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FIRST PRINCIPLES MODELING AND NONLINEAR OPTIMIZATION BASED ESTIMATION AND CONTROL OF A FLUID CATALYTIC CRACKING UNIT

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ABSTRACT. In this paper the output feedback NMPC approach is illustrated on a simulated fluid catalytic cracking unit (FCCU). This approach considers the most important features of a real-time control algorithm, which are often overlooked in simulation studies, contouring thus a framework for practical NMPC implementation. The most important features considered in the approach are: state and parameter estimation, efficient solution of the optimization, and computational delay. In the output feedback NMPC approach used in this paper, only measurements that are available in practice are considered, whereas the rest of the states are estimated together with uncertain model parameters using a moving horizon estimation (MHE) technique. The importance of taking this computational delay into account will also be assessed and a real-time formulation of the control approach is describes that includes the computational delay in the NMPC approach. The advantages of the proposed real-time approach are assessed through the simulated industrial FCCU application.

Keywords: Fluid catalytic cracking unit (FCCU), nonlinear model predictive control, moving horizon estimation, real-time control, multiple shooting, interior point algorithm.

1. INTRODUCTION

The fluid catalytic cracking unit (FCCU) is an important processing unit in an oil refinery. This process converts high molecular-weight gas oils into significantly more valuable, lighter hydrocarbon products. Any improvement, whether in design, operation or control, can result in dramatic economic benefits. The process is multivariable, strongly nonlinear, highly interactive, and is subject to many operational, safety and environmental constraints, posing challenging control problems. The competitive nature of the petrochemical industries drives the constant technological development of FCC processes, with the clear economic objective of improving productivity, while maintaining safety and environmental regulations. Due to its complexity, the modeling and control of FCCU poses important challenges (McFarlane et al., 1993). FCCU has become in the last decades the testing bench for many modern refinery control systems. This chemical process has been traditionally controlled by using algorithms on a linear time-invariant approximate process model, the most common being step and impulse response models derived from the convolution integral account (Qin and Badgewell, 2003). Linear model predictive control has proved its benefits in the petrochemical industries in the past two decades, however nonlinear model predictive control (NMPC) has the potential to achieve higher productivity by exploiting the advantages of taking process nonlinearities explicitly into Nonlinear model predictive control (NMPC) is a good candidate for the control of the FCCU, because of its ability to explicitly handle most of the aforementioned problems. First-principles model based NMPC requires full state information for the prediction, which is usually not available in practical applications. In the output feedback NMPC approach used in this paper, only measurements that are available in practice are considered, whereas the rest of the states are estimated together with uncertain model parameters using a moving horizon estimation (MHE) technique. The goal of state estimation is to reconstruct the state of a system from process measurements and a model. The state estimation is used to reconstruct the states and time-varying parameter for a process from a set of measurements. The concepts of observability and detectability provide conditions for state estimation to converge to the true value of the state and parameters (Russo et al, 1999). State estimators for physical processes often must address many different challenges, including nonlinear dynamics, state (e.g nonnegative concentrations, temperatures) and local optima, subject to hard constraints (Haseltine and Rawlings, 2003).

Industrial applications of model predictive control commonly use a constant additive disturbance model to compensate for model error. However, the use of a constant additive disturbance model may result in a poor or even unstable behaviour when there are significant unmodeled process dynamics or the plant is open-loop unstable. State estimation provides the mechanism to use more appropriate disturbance models (Russo et al, 1999). As a result, state and parameter estimation are a persistent topic for the research academy.

The paper is structured as follows: Section two presents the description of the plant. Section three and section four give an overview to the areas of moving horizon estimation and nonlinear model predictive control that have both attracted considerable industrial and academic interest over recent years.

2. DYNAMIC MODELING OF THE FCCU

The schematic diagram of the FCCU, for which the mathematical model was developed and the assessment of the NMPC has been performed is presented on Figure 1.

In the FCCU raw material is mixed with the regenerated catalyst in the reactor riser. The cracking reactions and coke formation occur in the riser and the products (gasoline, diesel, slurry) are separated in a fractionator. The deactivated catalyst due to coke deposition is regenerated in the regenerator.

