HYBRID MODEL OF A GASIFICATION PLANT

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Abstract: In this paper, a hybrid model of a gasification unit is presented, using linear representations and a discrete events (DES) supervisor based on automata. This supervisor chooses the best linear description at the occurrence of variations of plant's operative conditions, to assure the best prediction performance. Performances of the proposed hybrid model are discussed. *Copyright © 2005 IFAC*

Keywords: Hybrid Model, DES, Automata, Petri Nets, Hybrid Automata, ANOVA.

1 INTRODUCTION

In the recent years the need to enhance the efficiency level and the profitability of oil refineries as well as the commitment to meet precise production standards call for an increasing level of system automation (Garcia and Ray, 1995; Piovoso, 2000; Seborg, 1999). Furthermore, the existence of rigorous environmental standards together with the need to operate in high safety conditions contribute to the implementation of automatic systems of rising complexity. Recently, these plants commonly comprehend also electric energy production system using TAR as the primary energy source. This add further specifications relatively to safety and quality of server.

Different plant sections and different applications levels require the implementation of different control methodologies. Typically, control applications vary from low level process control (ordinary PID or more recent non linear or intelligent controllers), to the emergency situation management (diagnosis and fault controllers), up to the high level control of the entire plant (Supervisory controllers, management control). Both "time-driven" and "event-driven" dynamics are present and this clearly implies that for a correct modelization of oil refineries, hybrid models will be required (Zhu, 1993).

In the present paper, the identification problem of a refinery unit, namely the gasification process, in order to predict reaction's products has been addressed. This work is framed in a more general project that aims to assist and, in perspective to by-pass, a human supervisor in the managing of the low-level control. In this context, the problem of model acquaintance turns out to be essential in the development of suitable controllers for the automatic set-points generation.

2 PLANT'S DESCRIPTION

The IGCC (Integrated Gasification Combined Cycle) plant is a combine in the API refinery of Ancona, dedicated to the production of electric energy using refuses of crude oil refinement (*TAR*). Combined cycle plants like the IGCC, permit the recovery of the thermo-power station dump heat, using it for the production of steam which can be employed for feeding other industrial processes. The main IGCC components are a *gas-turbine* (*GT*), specially designed for synthetic gas combustion which is cascaded with a *heat recovery steam generator* (*HRSG*), for the recycling of the thermo-power contained in the *GT* waste gases; the steam produced in this boiler is then sent to other refinery units or utilized for electric-power production after an

expansion in a steam-turbine (*ST*). To recover for possible steam lack an auxiliary boiler, the *Auxiliary Steam Generator* (ASG), has been installed.

To minimize the pollution's emissions, the thermo-power station GT is not charged with the TAR (called also *charge oil*), but with a refinery gas produced by TAR's combustion, called *syngas*. The transformation from heavy hydrocarbon to syngas is called *gasification*. The efficiency of this transformation process depends on the mixture of reaction products and their heating values. The parameter used as a quality index for the gasification plant is the *CGE* (*Cold Gas Efficiency*), given by

$$CGE = \frac{LHV_{\text{Syngas}} \cdot w_{\text{Syngas}}}{LHV_{\text{Charge Oil}} \cdot w_{\text{Charge Oil}}}$$

where *LHV* is the *Low Heating Value* and *w* stands for *weighted flow*. Assuming a fixed charge composition ($\text{LHV}_{\text{Charge Oil}}$), and flows ratio quite constant, the efficiency is maximized when gasification reaction generates products with high LHV, such as H_2 (hydrogen) and *CO* (carbon's monoxide). Consequently, a quality index of the produced syngas can be chosen as the percentage of H_2 and *CO* contained in it, with respect to others undesired substances, such as CH_4, CO_2, H_2S, *COS*. Variations in the charge oil composition have a direct impact in the outcome products composition but, as shown in the block diagram in fig. 1, many other variables may influence the system. In particular, two manipulated variables have direct effect on the quality of the output syngas, the oxygen-oil ratio (O_2/*Oil*) and the steam-oil ratio (*Steam/Oil*). Indeed, oxygen feeds the reaction, whereas steam moderates it and atomizes the TAR. Disturbances of the system are the *QW* (quench water) injection and the *SW* (soot water) emission which indirectly influence the charge oil composition.

