PROCESS CONTROL OF AN OPEN PLATE REACTOR

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Abstract: A new chemical reactor, the Open Plate Reactor, is being developed by Alfa Laval AB. It combines good mixing with high heat transfer capacity. With the new concept, highly exothermic reactions can be produced using more concentrated reactants. A utility system to provide the reactor with cooling water is designed and experimentally verified. The utility temperature controller is based on a mid-ranging control structure to increase the operating range of the hydraulic equipment. A Model Predictive Controller is proposed to maximize the reaction yield under hard input and state constraints. Simulations show that the designed process control system gives high reaction yield and ensures that the temperatures inside the reactor do not exceed a predefined safety limit. *Copyright @ 2005 IFAC*

Keywords: heat exchange reactor, process control, mid-ranging, Model Predictive Control, Extended Kalman filter

1. INTRODUCTION

The syntheses of fine chemicals or pharmaceuticals, widely carried out in batch or semi-batch reactors, are often strongly limited by constraints related to the dissipation of the heat generated by the reactions. A new concept of heat exchange reactors, the Open Plate Reactor (OPR) developed by Alfa Laval AB, allows to perform complex chemical reactions with a very accurate thermal control. Thus, the OPR appears particularly suited to process intensification, as it allows at the same time an increase of reactant concentration and a reduction of solvent consumption. The sensors inside the reactor lead to better process knowledge and together with the possibility of multiple injection points they enable improved process control.

The paper is organized in the following manner. In Section 2 the OPR is briefly described and in Section 3 process operation and control objectives of the OPR are presented. In Section 4 the cooling system of the OPR is described. A temperature controller based on a mid-ranging control structure is designed and experimentally verified. In Section 5 a model predictive control approach is used for process control of the OPR. It is tested in simulations for a fast exothermic reaction. In Section 6 conclusions are drawn.

2. THE OPEN PLATE REACTOR

The OPR consists of a number of reactor plates, in which the reactants mix and react. On each side of a reactor plate there is a cooling plate, through which cold water is circulated. In this paper a simple first order exothermic reaction is considered, see Eq. 1.

$$A + B \rightarrow C \qquad (1)$$

In Fig. 1 a schematic figure of the first rows of a reactor plate is shown. The reactant A flows into the reactor from the upper left inlet. Between the inlet and the outlet, the reactants are forced by inserts to flow in horizontal channels. The inserts are specifically designed to enhance the mixing and at the same time the heat transfer capacity. The general flow direction inside the reactor plate is considered to be vertical. The concept relies on an open and flexible reactor

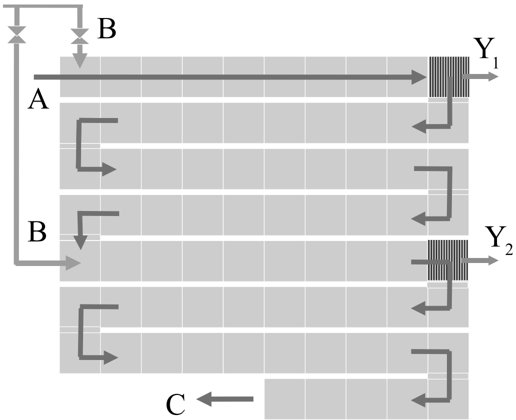

Fig. 1 A schematic figure of a few rows of a reactor plate. Reactant A is injected at top left and reactant B is injected at multiple sites along the reactor. Y_1 and Y_2 are internal temperature sensors used for process control and supervision.

configuration. The type of inserts and the number of rows in the reactor plate, which determines the residence time, can be adjusted, based on the type and rate of the chosen reaction. The reactant B can be injected in arbitrary places, typically in the beginning and in the middle of the reactor. Temperature sensors can be mounted arbitrarily inside the reactor, e.g. after each injection site. There can also be other sensors, such as pressure or conductivity sensors. The signals from the internal sensors are then used in the control system for emergency supervision and process control.

The cooling plates on each side of the reactor plate have vertical flow channels compared to the horizontal reactor channels, giving a cross-flow heat exchanger. However the general flow direction of the reactor flow is vertical, so the heat exchanger can be approximated as concurrent. A nonlinear model of the OPR was derived from first principles in (Haugwitz and Hagander, 2004b).

3. PROCESS OPERATION

The two main control signals of the OPR, see Fig. 2, are the injection flow distribution u_1, that is how large fraction of the reactant B that is injected at the first injection site, and the inlet temperature of the cooling water u_2. All other input variables are to be constant. All variables except concentration can be measured online. Another important design parameter is the location of the multiple injection sites. With fast exothermic reactions, most of the reaction heat will be generated near each injection point, which will lead to a local temperature maximum after each injection site.