The developed dynamic simulator consists of detailed models of: the feed and preheat system, reactor stripper, riser, regenerator, air blower, wet gas compressor, catalyst circulation lines and main fractionator. Based on the assumption given in Dupain at al. (2003) a five lump kinetic model (schematically shown on Figure 2) that predicts the yields of valuable products is proposed and included in the simulator. The resulted global model of the FCCU is described by a complex system of partial-differential- equations, which was solved by discretizing the kinetic models in the riser

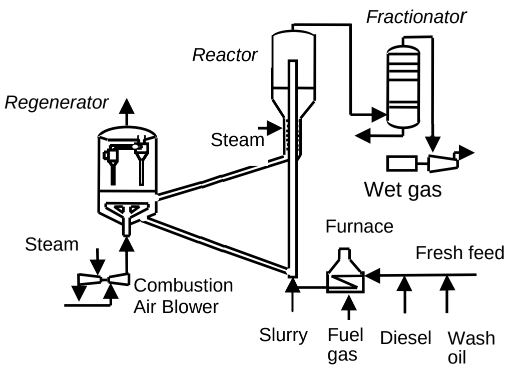

Figure 1. FCCU plant

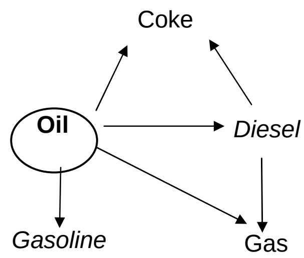

Figure 2. Five lump model for the catalytic cracking

and regenerator on a fixed grid along the height of the units, using finite differences. The resulted model is a very high order DAE, with 2143 ODEs (143 from material and energy balances and 2000 resulted from the discretization of the kinetic models). The model was implemented in C programming language for efficient solution and was used first to study the dynamics of the process and then in the NMPC controller.

3. MHE ALGORITHM

In a typical industrial application (FCCU) there is a need to reconstruct unmeasured states using a limited number of available measurements. A moving horizon estimator is employed for states estimation. The benefits arise because MHE incorporate physical state constraints into an optimization, accurately uses the nonlinear model, and optimize over a trajectory of states and measurements (Haseltine and Rawlings, 2003). The MHE estimator express as a nonlinear programming techniques (NLP) problem is as follows:

Problem P1:

$$\min_{x_{k-N},\theta_e} J_{MHE} = \sum_{j=k-N+1}^{k} \left\| y_i - y_i^{meas} \right\|_W^2 + \left\| \theta_e - \theta_e^{ref} \right\|_Z^2 \quad (1)$$

subject to: $x_i = f(x_{j-1}, u_{j-1}, \theta)$, $j = k - N + 1, ..., k$ (2)

$$y_i = g(x_j, \theta), \; j = k - N + 1, ..., k \quad (3)$$

$$\theta_{e,\min} \le \theta \le \theta_{e,\max} \quad (4)$$

where N is the estimation horizon, W, Z are weighting matrices and θ_e is a subset of model parameters selected for on-line adjustment. θ_e^{ref} is a set of reference values and $\theta_{e,\min}, \theta_{e,\max}$ are specified lower and upper bounds for the adjustment parameters; y_i denotes the output at discrete time j, and y_i^{meas} its corresponding measurement.

The second term in (1) penalize parameter moves away from reference values, while constraint ensure that parameter estimates stay within reasonable physical rages. In problem *P1* the inputs u_j, $j = k-N,...,k-1$ are known, applied inputs to system. The solution of problem *P1* results in $\hat{x}$ which is used to calculate an estimate of the controlled variable when this last quantity is not measured.

Figure 3 present comparatively, the simulation results of the model of the plant and simulation results using MHE algorithm in the presence of disturbance in the coke factor (*Kc*). The disturbance have an influence on the reactor temperature (T_r) and regenerator temperature (T_{reg}), on coke concentration on spent and regenerated catalyst (*csc* and *crgc*), on the regenerator and reactor catalyst inventory (W_{reg} and W_r), on the catalyst inventory on spent circulation lines (W_{sp}). The disturbance have also an influence also on the carbon inventory (W_c) deposited on the catalyst in regenerator and on the moles of carbon in regenerator (*n*). Coke factor has a small influence on the speed of catalyst in spent circulation line (*vsc*) and regenerated circulation line (*vrgc*). A small influence of the disturbance can be observed on the pressures of the system: combustion air blower sunction pressure (p_1), combustion air blower discharge pressure (p_2), reactor-fractionator pressure (p_5), regenerator pressure (p_6), wer gas compressor sunction pressure (p_7).