The aim of this work is to achieve a mathematical model of the gasification process, in order to predict reaction products (i.e. H_2 and *CO*) from variables trajectories measurements that primarily influence it. This is the first necessary step for the development of controller to suitably regulate the set points for oxygen-oil ratio and steam-oil ratio, in order to maximize the CGE. Currently, O_2/*Oil* and *Steam/Oil* flows are regulated by low-level controllers supervised by operators of a DCS console. The final purpose of the whole project is then to assist the operator and, in perspective, to free him from supervision tasks by means of a supervisor for these low-level controllers.

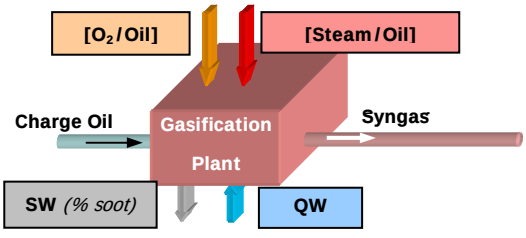

Fig. 1. Gasification Plant.

3 ASYM IDENTIFICATION OF THE MIMO INDUSTRIAL PROCESS

Many different approaches to the identification of the plant are possible. The choice made is to use a *black box* approach. This is motivated by the complexity of the outcoming model in terms of number of equations and parameters involved. Furthermore in the API refinery previous experience with simulators based on chemistry, kinetics and thermodynamics description of the plant, did not provide with satisfactory performances.

As usual for complex plant, the main problem to solve was the impossibility of making an identification experiment on the plant, such as a staircase experiment, a white noise or PRBS (*Pseudo Random Binary Sequence*) experiment (Zhu, 1993), on account of economic and safety reasons. The presence of an *on-line analyzer* of the outcome of the gasification plant, allowed to achieve historical series of the quality parameters that had to be predicted (H_2, *CO* that is, ultimately, *CGE*). Available data were the historical series of the plant (sampling time T_S = 5 minutes), with low signal to noise ratio, with limited spectrum and with a lot of spikes due to on-line analyzer calibrations. Hence, it was necessary to consider data taken over very long test time lag, while, in order to handle for the spikes presence, a supervised logical filtering function was implemented.

A linear dynamical model has been adopted to describe the system according to the fact that the process is regulated at given setpoints during the epochs of data collections for the identifications.
A ASYM (Zhu, 1993, Zhu, 1995, Zhu, 2001), identification method has been developed, which is an extension of ARX, ARMAX, Box Jenkins, traditional identification techniques. ASYM (or *two steps*), founded on Ljung asymptotic theory (Ljung, 1987) for MIMO processes, resulted particularly suitable for our purposes since it's focused on processes in refinery and oil industries, which can be characterized as continuous processes, with large scale and complexity, dominant slow dynamics, high and slow varying disturbances and local nonlinearities (Zhu, 1995). The advantages of this method if compared to others traditional identification methods is that it offers a procedural way to solve the problems of input design, model structure and order selection, numeric convergence and quantification of model errors, both in time's and in frequency's domains (Zhu, 1993).

Distributed parameter systems or, equivalently, infinite dimensional systems, are often required to mathematically describe many industrial processes. According to the asymptotic theory of Ljung it can be stated that it is natural to let the model order *n* depend on the number of observed data samples, $n = n(N)$. Typically, in order to have a model set large enough to contain the *"true transfer function"*

of an industrial process (or, equivalently, to give an approximation of the true dynamics), it will be allowed the order *n* to increase with the number of data samples *N* provided it is kept small compared to *N*. For the identifiability of increasingly higher order models, the process input is required to be persistently exciting with sufficient high order (Ljung, 1987, Zhu, 1993).