In Fig. 3 the temperature and yield profiles are plotted when there are two injection sites, one at the inlet and one in the middle of the reactor length for a exothermic reaction. The injection flow rate distribution $u_1 = 0.50$, i.e. 50% of the reactant B flow is injected at the inlet and 50% in the middle of the reactor. The cooling inlet temperature u_2 is 40°C. Together this set of control signals give the process two temperature maxima of $T = 87.3$ and 96.7°C. To maximize the productivity of the reactor, the local temperature maxima should be controlled to be of roughly equal height and they should be below a pre-defined temperature safety limit. In this case that would correspond to increasing reactant injection in the first point u_1 and decreasing the cooling temperature u_2.

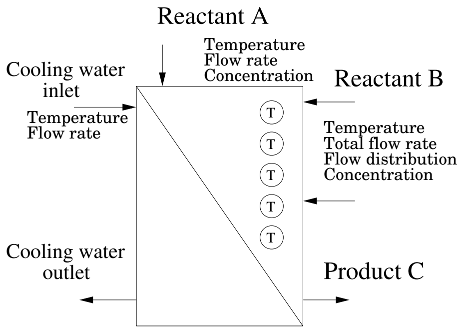

Fig. 2 The Open Plate Reactor as a schematic heat exchanger with reactions on one side and cooling water on the other side. There are multiple injection sites and internal temperature transmitters along the reactor length.

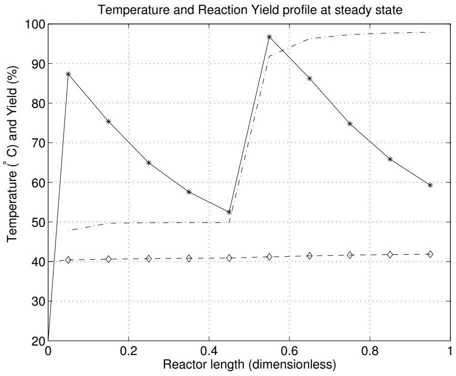

Fig. 3 Simulated temperature profile (solid) along the plate reactor with injection at two sites resulting in two temperature maxima at $T = 87.3$ and 96.7°C. Reaction yield (dash-dot) and cooling temperature (dashed).

3.1 *Control Objectives*

The overall control objective is to utilize the open plate reactor maximally in a safe way. This implies that the reaction is to be completed within the reactor and that the reactants are to be fed in the right stoichiometric proportions. Highly concentrated solutions should be used and there should not be any side reactions. Suitable safety margins should be maintained in for instance temperature.

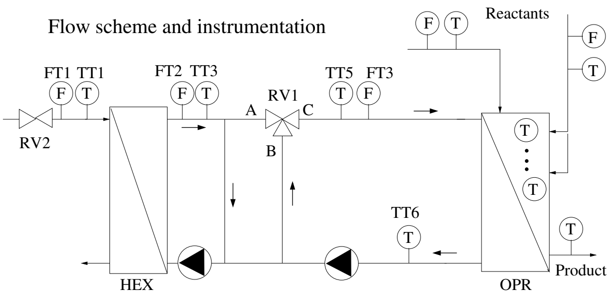

Fig. 4 Flow configuration with a three-way control valve with recycle around the heat exchanger (HEX) and the OPR.

The most important output variable is the reaction yield γ, which is defined as

$$\gamma = \frac{c_{product}}{(c_{product} + kc_{reactant})} \tag{2}$$

where the concentrations c are at the reactor outlet and k is the stoichiometric coefficient. The control objective for the OPR can be stated as an optimization in γ with both input and state constraints, which can for example be solved with Model Predictive Control (MPC), see Section 5. The objective is to calculate

$$\max_{u \in \mathscr{U}} \gamma(x,u,d) \tag{3}$$

where x are the states temperature and concentration along the reactor, u are the control signals and d are exogenous disturbances. The maximizing u calculated in the optimization in Eq. 3 is passed on as reference values for the injection flow distribution and the cooling temperature controller, see Section 4.1.

4. UTILITY SYSTEM

To get the desired flow rate and temperature of the cooling water, given by the optimization in Eq. 3, into the cooling plates of the OPR, a utility system has been designed and tested. The flow configuration in Fig. 4 is a standard flow circuit for heating or cooling purposes, see (Petitjean, 1994). All notations in this section is taken from Fig. 4. With recycle of the water coming out from the OPR directly back to the control valve RV1, the speed of the temperature control can be significantly improved and the flow rate $FT3$ is kept almost constant. The utility system and its control is further described in (Haugwitz and Hagander, 2004b)

The second recycle, around the heat exchanger HEX to the left, is implemented to keep the flow rate through the heat exchanger $FT2$ constant, regardless of the current valve position of RV1. Even though the performance and the flexibility increases with the two recycle loops, they add complexity to the dynamical analysis of the cooling system, see for example (Morud and Skogestad, 1996).

