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INDUSTRIAL CHALLENGES IN MODELING OF PROCESSES AND MODEL REDUCTION

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Abstract: Currently a shift of focus towards 6-sigma quality and market responsive operation has been initiated in the chemical processing industries. The fast evolution of products and processes enforced by fierce global competition and by tightening legislation are major forces for new application development approaches and for new technologies. The need of high performance non-linear model based control, optimization, monitoring and soft sensing applications and the cost driven necessity of re-use of models and results of earlier engineering effort will be explained to be the drivers for the current and future industrial challenges in (hybrid) modelling and system identification. These market developments require more extensive application of (non-linear) rigorous models extended with empirical model components to achieve the model accuracy requirements, the coverage of wide process operating ranges and minimization of engineering costs, which cannot be attained by application of pure black box modelling approaches. Besides the techniques applied for hybrid modelling and parameter estimation, the paper also discusses the techniques needed for model reduction, model tracking and state estimation to make the high performance model based applications work properly. An overview with some results is given of the techniques applied and tested in our current R&D industrial pilot projects.

Keywords: Model reduction, Process Control, Model Based Control, Industrial Automation, Plantwide Optimization, Chemical Processing Industry, Process Operations, Manufacturing Execution Systems

1. INTRODUCTION

Over the past decades processing industries have been facing significant changes, both in the marketplace as well as in society. The marketplace has turned from a quasi-infinite market, with only limited and mostly local competition in the 1970s, to an almost completely saturated and extremely competitive global world market at present. Society has become well aware of the limitations of our earth's ecosphere in handling the effects of our rapid consumption of fossil fuel reserves and large growth of emissions. Industries are confronted today with ever tightening legislation with respect to the environmental impact of their production, the use of natural resources, and the disposal or recycling of their products. They are getting full responsibility for all future effects of their production processes as well as of their products and by-products on people and environment. Hence, industries have to move towards a competitive and sustainable production on demand at tight operating constraints as well as product quality and variability specifications in order to cope with these changes.

To get a clear understanding of the problems process industry is facing, an analysis needs to be made of the way processes are operated today in comparison with market demand and market opportunities (Backx et al, 2000; Pantelides et al. 2004; Britt et al., 2004).
At present the Chemical Processing Industries are still largely operating their production facilities in a supply driven mode of operation. This implies that no direct link exists in most companies between actual market demand and actual production. Products are to a large extent produced cyclically in fixed sequences. Delivery of orders is mostly handled from stock of finished products or from intermediates that only require finishing.

The highly competitive market on the contrary imposes a strong need for flexibility with respect to the production of a broad variety of product types and grades at time-varying capacities. Good prices can only be made during those time periods where a product is asked for in the market. Hence, production capacity and product quality must become predictably controlled to enable and support market driven marketing and sales. On-time delivery of the right product at the right quality at a competitive price at the right location must be guaranteed as a minimum. Despite the need for high flexibility, delivery on demand has to be achieved by the industries without building up large stock volumes of intermediates or products. In addition price pressure enforces producers to process a broad variety of market available feedstock materials and utilities at loosely specified properties for producing products at tight -6-sigma- quality specifications.

Examples from two different industries are presented next in order to illustrate the trends. Supply of polymer products to the automotive industries is taken as a first example. Currently, most of the polymer suppliers work with yearly renewable, preferred supplier type contracts. These contracts settle the base prices as a function of the ultimately requested volume of delivered product. Detailed orders for specific deliveries are placed up to just a few weeks before the requested moment of delivery. Significant penalties are agreed upon for late or off-spec deliveries.
Considering the broad range of polymer grades requested by the market, flexibility in manufacturing and tight quality control are absolute requirements for polymer suppliers to stay in business. Capital productivity and hence economic success highly depend on their manufacturing flexibility.