The asymptotic theory results guarantee the consistence of model estimates and transfer functions error with Gaussian distribution at each frequency. The result is independent from the model structure as the order is allowed to increase with the number of data points (experiment duration time), (Zhu, 1993). Assuming the cross spectrum $\Phi_{u\xi}(\omega)$ between *u(t)* and *ξ(t)* to be null (i.e. open-loop assumption), the asymptotic variance of the process model can be approximated as follows:

$$\mathrm{Var}\left[\hat{G}_N^n\left(e^{j\omega}\right)\right] \approx \frac{n}{N}\cdot\frac{\Phi_v(\omega)}{\Phi_u(\omega)} \qquad (1)$$

Equation (1) states that the variance of the model transfer function *at a given frequency* is proportional to the (output) noise-to-signal ratio, and to ratio of the model order to the number of data samples.

3.1 The Identification Method

The adopted approach consisted in starting with a high order model estimation followed by a suitable model reduction so to arrive at more compact and fruitful models avoiding numerical problems. As asymptotic properties of the transfer function estimates are independent of the model structures (Zhu, 1993), a model structure simple as possible for the high order model (equation error models, such as ARX) has been adopted. This ensured analytical solution, a global minimum for all *n* and *N* and consistent and efficient estimates, if residuals could be proven to be Gaussian, zero mean white noise (Ljung, 1987).

The main steps of the identification procedures in a SISO case can summarized as follow:

STEP 1. High order model estimation

Estimate a high order *($n \approx 30$)* equation error model;

STEP 2. Model reduction

The model that results from Step 1 is often over-parameterized. Since the variance is proportional to the order *n*, model reduction can reduce the variance, if it is properly performed. The asymptotic theory shows that, in the frequency domain, the high order model follows approximately a Gaussian distribution with the variance given by (1). Regarding the frequency response of the high order estimates as the *noisy observations of the true transfer function*, then the maximum likelihood principle can be applied. Since the high order model (observation) follows a Gaussian distribution, the reduced model is consequently assumed to be an asymptotic maximum likelihood estimate; this will lead to an asymptotically efficient (minimum variance) estimate of the frequency response. Solving this problem calls for a non-linear minimization algorithm, such as an output error identification method.

The first step is to collect the external inputs that have been used in the identification experiment, and filter them by the inverse of the disturbance model. Then, simulation of the high order model using a filtered input is necessary to finally obtain the new input/output data. The parameters of the reduced model are calculated by using an *output error method* (Ljung, 1987; Zhu, 1993). Similarly it can be operated on the estimate of the disturbance model of the high order. Thus, the reduced process model and the reduced disturbance model are easily computed. The final model has a Box-Jenkins structure.

STEP 3. Deriving an upper bound modelling errors

Errors of the high order model follow asymptotically a normal distribution with variance given by (1). Therefore a $3\cdot\sigma$ upper bound of the errors of the high order model can be defined and used for the reduced model G^l, since model reduction will reduce the model error (Zhu, 1993). Thus the following can be stated:

$$\left|G^o\left(e^{j\omega}\right) - \hat{G}^l\left(e^{j\omega}\right)\right| \le 3\cdot\sqrt{\frac{n}{N}\cdot\frac{\hat{\Phi}_v(\omega)}{\Phi_u(\omega)}} \text{ w.p. 99.9 \%} \quad (2)$$

where $\hat{\Phi}_v(\omega)$ can be estimated by step 1 calculations and $\Phi_u(\omega)$ can be calculated from the measurement.

3.2 The MIMO Identification Method

In order to be applied to the problem of interest in the actual work, a suitable extension of the identification technique described in the previous so to pertain to MIMO systems is needed. Further details of the identification method for MIMO processes, not reported here for sake of simplicity, can be found in (Zhu, 1993).

3.3 Validation

Although a non-linear minimization algorithm is necessary for the computation of the reduced model, the adopted solution has to be preferred to the use of a minimum prediction error method. First, the influence of the disturbance is reduced greatly when using the data from the simulation of the high order model, instead of the original data. Secondly, poor local minima are detected. In facts, if the minimization algorithm converges to the global minimum, the frequency response of the reduced model should lie in the middle of the fluctuating frequency response of the high order model due to the smoothing effect of model reduction. If this is not

the case, a local minimum is detected and in order to avoid the problem, a different initial estimate is assigned and the minimization algorithm restarted.