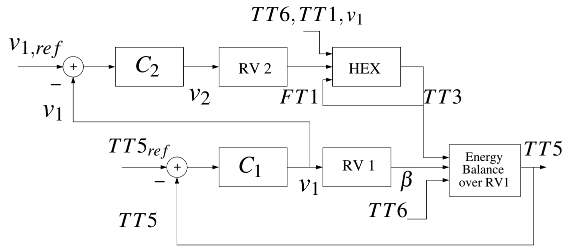

Fig. 5 Mid-ranging control structure of the utility system. PI-controller C_1 controls the cooling inlet temperature $TT5$ and C_2 acts such that v_1 works around a desirable working point specified by $v_{1,ref}$.

4.1 *Temperature control*

The cooling temperature $TT5$ should follow the reference temperature $TT5_{ref}$, given by the MPC optimization, see Section 5. The main control signal v_1 of the temperature controller is the desired position of the control valve RV1. The valve opening gives the flow ratio β, i.e. how much of the flow that go through port A divided by the total flow through port C. The second control signal v_2 is the position of control valve RV2, which indirectly controls the temperature $TT3$, see Fig. 4. By combining the two control signals in a mid-ranging control structure, see Fig. 5, the cooling temperature $TT5$ can be controlled, and in addition the control valve RV1 can work around some operating point, e.g. 50%, to avoid valve saturation. The term mid-ranging refers to a control structure used when two inputs signals are used to control a single output variable, see (Allison and Isaksson, 1998).

There are several advantages with the mid-ranging structure compared to using a constant cooling flow rate $FT1$. First, the operating range of the utility system is largely increased and valve saturation can be avoided. Second, the performance can be increased for large set-point changes. Third, the utility system will be less sensitive for external disturbances. The disadvantage is that the v_2 will act as a load disturbance to v_1, which might decrease the transient performance.

4.2 *Tuning the mid-ranging control structure*

The positions of the control valves RV1 and RV2 are controlled by two PI-controllers with nonlinear gain to compensate for nonlinear valve characteristics. Transfer functions from v_1 and v_2 to the cooling temperature $TT5$ are identified from experimental data. The block diagram in Fig. 5 is rewritten to a dual cascade structure, in which the controllers are tuned with the λ-method, described in (Åström and Hägglund, 1995). The tuning procedure is described in more detail in (Haugwitz and Hagander, 2004a).

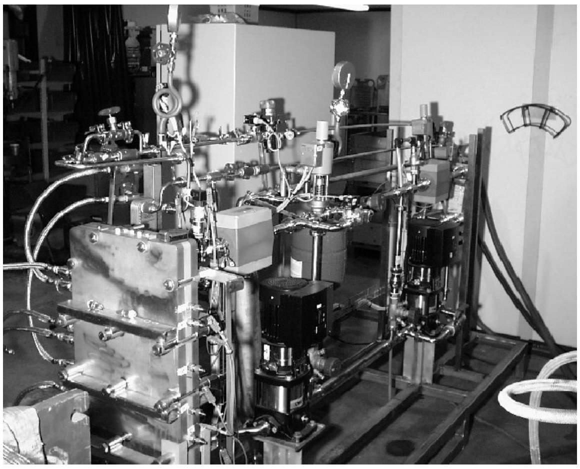

Fig. 6 The experimental setup at Alfa Laval laboratory in Lund. The OPR is seen to the left and the utility system to the right. Note the injection pipes on the left side of the OPR and the thermocouples along the right hand side of the OPR.

4.3 *Experiments on the utility system*

An experimental set-up was constructed at the test lab of Alfa Laval AB in Lund, see Fig. 6. There were several objectives with the experiments. First, to verify the hydraulic and thermodynamic design of the utility system. Second, to analyze the coupling between the plate reactor and the utility system including the sensitivity to disturbances. Third, to design a control system for the utility system.

The plate reactor was assembled with one reactor plate and a cooling plate on each side. For simplification, instead of using chemicals and having exothermic reactions, standard water was used as reactant A and super-heated steam was used as reactant B. The steam is injected along the left side of the OPR, see Fig. 6. The steam injection does not give the same dynamics as a chemical reaction, but the steam can still be approximated as a very fast exothermic reaction.