A second example is taken from the oil refining industries. Tightening legislation on fuels and permitted exhaust gas composition has resulted in more detailed and tighter fuel composition specifications. Consequently, complexity of fuel manufacturing has been increasing. At the same time, legislation on waste reduction and market pressure has forced refineries to further process heavy residues. Since crude feedstock quality is slowly degrading over time, high quality feedstock prices are increasing rapidly. Consequently, cheaper feedstock materials of lower and diverse quality are going into the market. Feedstock switch frequency is increasing to exploit economic opportunities in processing low priced raw materials. Economic performance of refineries is depending more and more on their flexibility to being able to handle and quickly change-over between a wide range of feedstock materials driven by availability, price and opportunities to meet delivery at market demand. Operating point switching facilitates the processing of a variety of feedstocks to minimize raw material cost, the processing of heavy residues to reduce waste streams, and the production of the right product qualities on demand. Capital productivity is continuously driven to its maximum by pushing total throughput despite of continuously varying operating conditions.

The examples clearly demonstrate the need to enable production plants to be operated in a deliberately dynamic mode, covering feasible, wide operating ranges. Today many companies produce products at lowest possible costs in a lean operation with minimum overhead costs and no significant investments in upgrade of operation support technologies that focus on market driven production and innovation. Longer term these enterprises will experience that the average residence time of products in their warehouses will be long in comparison with the average residence time of products in warehouses of companies that have strongly invested in directly linking production to market demand and innovation. Margins will continuously be under extreme pressure for a significant part of the volume produced due to market saturation effects and due to mismatch between market demand and supply from stored products. The average capital turnaround cycle time will remain poor, despite a limitation of the number of grades produced per plant. This will continue putting pressure on the ultimate business results of these companies.
Only those enterprises will be successful in the longer run, which will be able to exploit opportunities by quickly adapting to market dynamics. Critical issues are flexibility with respect to volume, type and grade of products, transition time and cost, predictability of production, reproducibility of transitions and tight quality control. Consequently, manufacturing will have to move from largely steady-state operation to an intentionally dynamic operation of the plant (Koolen, 1994; Backx et al., 1998). Companies that have invested in flexible and innovative operation are the ones that are setting the scene for turning around the way of working in the Chemical Processing Industries (CEFIC, 2004-1,2). These companies are doing the same as the ultimately successful companies in the Consumer Electronics and Automotive Industries did 20-30 years earlier: Operate production directly driven by market demand to the extent feasible. Companies doing so now are facing tough times however, as their total production costs, due to their focus on flexibility and innovation, initially appear to be higher. They have to make significant investments in adapting their operations, production and internal organisation to enable the flexible operation. Ultimately, these companies will see their overall performance rapidly improve due to the increase of capital turnaround, the better margins related to improved flexibility, their ability to better adapt to changing market conditions and their capability to timely deliver at (changing) specifications and varying volumes of product demand. A significant

improvement of economic performance results when the response of production to orders received is coupled directly. This of course requires predictable performance in manufacturing. Focussing operations on enabling market driven operation of processes opens up the opportunity for best economic performance. It ultimately ensures that production of ordered products starts after orders have been received and that the products are delivered to customers immediately after production so enabling shortest possible capital turnaround and significantly improved capital productivity.

Innovation in future process technologies must in the first place aim at a high degree of adaptability of manufacturing to fluctuations in market demand covering operations as well as process and equipment design. The constraints imposed upon production result in increasing complexity of processes and of their operations. More sophisticated, model based operation support systems will be required to exploit freedom available in process operation (Backx et al., 1998).

2. MODELING REQUIREMENTS IN THE CONTEXT OF MARKET DRIVEN PROCESS OPERATIONS

Two challenges have to be faced in order to move towards intentional dynamic and supply chain conscious market driven plant operation:

- Fully integrated technologies are needed that make transparent operation of plants and their processes as part of supply chains feasible to enable the implementation of dynamic operation in industrial practice. In addition also a significant change in the culture of operators and plant management will be required. Dynamics has to be accepted as a further opportunity for performance improvement rather than considered as a strange, undesired and even dangerous phenomenon outside the scope of normal process operations.
- In addition, built up knowledge of processes and plants has to be condensed preferably in re-usable, well documented, generally applicable so called Reference Models, which are continuously updated and refined to reflect state-of-the-art understanding of plant and process behaviour (Foss, et al., 1998; Pantelides, 2003). These reference models at their turn may form the basis for highly automated updating of applied model based (dynamic) optimisation systems, (non-) linear control systems, process monitoring systems, soft sensing systems, etc. In these systems information on operational objectives and manufacturing status must be transparent at all levels of the automation hierarchy, since the operators will ultimately become the proprietors of the process (Clark, et al. 1995; Han, et al., 1995). Instead of merely executing process operation tasks targeting at process variables, operators will move towards making productivity decisions on the basis of real-time business variables derived from actual and model based process measurements and enterprise policy.