For model validation many criteria based on different index such as FPE, AIC, MDL, the variance of the error, or whiteness test of residuals, can be found in literature. Nevertheless, these criteria not perfectly apply to the ASYM method which is not based on the research of the true order of the process but instead, it searches for an order so that the best frequency response estimate can be obtained.

The idea is to build an Asymptotic Criterion (ASYC) index as follows: if the reduced model is allowed to deviate from the high order model the same amount as the error of high order model (measured by its variance), there are reasonable chances that the reduced model is most close to the true frequency response. Based on this observation, the ASYM method of validation (Zhu, 1995; Zhu, 2001) suggests to choose the order such that the difference between the high order model and the reduced model (in the frequency domain) approximately equals the variance of the high order model. The same idea can be applied for determining the order of the disturbance model. It is important to remark that, in this method, the selected order is usefully related to the noise-to-signal ratio, and so to the experiment time. For a given process, if the noise level is high and the experiment time is short, the selected order of the reduced model will be low. For the same process, the selected order will increase if the power of the test signal and/or the experiment time increases.

Error Bound Matrices

A method of grading the models (Zhu, 1995) has been implemented: this is done by comparing the relative size of the bound with the model over the low and middle frequencies.

Some Problems

The introduction of the ASYC index and the use of the error bound matrices were not sufficient to solve the problems at the validation stage. In particular, all the criteria above were more or less satisfied with different order models, made with different training data, and there was not significant differences in the one-step predictions. Nevertheless, if the prediction horizon was increased, the differences between two different order models (and also between different training epochs) became important. This produced two main problems, that is the difficulties to detect the best model and the difficulties to establish if the performance deterioration in different epoch derived from an incorrect choice of the model, or from external causes, such as an alteration in charge oil composition (that is in changed operative condition). Statistical tests for the hypothesis verification were thus adopted, in particular Analysis Of Variance tests (ANOVA). ANOVA test had fixed the best model for each training epoch, and the models found had not the same order. Thus it was concluded that in the various epochs dynamics had really changed, as a result of variations of charge-oil composition.

With the historical series at disposal, three regions have been singled out, with three different compositions of TAR, in terms of sulphur's percentage and carbon-hydrogen ratio. Three optimal models, with three different orders represent the system were built.

4 HYBRID MODEL

In order to assure the best prediction performance a supervisor system that enforce a switching behavior between the estimated models at the occurrence of variations of plant's operative conditions has been developed. The adopted approach involve the theory of *discrete event systems* (DES) oriented to the generation of a *hybrid model*.

In recent years, a variety of models have been introduced for hybrid systems (Koutsoukos, *et al.* 1998; Lemmon *et al.*, 1999; Stiver, *et al.*, 1996). These models generally describe the continuous part of the system by a set of ordinary differential equations and represent the discrete part of the system by a discrete-event system. The discrete-event model which has been most widely used in the past is the finite automaton. Finite automata provide a particularly convenient method for hybrid system modeling. In spite of this success, however, there are some significant limitations in using finite automata in the modeling, analysis and synthesis of hybrid control systems. The main limitation concerns the complexity of such automata when used to design control supervisors, and particularly when used to model concurrent processes. Concurrent systems are systems in which several subsystems are operating at the same time. The problem here is that the state space for a finite automaton representing the various discrete operational states that a network of concurrent systems can generate will grow non linearly with the number of processes. This means that automata based methods for hybrid modeling have an intrinsic limitation when dealing with highly concurrent processes.