The first experiment is to keep the TT5 temperature constant despite varying heat release inside the reactor. For notations, see Fig. 4. The change in cooling outlet temperature TT6 corresponds to a decrease in heat release of 50 %, a very large and sudden change. In this case, the mid-ranging control is disabled and only the PI-controller for RV1 is active. In Fig. 7 it can be seen that the controller manages to keep the cooling temperature TT5 almost constant.

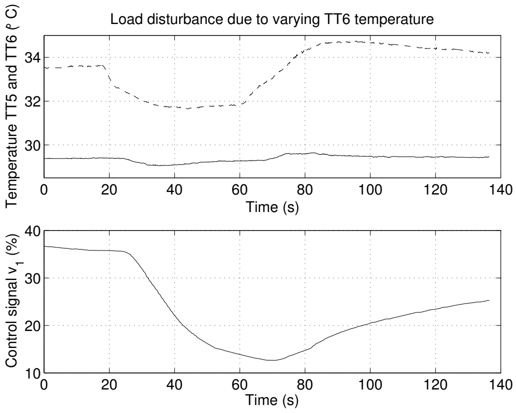

Fig. 7 Experiment in load disturbance, when heat load in the reactor is varied, which gives varying TT6 temperature (dashed). The controlled variable TT5 (solid) remains almost constant.

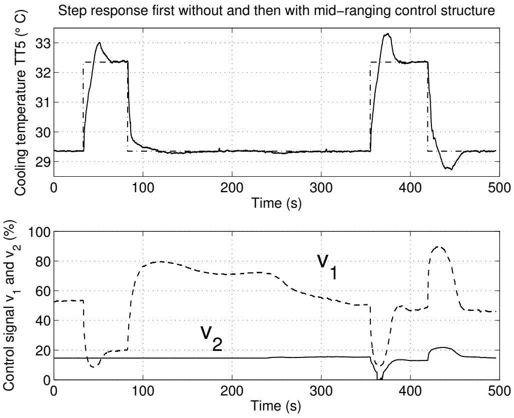

Fig. 8 Experiment using mid-ranging control structure with the cooling inlet temperature (solid) and the reference (dash-dot) in the top plot and the two control signals v_1 and v_2 in the lower plot. Note that v_2 (solid) is constant during the initial step and only v_1 (dashed) is used for control purpose. Mid-ranging is enabled at $t = 240$ s.

The mid-ranging control structure is also tested in a series of experiment, see Fig. 8. A step sequence in temperature reference is made first without mid-ranging, where v_2 (solid) is constant, leading to a constant cooling flow rate $FT1$. The step sequence is then repeated using mid-ranging. The control parameters for v_1, the first PI-controller, are the same for both experiments. After the first step in the reference signal, the control valve v_1 (dashed) position goes down from 50% to 20% open, which can severely limit the operating range of the cooling system. The mid-ranging is enabled at $t = 240$ s. With the mid-ranging, the v_1 returns to 50% after about 30 seconds. There is however a small increase in the overshoot of the step response, due to the mid-ranging control and the cross-couplings in the cooling system. Further tuning could improve the dynamical behavior of the system.

5. MODEL PREDICTIVE CONTROL OF THE OPR

The OPR control problem contains hard input and state constraints and the main objective is to maximize the reaction yield. A nonlinear model of the OPR, derived from first principles, is taken from (Haugwitz and Hagander, 2004b) and a linear MPC controller is developed based on notations from (Maciejowski, 2002). The nonlinear model is linearized around a non-optimal working point (x^0, u^0) and is sampled with $h = 1.0$ s to a discrete-time system.

$$x(k+1) = Ax(k) + [B_1\, B_2][u_1\, u_2]^T + B_d d \tag{4}$$

$$y = C_y x(k) \tag{5}$$

$$z = C_z x(k) \tag{6}$$

The plate reactor can be approximated as a tubular reactor and is discretized in 10 elements. There are five states in each element, the reactor and cooling water temperature and the concentrations of the two reactants and one product, see Eq. 11. That gives the linear model 50 states. The state vector x is then augmented with two constant disturbance states x_d and a constant parameter state x_p to be used in estimation later. It leads to integral action against unmeasured disturbances in the inlet concentrations and a unknown model parameter, see e.g. (Pannocchia and Rawlings, 2003). The two control signals are injection flow distribution u_1 and cooling temperature u_2. There are 7 possible inlet disturbances d, see Fig. 2, but only the inlet concentrations are unmeasured. The available state measurements y are the temperatures inside the reactor and the inlet and outlet temperature of the cooling water, in total 12 signals. The reaction yield was defined in Eq. 2 and has a maximum, when the outlet reactant concentrations are minimized. The controlled variables z are therefore chosen to be the outlet concentrations of the two reactants. The cost function to be minimized is

$$V(k) = \sum_{i=1}^{H_p} ||\hat{z}_{k+i|k} - r_{k+i|k}||_Q^2 + \sum_{i=0}^{H_u-1} ||\Delta\hat{u}_{k+i|k}||_R^2 \tag{7}$$