Market driven process operation puts extremely high requirements on predictability and reproducibility in process operation. One needs to be able to produce products at adjustable specifications in predefined, tight time slots and in changing volumes. Flexibility and timing are key parameters that drive performance. Technologies that support such process operation have to provide the functionality to operate processes this way.

The problems faced by process industries to turnover production control from supply driven process operation to market driven process operation may be summarized by the following problem statement:

Given an industrial scale production plant that forms one link in a supply chain, provide the model based technologies for this plant that:

- *Enable flexible, dynamic operation of the plant in such a way that imposed operating constraints related to safety, ecology, plant lifetime and plant economics are always satisfied*
- *Support continuous improvement of the plant and its operations to drive the plant towards conditions that comply with supply chain optimum operation within a pre-defined, feasible operating envelope for the plant*
- *Operate the plant in accordance with process conditions that push for maximization of capital productivity of the company the plant belongs to.*
- *Exploit freedom in plant operation to maximize capital productivity of the plant over plant lifetime*

Assuming that best performance is achieved, if plants are operated in an anticipative way by exploiting detailed knowledge of dynamic behaviour of the plants, this problem definition clearly links to the following set of sub-problems related to modelling and model reduction (cf. fig. 2.1):

- Enable fast and accurate modelling of application relevant dynamic process behaviour using detailed knowledge of processing equipment, materials and chemistry (Marquardt, 1995; Pantelides, 2003): apply *Reference Models* to make cost effective and market responsive, innovative operation feasible
- Extract application relevant information for various model based applications (e.g. model based optimisers, model based control systems, model based soft sensors, model based monitoring systems, model based research and development of processes and equipment, …) in fast and robustly computing approximate models in a highly automated way: enable development of *Reduced Models* that robustly and accurately reflect relevant system characteristics.

- Realize continuous improvement of knowledge of processing equipment, materials and chemistry stored in *Libraries*. These libraries have to contain model building components that represent the state-of-the-art of the knowledge that should be applied throughout the company for R&D, Design, Process & Systems Engineering, Monitoring, Maintenance and Operations.
- Create model adaptation mechanisms that enable closed loop adjustment of specific approximate model parts to overcome remaining inaccuracies and imperfections of the applied reduced complexity, approximate models.

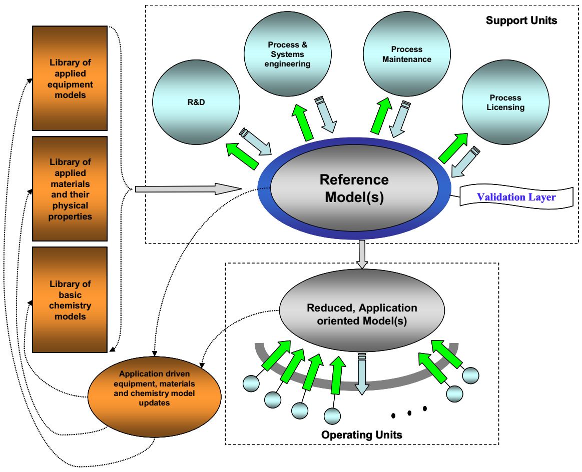

Fig. 2.1 The Reference Model concept

The model based applications have to use all freedom available in plant operation for continuously driving the plant to the operating conditions that best comply with a selected balance of most of the time mutually conflicting objectives.

