x_{c,na}$) and the jacket temperature (T_{jacket}). The volume of the reactor is constant. The requirement for the hybrid model is to describe the dynamic and static behaviour of the molecular weight distribution (MWD) and the conversion ζ. The MWD can be characterized by the chain termination probability q.

To describe the dynamics accurately, it appeared to be necessary to incorporate all balances involved. The design focuses on reducing a complex set of static relationships by overall fuzzy sub-models. The reaction rates for the chain propagation, chain termination, catalyst activation and catalyst deactivation, determine the shifts in the component balances. For these rates, fuzzy relationships are built.

Table 1 Examples for hybrid modelling.

Process	Example	Approach dynamics	Approach statics
ideally mixed	polymer CSTR	all dynamics by balances are considered	sensitivity analysis to design reduced relationships
distributed	pulp digester	maintaining PDE's, order reduction by combining of phases, components and sections by physical insight	
chained	batch distillation column	covering the essential dynamics by global dynamics	approximating of overall behaviour

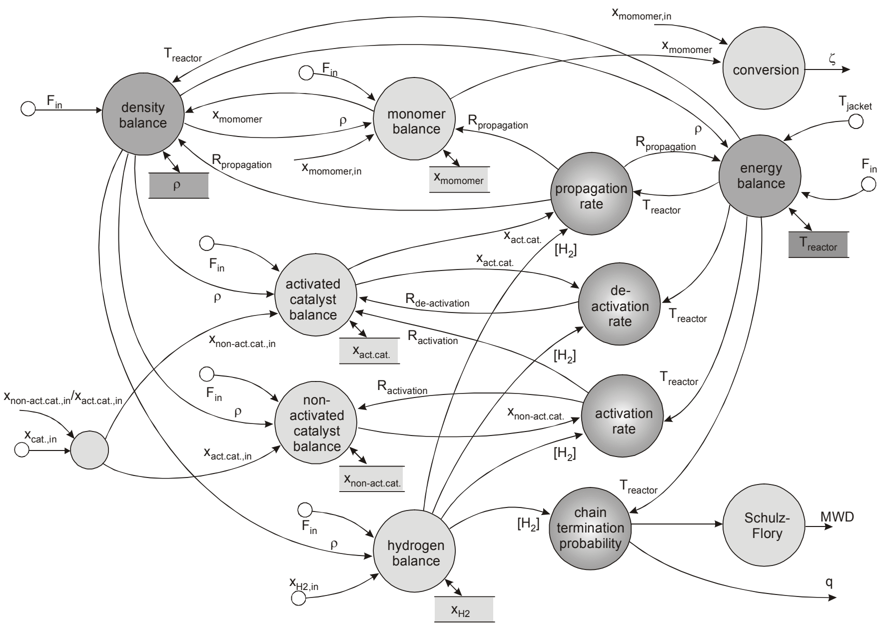

Fig. 3. Hybrid model DFD of polymer reactor.

From the sensitivity analysis, it appeared that the jacket temperature T_{jacket} and hydrogen fraction x_{H2} are the dominant influences. Therefore, in the fuzzy relationships the reaction rates are assumed to depend on those two variables and also on the related component fraction. Hereby, an overall description of the reaction rate is derived and it is not necessary to describe explicitly the adsorption rate from the monomer into the amorphous polymer phase. Fig. 3 shows the hybrid model. Several data sets with different number of data points were used to fit the model. The following conclusions could be drawn:

- The dynamic behaviour of the hybrid model is identical to the behaviour of the simulation model.
- For the static behaviour, reduction of the original model could be achieved. However, the behaviour shows deviations in some areas of the operating range for which the sensitivity is large (T_{jacket}).
- From reduced data sets it appeared, that still an accurate hybrid model could be designed, although it was more difficult to find a good set of clusters and extrapolation became less reliable.

3.2 Distributed process: pulp digester

A pulp digester has been used as an example for a distributed process. The original model is the so-called Purdue Model (Smith and Williams, 1974), which is a detailed and industrially accepted digester model. The continuous pulp digester converts wood chips into a cellulose fibre pulp by delignification by means of a hot solution of sodium hydroxide and sodium sulphide, referred to as the liquor. The digester is essentially a tubular reactor, where wood chips travel from the inlet at the top to the outlet at the bottom of the digester. The digester is divided into five functional zones: the co-current impregnation, heating and cooking zones, the counter-current washing zone and the co-current cooling zone. The actual delignification takes place in the cooking zone. The most important input of the digester variables are the wood chips flow ($\phi_{wood,in}$), the liquor flow ($\phi_{liqour,in}$) and the heat supply ($Q_{heating}$). The requirements for the hybrid model are to describe the dynamic and static behaviour of the key variables Kappa number ($\kappa\#$) and the yield (γ) according to the physical model. The $\kappa\#$ is a measure for the amount of lignin in the wood chips.