In this paper, a representation of a DES in terms of rectangular hybrid automata is adopted. In order to solve problems related to the realization of a supervisor containing many concurrent processes an innovative approach developed by the authors, has been followed. The method, not presented in this contest, consisted in considering the model in term of a particular class of Petri nets (Reisig, 1985), *finite state machine*, thus allowing to limit the dimension explosion of the state-space representation. In fact, the capability of obtaining composition rules in a closed form, typical of automata, is joined to the high efficiency, in dimensional terms, of Petri nets (Barboni, 2002)

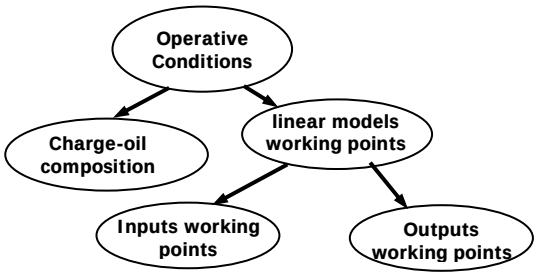

Fig. 2. Operative conditions acting in the process

5 SUPERVISOR'S MODEL WITH AUTOMATA

From the validation process described in the previous, it has been concluded that one single model was not sufficient to assure good predictions, especially in the case of large prediction horizons. Three elementary operative conditions, or *specifications* were identified, charge charge-oil composition been obviously one (see fig. 2). The other *operative conditions* which could affect the choice of the best model for the plant were discovered during validation. In particular, since linear models were used, it was important to take into account the *working points* ***(****inpust* and *ouputs****)*** around which these models were identified.

For each elementary *specification*, an automaton was built to determine the more suitable model responding to events generated by variations of the variables related to the considered specification. In particular, to every state of each automata was associated, as output, a model, and switching between the various states (models) was performed at the occurrence of events springing by variations of the considered operative condition. In this way, partial descriptions of the entire system are obtained, represented by each single hybrid automata generated. Then, the single automaton were combined by parallel composition to obtain the whole supervisor (Cassandras and. Lafortune, 1999).

5.1 The Hybrid automata construction

The construction of a single automaton which models the system behavior with respect to charge-oil's data is described in the following. To build a hybrid automaton (Lemmon, *et al*. 1999; Kopke, 1996; Henzinger, 1997) its *graph*, *invariants*, *initial conditions*, *activity rectangles*, *guard equations* and *events* must be defined. The continuous state space must be quantized in order to generate the discrete state: this procedure is equivalent to realize that part of the interface which is usually called *generator* (or *quantizer*) (Lunze, et al.2001). From the analysis of charge-oil's composition, three working regions were recognized, corresponding to three different C/H ratios and sulphur percentages, and a suitable model was built for each region. Every state will have the corresponding model as invariant; initial conditions will be given by the vector (of the same length of the

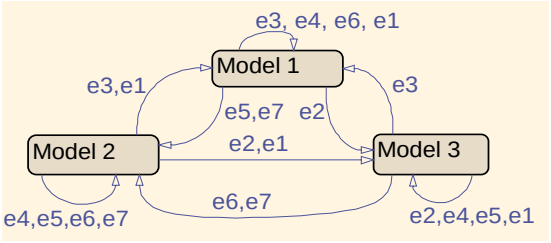

Fig. 3. Non-deterministic automaton for the specifications of charge-oil's.

memory of the system) of the last values assumed by the continuous state *in the discrete state preceding the actual state*. The activity rectangles correspond to the intervals in table 1: note that activity rectangles of the three states overlap. Guard equations are reported in table 2.

Table 1 Invariants definition

Invariants	Model
$3.8 \le S \le 4.5$ $8.54 \le C/H \le 9.35$	$\mathcal{M}_1$
$3.8 \le S \le 4.5$ $8.88 \le C/H \le 10.20$	$\mathcal{M}_2$
$4.5 < S \le 5.2$ $8.88 \le C/H \le 10.20$	$\mathcal{M}_3$

Table 2 Guard Equations

Guard Equations	event
$(8.54 < C/H \le 8.88) \wedge (4.6 < S \le 5.2)$	e_1
$(8.88 < C/H \le 10.2) \wedge (4.6 < S \le 5.2)$	e_2
$(8.54 < C/H \le 8.88) \wedge (3.8 < S \le 4.6)$	e_3
$(8.88 < C/H \le 9.35) \wedge (4.4 < S \le 4.6$	e_4
$(9.35 < C/H \le 10.2) \wedge (4.4 < S \le 4.6)$	e_5
$(8.88 < C/H \le 9.35) \wedge (3.8 < S \le 4.4$	e_6
$(9.35 < C/H \le 10.2) \wedge (3.8 < S \le 4.4)$	e_7

What is obtained from the previous process is a non-deterministic automaton which is depicted in fig. 3.