3. STATE-OF-THE-ART IN MODELLING AND MODEL REDUCTION

Model based applications require the models to satisfy very specific properties. The specific requirements imposed depend on the application. Most of the literature on modelling and model reduction is related to specific applications discussed. No structuring of modelling and model reduction techniques has been discussed in literature yet.
Two types of modelling approaches are applied in the (petro-)chemical processing industry for the development of model based applications:

– Empirical modelling (black box modelling)
– First principles based modelling

Empirical modelling techniques are the techniques that are applied extensively in industry for the development of model predictive control systems, inferential control systems and soft sensors. The process identification techniques applied for empirical modelling have been given broad research attention the past two decades in a predominantly linear model context covering model structure (Ho et al., 1966; Willems, 1986, 1987; Ljung, 1987; Backx et al., 1992), parameter estimation (Åström et al., 1971; Eykhoff, 1974; Richalet et al., 1978; Ljung, 1987; Söderström et al., 1989; Heuberger, 1990; Verhaegen et al., 1992; Van Overschee et al., 1993; Zhu et al., 1993; Falkus, 1994; Van den Hof et al., 1994; Van Overschee, 1995; De Vries et al., 1998), model reduction (Ho et al., 1966; Zeiger et al., 1974; Moore, 1981; Pernebo et al., 1982; Backx, 1987; Heuberger, 1990), closed loop identification (Forssell et al., 2000; Van Donkelaar et al., 2000; Zhu, 2003) and parametrization and estimation of model uncertainty (Ljung, 1987; Zhu, 1991; Falkus, 1994; Hakvoort, 1994; Van den Hof et al., 1994; De Vries, 1994; Reinelt, et al. 2002). Process identification techniques focus on accurate modelling of process dynamics, which are relevant for process control. The techniques applied –model parameter estimation on the basis of input-output process data generated by persistent excitation of process inputs during sufficiently long time- result in models that have both good observability and good controllability. The models obtained reflect the approximated linear dynamic behaviour of the processes observed during the data generation. The models are valid for the operating window covered during testing, but in general cannot be applied reliably for operating conditions, which have not been covered during testing.
First principles based modelling techniques apply basic physical/chemical/biological laws and mechanisms –mass balances, energy balances, momentum balances extended with constitutive equations- to construct models. As the models are based on basic laws, they have wide range validity in general. A main problem in creating models that accurately reflect actual process behaviour is stemming from the fact that no direct process information is used to select the mechanisms included in the models. Especially accurate modelling of process chemistry appears difficult due to inaccurate knowledge of main reaction complexes and reaction kinetics. Physics related process behaviour of applied equipment can be modelled accurately in general by application of the conservation laws. Accurate modelling of physical properties of materials mostly results in complex models with much redundancy. Model inaccuracies always remain due to inaccurately known physical properties, reaction complexes and reaction kinetics. Models resulting from first principles modelling therefore always will require adaptation to align them with actually observed process behaviour (Briesen et al., 2000). This implies that adjustments of the models based upon actual process measurements are a necessity to assure that the applied models reflect actual process behaviour. The actual model accuracy and model content requirements are a function of the specific application of the models: Model based research and development, model based (dynamic) optimization, model predictive control, inferential control, model based soft sensing, model based process monitoring, process performance analysis ….

The requirements involve the range of dynamics covered (time scale), the operating range covered, specific process mechanisms covered and model components applied for model adaptation.

State-of-the-art model reduction techniques in general focus on two main requirements imposed on the reduced model:

– Extraction of model behaviour relevant for the application (relevant range of dynamics, applied operating window)
– Reduction of model complexity to enable faster simulations (relevant process mechanisms, restriction to the actual operating window, approximate modelling)

In general closed loop applications impose restrictions on the range of dynamics covered by the reduced model, the operating window covered and the condition number of the reduced model. Due to limitations in the range of dynamics, accuracy and reproducibility of actuators and sensors only two decades of dynamics can be handled in most industrial model predictive control applications. As model predictive control systems predominantly are focussing on disturbance rejection (time varying) linear models can be applied for actual control in general. This also applies for model based control systems for transition control and batch control. In addition the models applied in model predictive control and closed loop optimization applications may not contain too small gain directions. If a model would contain very small gain components, the controller or optimizer would directly use these directions for achieving its objectives by generating large input amplitudes in these small gain directions. Even small model inaccuracies in these directions result in very poor controller or optimizer performance due to the large input amplitudes applied in not exactly right directions.