The apparent choice is to derive the hybrid model structure from the original simulation by a form of model reduction. However, it appeared to be difficult to simplify the dynamics. The wood flow rate differs from the liquor flow rate. Both flows exchange constantly components and energy. Consequently, the results of temperature and composition changes at the entrance propagate with the fastest flow and at the outlet, a transition area can be seen which duration is determined by the flow rate difference. However, flow rate changes show different dynamic behaviour. A rate change accelerates or decelerates the gradient present in the reactor and therefore influences the outlet directly. To describe the dynamics of the sections accurately, it appeared to be necessary to maintain the PDE's. Yet, it is possible to obtain a substantial reduction in the dynamics and statics. The number of column sections is reduced from 10 to 4, the free liquid and the entrapped liquid phase were combined and the number of components was reduced from 19 to 13. The chosen hybrid model structure of one section is shown in Fig. 4. The data were obtained from nine identification sets and for the validation eight sets were available. The sub-model outputs were derived from observed behaviour by PI-estimation. The hybrid model showed errors mainly caused by the model reduction. Therefore, the fuzzy sub-models were adjusted to improve the performance by optimisation. Fig. 5 shows the static result of the hybrid model for the $\kappa\#$ due to step changes in the heat supply.

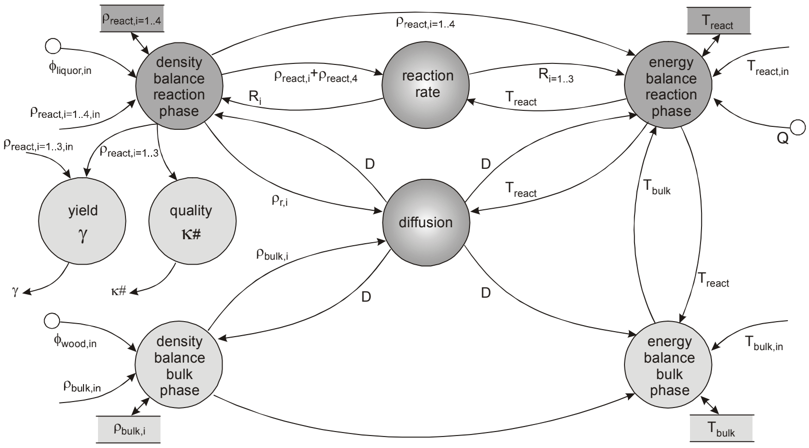

Fig. 4. Hybrid model of one section of a pulp digester. i denotes the different components.

The following general conclusions can be drawn:

- The dynamic behaviour of the hybrid model is identical to the behaviour of the simulation model.
- The static behaviour shows that with respect to interpolation, the hybrid model performs well and with respect to extrapolation the performance is limited by the quality of the fuzzy models.
- By the optimisation the error reduction in κ# is significantly for the 8 validation sets: factor 15 to 50. The error in γ was already small.
- A complete fuzzy model for κ# and γ based on a second-order ARX model with dead time compensations performed inferior in comparison to the hybrid model. This is most likely caused by a lack of dynamic training data.

3.3 Chained process: batch distillation

The example of the chained process is a batch distillation column. The objective is to develop a model that can simulate a batch run, including start-up. A batch process requires a model with a relatively large operating range, because the bottom composition shifts continuously due to exhaustion. The start-up behaviour of the model before the vapour flow reaches the condenser is not incorporated, as it is not represented by the measurements. Based on physical considerations, a model structure can be derived which correlates properties like the amount and composition in the bottom vessel and the energy input to the

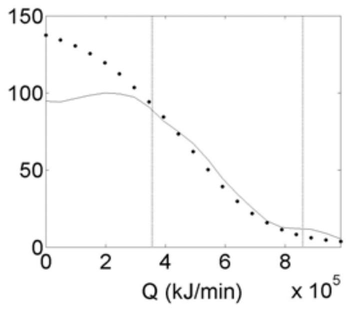

Fig. 5. Static extrapolation results for κ# as a function of $Q_{heating}$. Solid line: hybrid model. Vertical lines indicate the identification domain.

development of the vapour flow and top composition. Fuzzy logic can be used to derive the description from the observations, without the need for rigorous tray-to-tray modelling.

The framework has to consist of at least three balances describing the long-term development: the total mass balance, the component balance considering the average column composition x_{col} and the heating-up of the column. The most important input variable is the reflux fraction R^*. The output variable is the top fraction x_{n+1}. Three different hybrid models for the top composition x_{n+1} will be developed for comparison, each incorporating a different level of a priori knowledge.