The goal of MHE is to reconstruct the state of a system from process measurements and estimate the unknown model parameter *Kc*. Figure 3 also presents the evolution of the states of the FCCU model using eleven measurements: T_r, T_{reg}, *vrgc, vsc* and the pressures in the system (p_1, p_2, p_5, p_6, p_7), considering errors in the initial states of the model. As can be seen from the Figure 3, a few states are unobservable: W_{reg}, W_r, W_c, W_{sp} and *n,* however the estimator achieves excellent performance in estimating the unknown model parameter.

4. NONLINEAR MODEL PREDICTIVE CONTROL

4.1 Formulation of the algorithm

NMPC is typically implemented as a two-step algorithm: state estimation and prediction to minimize a specified control objective function. An NMPC algorithm must also be formulated must also be formulated to ensure integral action in the feedback path. We consider the following general differential- algebraic optimization problem, as the starting point for the development of state estimation and predictive control algorithms:

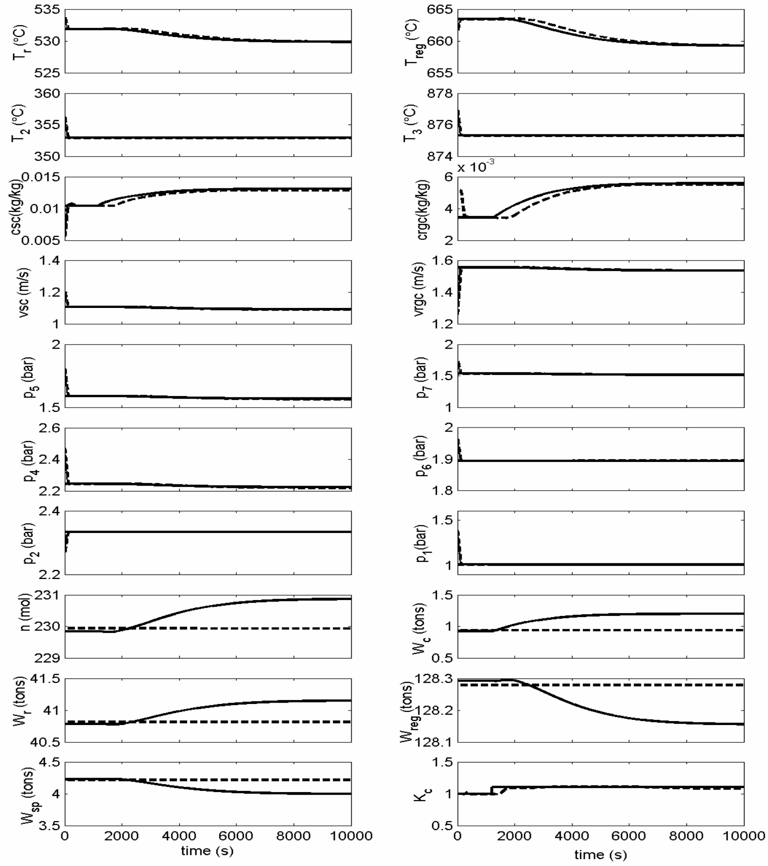

Figure 3. Performance of the MHE in the case of errors in the initial states and disturbance in K_c (10 % increase at t= 20 min) plant data modeling results (solid line); MHE results (dotted line)

Problem P2:

$$\text{Minimize } J = \phi(x(t_f), t_f + \int_{t_0}^{t_f} L[x(t), u(t), t]dt \quad (5)$$

$$\text{subject to: } \dot{x}(t) = f(x(t), u(t)) \quad (6)$$

$$G(x(t), u(t)) = 0 \quad (7)$$

$$H(x(t), u(t)) \leq 0 \quad (8)$$

where J is the state estimation or predictive control objective function, $x(t)$ and $u(t)$ are the state and input vectors, respectively, and F and G represent the mechanistic system model, a coupled set of ordinary differential and algebraic equations. H represents bounds on system variables or other linear or nonlinear constraints.