Similar requirements apply for soft sensing, inferential control and observer applications to achieve robust performance (Marquardt, 2001; Antoulas, 2005).

4. INITIAL STRUCTURING OF THE MODEL REDUCTION TECHNIQUES

In order to support minimum effort design and maintenance of model based applications in chemical processing, the reference model concept may be applied. This concept assumes that a reference model is developed and maintained that reflects all process knowledge available from R&D, process and systems engineering, process operations, process control and optimization. The reference model reflects all relevant process knowledge available at any time first principles based, if necessary extended with empirical model components. The reference model only approximates actual process behaviour. Therefore it always will be inaccurate to some extend and on-line adaptation of the derived model on the basis of measured process behaviour will be necessary.

The reference model will become too complex on the other hand for most applications as it will be based on rather generic library components that reflect knowledge obtained from a wide range of research, development, design, monitoring, maintenance and operation activities. Model approximation and model reduction techniques are required to extract the relevant behaviour for specific applications in sub-models. To derive approximate models that match the needs, specific model reduction and model approximation procedures need to be developed for this purpose. Such model reduction procedures do not exist yet. The EC funded 6th Framework Program Marie-Curie Training Network project PROMATCH focuses on the development of these techniques. To enable appropriate model reduction aiming at approximate initial process models that reflect all application relevant process dynamics with minimum complexity, a procedure will be elaborated on based on a selection of the following categorized techniques:

– Selection of main process mechanisms in a well balanced way by application of physical/chemical model reduction (Tatrai, et al. 1994; Androulakis, 2000; Vora et al., 2001; Petzold et al., 1999; Briesen et al., 2000; Maas et al., 1992; Ganguly et al., 1993).
– Selection of relevant operating windows and relevant dynamics by using projection methods (Inertial methods, Galerkin projection methods, Proper Orthogonal Decomposition methods) and Krylov subspace methods (Armaou et al., 2001; Rathinam et al., 2003; Adrover, et al. 2002; Kunisch et al., 2002; Shvartsman, et al. 2000; Novo, et al. 2001; Garcia-Archilla, et al. 1999; Bai, 2002; Jaimoukha, 1997; Heres, 2005)
– Reduction of the model complexity by non-linear model reduction (Löffler et al., 1991; Lohmann, 1995; Lall, et al. 2002; Mossayebi, et al. 1992; Desrochers et al., 1980)
– Selection of relevant process dynamics by application of numerical reduction methods (Baldea et al., 2006; Lee, et al. 2000; Carpanzano, 2000; Kumar, et al. 1998; Sun et al., 2005; Hedengren et al., 2005)

In addition to the direct use of the techniques summarized above, it seems important to evaluate these techniques additionally under closed-loop conditions imposed by real-time feedback control and feedback optimization algorithms.

5. EXAMPLE

MPC control based upon detailed CFD models of a glass forehearth is used to demonstrate the rigorous model based approach. This example has been worked on as part of a research project funded by the Dutch government (REGLA project funded by the E.E.T. program).

The objective of the controller is to stabilize the temperature of the glass that is delivered to the forming machines in order to improve the so-called workability of the glass. The workability of glass, or the ease with which the glass can be used for forming the final product, depends largely on the viscosity and therefore on the temperature and temperature distribution of the glass melt.

A new approach to set-up control models:

– The approach starts with setting up a separate CFD model for the feeder under consideration. This model is validated, as the performance of the controller will depend largely on the quality of this underlying model.
– Subsequently, dynamic tests are performed upon the CFD model. The simulation tests couple the response of temperatures and flows in the feeder to changes in the input. Proper Orthogonal Decomposition (POD) is applied for model reduction.
– The resulting approximate model is used to achieve constant temperatures and setpoints at the exit of the feeder even for the case of disturbances in the melt entering the feeder or disturbances in the feeder itself.