I. Only long term dynamics

$$x_{n+1} = f_{\text{fuzzy}}\left(R^*, x_{col}, V\right) \tag{1}$$

II. The dynamic behaviour is incorporated by an ARX structure:

$$x_{n+1,k+1} = f_{\text{fuzzy}}\left(x_{n+1,k}, R_k^*, x_{col,k}, V_k\right) \tag{2}$$

III. The first-order overall column dynamics can be described by:

$$\frac{dx_{n+1}}{dt} = \frac{1}{\tau_{x,column}}\left(x^*_{n+1} - x_{n+1}\right) \tag{3}$$

where x^*_{n+1} is the pseudo static fraction described by a fuzzy relationship.

$$x^*_{n+1} = f_{\text{fuzzy}}\left(R^*, x_{col}, V\right) \tag{4}$$

Fig. 6 shows the structure of model III.

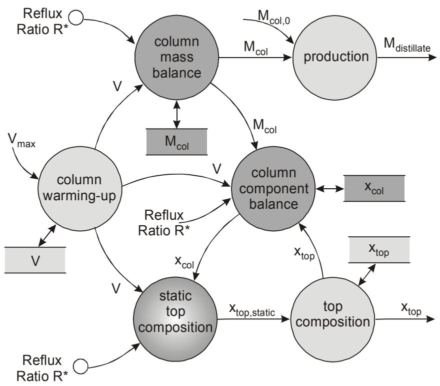

Fig. 6. Hybrid model of batch distillation column

For the identification three data sets and two validation sets were available, which all have different initial bottom amounts and compositions. For model III, the output x^*_{n+1} of Eq. 4 is estimated using a PI-estimator. During the batch, the top fraction is controlled by the reflux. To test whether the models behave like the process itself, the derived hybrid models are used to simulate batch runs using constant quality control. Fig. 7 shows the results for simulated batch runs with initial conditions taken from one of the three batch runs.

For model I the controller gain is negative. This means that in order to increase product quality, the reflux fraction R^* is decreased, which results in a production which is higher than the theoretical maximum. This behaviour is caused by the fact that model I neglects information about the dynamics of the relationship between R^* and x_{n+1}, which is characterized by the dominant time constant. Model II performs considerably better during simulation. The manipulated variable follows the measurements more closely. However, when the controller is switched on, R^* is increased and becomes temporarily larger than 1. This results in a slight inverse response in the production curve, which is not possible in practice. It was found to be caused by the fuzzy model. Model III approximates the measured production well. The dynamics of all trays can be reduced to a first-order time constant, which is a property of chained processes. This time constant is only constant when the process operates under constant quality control (Van Lith *et al*. 2003).

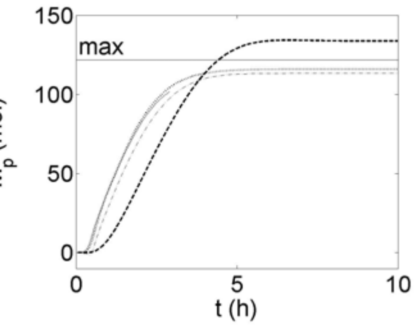

Fig. 7. Batch distillation simulations: measurements (solid line), model I (dashed), model II (dash-dot) and model III (dot).

4. CONCLUSIONS

Three examples of hybrid modelling have been worked out for typical types of process dynamics: an ideally mixed, a distributed and a chained process. Separation of the dynamics from the statics makes it possible to describe the dynamic behaviour well. For the ideally mixed process, it was necessary to incorporate all balances. For the distributed process the number of sections and phases could be reduced, but the PDE's have to be maintained. Only for chained processes a large reduction in the dynamics based on process knowledge is possible. In all examples the fuzzy sub-models are able to describe the steady state well over a large operating range.

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Table 2 Fuzzy sub-model characteristics of polymer reactor, digester and batch distillation column.
(remark: each membership function is described by 4 parameters)

dependent variables	independent variables	# membership functions	# parameters premise part	# parameters consequence part	# weighing parameters
		polymer reactor			
q	$[H_2]$, $T_{reactor}$	3	2x3x4=24	3x(2+1)=9	-
R_i	$x_{non\text{-}act.cat.}$, $[H_2]$, $T_{reactor}$	2	3x2x4=24	2x(3+1)=8	-
R_p	$x_{act.cat.}$, $[H_2]$, $T_{reactor}$	3	3x3x4=36	3x(3+1)=12	-
R_d	$x_{act.cat.}$, $[H_2]$, $T_{reactor}$	3	3x3x4=36	3x(3+1)=12	-
		pulp digester			
R_1	ρ_1, ρ_4, T_{react}	4	3x4x4=48	4x(3+1)=16	0
R_2	ρ_2, ρ_4, T_{react}	6	3x6x4=72	6x(3+1)=24	6
R_3	ρ_3, ρ_4, T_{react}	6	3x6x4=72	6x(3+1)=24	6
D	T_{react}	2	1x2x4=8	2x(1+1)=4	0
		batch distillation column			
$x_{top,static}$	R^*, V, x_{col}	3	3x3x4=36	3x(3+1)=12	-