4.2. Efficient solution of the NMPC optimization via multiple shooting

Problem P2 can neither be solved by typical nonlinear programming (NLP) techniques nor by optimal control methods. In general, NLP methods cannot optimize continuous systems while optimal control methods do not handle algebraic constraints for G and H. Considering the discrete nature of the online control problem, a convenient approach to solving Problem 2 is to formulate discrete approximation to it that can be handled by conventional NLP solvers. An alternate formulation for discrete approximation of the problem for nonlinear model predictive control is adopted for its generality (*Problem P3*). The prediction horizon $[0, t_f]$ is divided into p equally spaced time intervals, Δt, with discrete time $k+i$ representing $t = i\Delta t$, $i = 0,1...p$.

Problem P3:

$$\min_{u_{k/k}, u_{k+1/k} \ldots, u_{k+m-1/k}} J_{NLMPC} = \sum_{j=k+1}^{k+p} \left\| y^c_{j/k} - d_k - y^{ref}_j \right\|^2_Q + \sum_{j=k}^{k+p} \left\| u_{j/k} - u^{ref}_j \right\|^2_R + \left\| \Delta u_{j/k} \right\|^2_S \quad (9)$$

subject to: $x_{j/k} = f(x_{j-1/k}, u_{j-1/k}, \theta)$, $j = k+1, ..., k+p$ (10)

$$y^c_{j/k} = g(x_{j/k}, \theta), \; j = k+1, ..., k+p \quad (11)$$

$$y^c_{\min} \le y^c_{j/k} \le y^c_{\max}, \; j = k+1, ..., k+p \quad (12)$$

$$u_{\min} \le u_{j/k} \le u_{\max}, \; j = k, ..., k+m-1 \quad (13)$$

$$\Delta u_{\min} \le \Delta u_{j/k} \le \Delta u_{\max}, \; j = k, ..., k+m-1 \quad (14)$$

$$u_{j/k} = u_{j-1/k}, \; j = k+m-1, ..., k+p-1 \quad (15)$$

where p is the predicted horizon, m is the control horizon, $u_{j/k}$ is the process input and $y^c_{j/k}$ is the controlled output variable at discrete time j calculated from information available up to discrete time, k. $\Delta u_{j/k} = u_{j/k} - u_{j-1/k}$, $j = k, ...k+m$, are present in the objective function to allow excessive input moves to be penalized and const rained if necessary, d_k is an estimate of unmeasured disturbance at time k, and is required in the control formulation to ensure offset free operation of the controller.

At each control interval, the entire *Problem P3* is solved but only the input $u_k = u_{k/k}$ is implemented. Q, R, S are the weighting matrices and θ is a vector of model parameters. The trajectories of target, y^{ref}, u^{ref} are obtained from the solution of an off-line dynamic optimization problem.

A very efficient solution technique for the problem (9)-(15) is based on the multiple shooting approach (Diehl, 2001; Franke and Arnold). This procedure consists of dividing up the time interval $t \in [t_0, t_f]$ into a series of grid points $[t_0, t_1, t_2, \ldots, t_f]$. Note that the grid points do not necessary correspond to the discretization points in the definition of problem *P*2. Using a local control parameterizations a shooting method is performed between successive grid points (see Figure 4). The differential equations and cost on these intervals are integrated independently during each optimization iteration, based on the current guess of the control. The continuity/consistency of the final state trajectory at the end of the optimization is enforced by adding consistency constraints to the nonlinear programming problem. A set of starting values for the state and adjoint vectors is required at each grid point in time, and continuity conditions for the solution trajectory introduce additional interior boundary conditions, which are incorporated into one large zero-finding problem to be solved. The solution of Problem *P2* is performed using an NMPC tool (Nagy *et al.*, 2004) based on the sequential-quadratic-programming (SQP) type optimizer HQP, which is used in conjunction with the implicit differential-algebraic-equation (DAE) solver, DASPK, for robust and fast solution of the model equations.