The resulting control model, which is derived from these CFD simulation tests, can be used for a large set of working points (e.g. a large range of loads) instead of for one single working point, as the response of the feeder to large variations in disturbances and process settings is determined. Consequently, the control model does not have to be rebuilt when a different working point for the feeder/furnace is selected due to e.g. the production of a different product (as long as the type of glass does not change). It is a fast way of setting up a complete control model without any risk for production.

The resulting control scheme for the industrial feeder is shown in figure 5.1. The temperatures in the feeder are controlled via the set-points of three PID controllers that adjust the fuel supply to the three zones in the feeder. These PID set-points are the result of the MPC, which reads the values of the 9-grid thermocouple at the feeder exit. Based on the fast reduced model describing the dynamic behavior of the feeder, the MPC determines the optimal values of the PID set-points such that the desired temperature (homogeneity) at the feeder exit is attained. Next to the control objectives (desired temperature and temperature homogeneity at the feeder exit), also several constraints are imposed to the MPC: the glass melt temperatures in the feeder may not exceed and drop below certain values; also the rate of fuel adaptation is constrained to avoid instabilities in the feeder. These constraints limit the flexibility of the feeder operation and hamper the identification of the optimal feeder settings (optimal PID set-points to ensure stable production at the desired glass melt temperature (homogeneity)) when CFD models are not consulted.

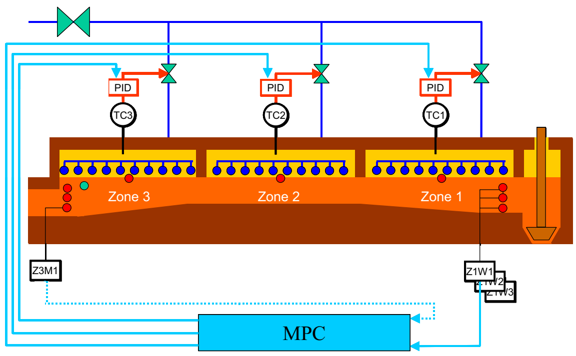

Figure 5.1: Control scheme for the industrial feeder.

Although the feeder entrance temperature (homogeneity) is measured continuously, in the field test of the MPC this information has not been taken into account. Incorporation of the entrance temperatures in the MPC (indicated by the dotted line in figure 5.1) would allow the MPC to anticipate in the feeder (by adjusting the PID set-points) on temperature disturbances from the refiner.

The application of the described MPC feeder control has been extensively tested on various production campaigns for a production feeder in emerald green container glass manufacturing. Figure 5.2 shows the impact of the controller on the average 9-point grid temperature, which is the main objective for the controller. In manual control mode, deviations in temperature in the 9-grid exceed +/ 2.5 degrees C, in some instances even more. It is clearly seen that the feeder temperatures become very stable (+/ 0.5 degrees C) once the controller is switched on. It should be noted, that the smallest change in temperature that is detected by the thermocouples is 0.2 degrees C, which makes the capabilities of the controller even clearer. Besides the increased stability, changes in set points are realized within a short period of time. Even automated transitions between largely different operating points (95 ton/day – 135 ton/day; different glass gob temperatures) have been performed successfully.

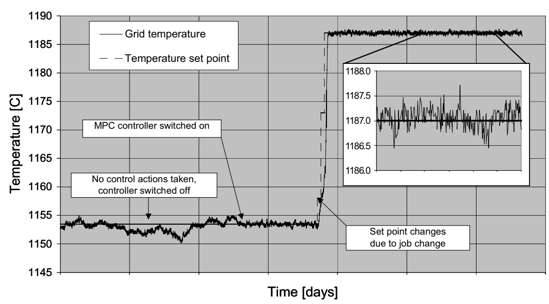

Fig. 5.2 Wide operating range POD reduced model based controller performance

6. CONCLUDING REMARKS

Changing market conditions enforce chemical processing industries to better utilize process capabilities. Process operation needs to be closer tied with market demand to improve capital productivity. Model based techniques require dedicated models that reflect application relevant dynamics with sufficient accuracy for the relevant operating range. New concepts have been discussed that are based on the development of a reference model and subsequent derivation of approximate, reduced process models. The approximate models are derived from the reference model by using an adequate model reduction/ model approximation method. This requires a highly automated, minimum engineering effort model reduction technology.

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