Operating in a similar manner, the automaton that consider the working points of the two inputs (O_2*/Oil* and *Steam/Oil*) have been constructed. To define the activity rectangles, a function of mean value and standard deviation of the signal used for identification has been adopted. Finally, two more automata were constructed to account for the specification of the output working points (here not reported).

Since, as it can be easily verified in fig. 3, the computed automata were not deterministic, before proceeding further standard procedure for the construction of the observer has been applied (see for ex. Cassandras and Lafortune, 1999).

5.2 Automata composition

The final composition of the observer automata, resulted in a *"shuffle"* this implying the final state space dimension to be given exactly by the dimension of the Cartesian product of the state spaces of each single component. To overcome to this significant growth of state space dimension, a particular class of Petri nets (*finite state machine*)

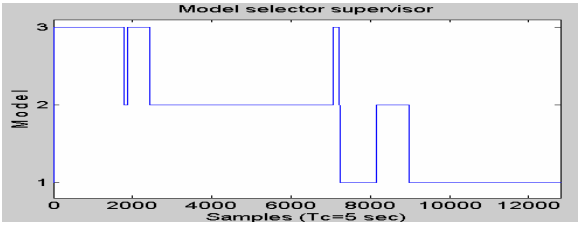

Fig. 4. Output of the model selector supervisor

was used and a representation of a DES alternative to finite state automata is provided. This allow the realization of a supervisor containing many concurrent processes, without letting the dimension of the state-space representation grow up excessively. In this approach, the capability to obtain composition rules in a closed form, typical of automata, is joined to the high efficiency, in terms of dimension, of Petri nets.

5.3 Supervisor for model selection.

In each single developed automaton, outputs values were in a bi-univocal dependence with the automaton states: each state was, de facto representing a single model. As a result of the observer computation and the final automata composition, the output function was not anymore always univocally defined. In most states, a simple heuristic based on the assignment of probabilistic weights to each model could be applied which assured the output of the supervisor (i.e. the best model) to be univocally defined. In few other cases, two or three model could fit in the same manner. In order to solve this problem, a more complex heuristics was determined which assigned weights to the output function of each automaton, according to an empirical hierarchy of "importance" of the phenomena they represent.

Finally, a further improvement of the system was made in order to avoid chattering phenomena observed in the first experimental tests. More specifically, the generation of the events of the automaton was no longer based on punctual values of the inputs and the outputs of the plant, but it has been modified by the introduction of a sort of "memory".

This outputs of the model supervisor are depicted in fig. 4, where values 1, 2, 3 on the vertical axis refer to the choice of the respective model as representative of the system in the current operative conditions.

6 CONCLUSION

The aim of this paper was to achieve a mathematical model of the gasification plant of API refinery's IGCC station. Processes identification was required in order to perform prediction on system performances and, as final future goal, to design a suitable controller to optimize cold gas efficiency.

For the identification and the validation processes data over sufficiently large epoch were avialable. The computed models have been tested on data different than the ones used for the identification but relative to the same epoch. These models have shown to be capable to predict the characteristics of the considered reaction products in a satisfactory way keeping the average prediction error lower than 2% in the case of 50 minutes prediction (10 step ahead), and lower than 7 % in the case of about 6 six hours predictions.

From an operative point of view, results in terms of prediction capability are very positive, also with large prediction horizon, validating the black-box identification approach as a valuable tool in the modelization of multivariable industrial processes. The actual validation of the adopted approach requires to test the system in condition different from that of the identification phase. This will be the next necessary step of the present research.

From a methodological point of view it can be stated that the need of a hybrid model is confirmed, since best performances are guaranteed using more than one model. Once the validation phase will be completed, the result achieved in term of plant identification should finally be applied for a synthesis of a controller to optimize the CGE of the plant.

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