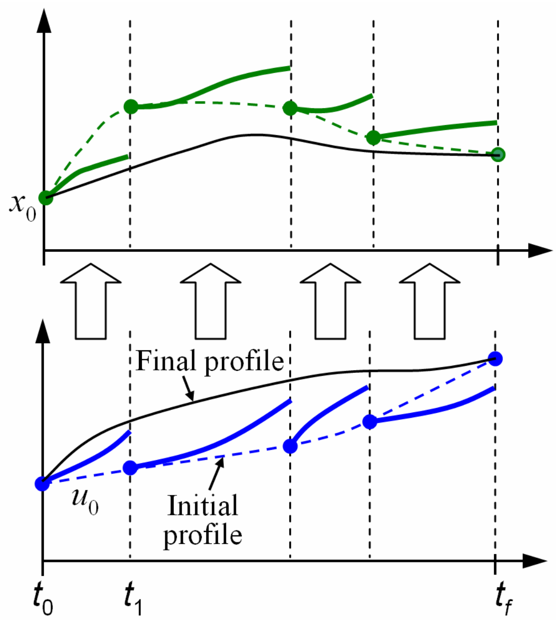

Figure 4. llustration of the multiple shooting approach.

4.3 Real-time NMPC algorithm

The solution of problem *P2* requires a certain, usually not negligible, amount of computation time d_k , while the system will evolve to a different state. In this case the optimal feedback control $u^{\star}(t_k) = [u_{0|t_k}, u_{1|t_k}, \ldots, u_{N_p|t_k}]$ computed in moment t_k corresponding to the information available up to this moment, will no longer be optimal. Computational delay d_k has to be taken into consideration in real-time applications. In the approach used here, in moment t_k, first the control input from the second stage of the previous optimization problem $u_{1|t_{k-1}}$ (which corresponds to the first stage of the current optimization) is injected into the process, and then the solution of the current optimization problem is started, with fixed $u_{0|t_k} = u_{1|t_{k-1}}$. After completion, the optimization idles for the remaining period of $t \in (t_k + d_k, t_{k+1})$, and then at the beginning of the next stage, at moment $t_{k+1} = t_k + \Delta t$, $u_{1|t_k}$ is introduced into the process, and the algorithm is repeated. This approach requires real-time feasibility for the solution of each open-loop optimization problems ($d_k \leq \Delta t$).

4.4. MHE-NMPC of the FCCU

Simulation results of a combined NLMPC-MHE algorithm are shown in Figure 5 together with the open loop simulation in the case of 5% decrease in the coke formation factor. The controlled variables: the temperatures in the reactor and regenerator are shown in Figure 6, whereas the control inputs are the input flow rate in the reactor riser and the valve position on the regenerated catalyst pipe. In the simulation a sampling time of 2 minutes and a control horizon of one sampling time were used. The prediction horizon for the NMPC is 50 sampling periods, whereas the horizon of the MHE is 30 sampling instances in the past. It can be seen that the MHE is able to estimate unmeasured states and the model parameters very well. Although some of the states are not estimated they are kept within the boundaries of physical limits due to one of the major advantages of MHE, i.e., bounds on the estimated states can be incorporated in the optimization problem easily. The overall performance of the MHE-NMPC is very good; the temperatures are kept within a narrow band of variation compared to the open loop response of the process. It can be seen that the unknown model parameter is estimated with no offset in about one hour, and the disturbance is rejected in about two hours by the NMPC.

The CPU times corresponding to the MHE and NMPC calculations are presented in Figure 7. The dimension of the optimization for the NMPC is only two since a control horizon of only one sampling time, whereas the dimension of the optimization problems from the MHE is 19 (18 states plus one model parameter), leading to a significantly higher computational burden. Figure 6 demonstrates that the computational time scales only linearly with dimension of the optimization problem due to the efficient multiple shooting approach used, and the maximum total computational time (approximately 20*s*) is well bellow the sampling time (120*s*). The results demonstrate that efficient optimization algorithms can guarantee the real-time feasibility of the MHE-NMPC implementation even when a model with 2143 ODEs is used.

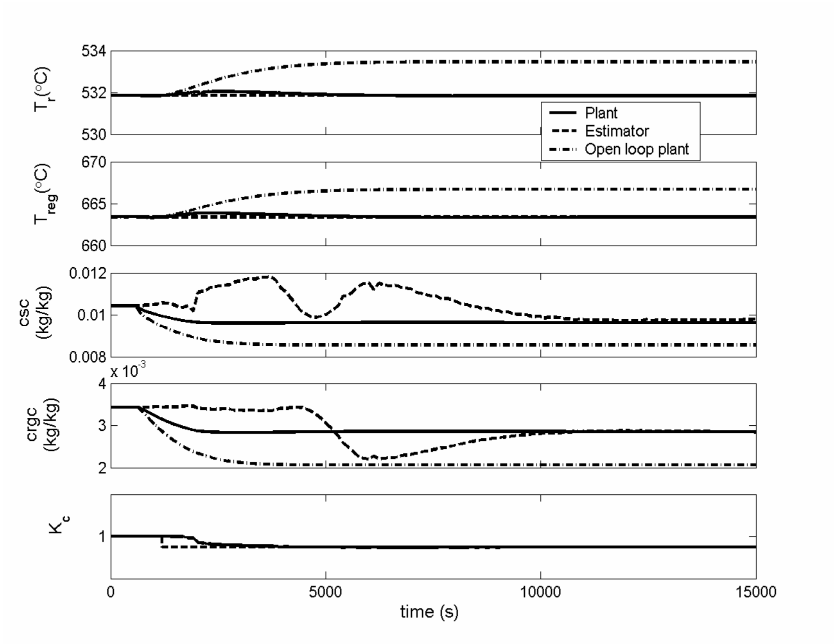

Figure 5. Simulation results of the MHE-NMPC of the FCCU

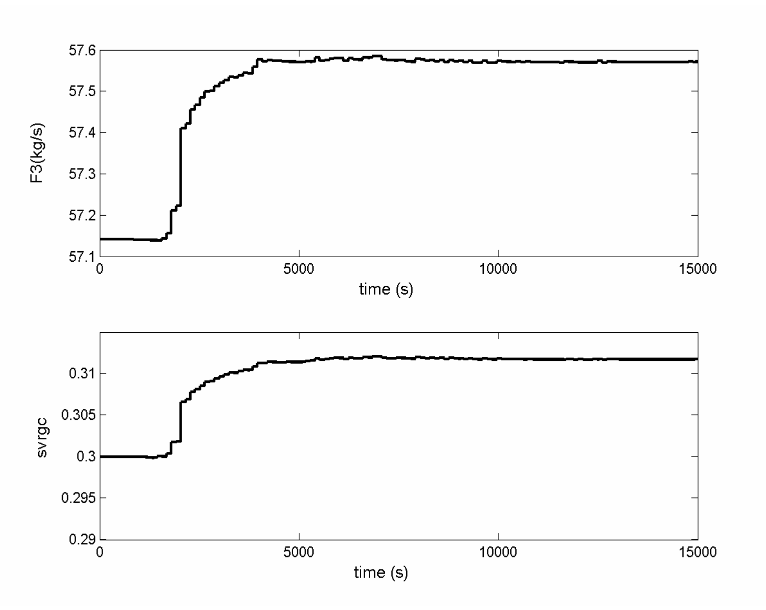

Figure 6. The controlled variables of the MHE-NMPC of the FCCU

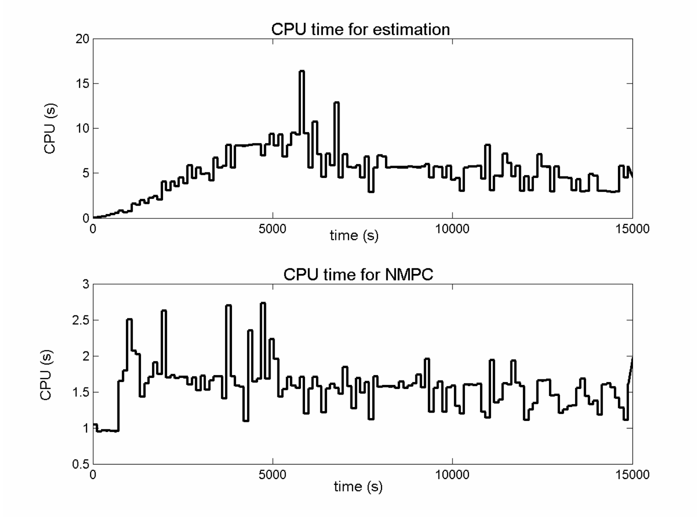

Figure 7. CPU times required for the optimization problems from the MHE and NMPC

5. CONCLUSIONS

The paper assesses the performance of a moving horizon estimation based nonlinear model predictive control approach in the case of a highly complex industrially relevant process the FCCU. The estimation of model states and parameters is critical to the success of model based process monitoring and control applications. Simulation results demonstrate that using state-of-the-art optimization algorithms and software advanced control and estimation strategies can implemented on complex industrially relevant problems.

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