The constant reference signals are set to $r = [0 \quad 0]^T$, corresponding to all reactants consumed and γ = 100%. The prediction horizon is chosen as $H_p = 160$, so that all important process dynamics can be observed within the prediction window. The control horizon $H_u = 8$ and the weight matrices for the output and the control signals are chosen as $Q = 10^{-5} \cdot \mathbf{I}$ and $R = [1000 \quad 0; 0 \quad 1]$.

There are hard constraints on the temperature inside the reactor due to safety concerns, $T_i \leq T_{max} = 90°C$, where T_i is the temperature in the i:th element of the model and $1 \leq i \leq 10$. There are also constraints on the control signals $0.1 \leq u_1 \leq 0.9$ and $10°\text{C} \leq u_2 \leq 70°\text{C}$. and the change in control signals, $|\Delta u_1| \leq 0.2$ and $|\Delta u_2| \leq 1$.

The MPC controller and the nonlinear model of the OPR are implemented in Matlab/Simulink. An extended Kalman filter (EKF), which provides state, disturbance and parameter estimation to the MPC controller, is designed based on (Dochain, 2003). It uses the full nonlinear model of the process and calculates the covariance matrix $P(\hat{x})$ as the solution of the dynamical Riccati matrix equation, which minimizes the variance of the estimation error, see Eq. 10. R_1 and R_2 are the variances of the process and measurement noise, respectively.

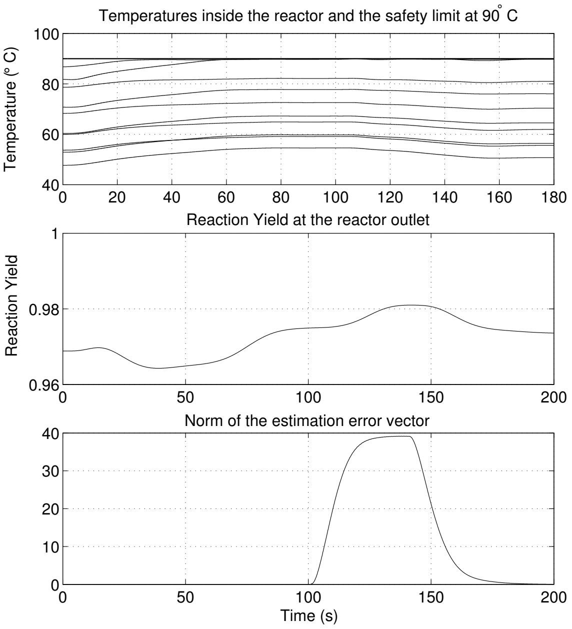

Fig. 9 Upper plot: Temperature in the 10 elements of the reactor. Middle plot: Reaction yield at the reactor outlet. Lower plot: The norm of the estimation errors is nonzero during the changes in inlet concentrations.

$$\frac{\mathrm{d}\hat{x}}{\mathrm{d}t} = f(\hat{x}, u, d) + K(\hat{x})(y - \hat{y}) \tag{8}$$

$$K(\hat{x}) = P(\hat{x}) C_y^T R_2^{-1} \tag{9}$$

$$\frac{\mathrm{d}P}{\mathrm{d}t} = -PC_y^T R_2^{-1} C_y P + PA^T(\hat{x}) + A(\hat{x})P + R_1 \tag{10}$$

The reaction used in the simulations is oxidation of thiosulfate by hydrogen peroxide.

$$2Na_2S_2O_3 + 4H_2O_2 \rightarrow Na_2S_3O_6 + Na_2SO_4 + 4H_2O \tag{11}$$

The kinetic reaction parameters are $k^0 = 2 \cdot 10^{10}$ L/(mol s), $E_a = 68200$ J/mol and $\Delta H = -586000$ J/mol thiosulfate, indicating that the reaction is fast and exothermic. The dynamic model of the cooling system and its controller from Section 4 is not included in the process model of the MPC, but is used in the simulations.

5.1 *Simulation results*

The process starts at rest in a non-optimal operating point and it is assumed that the observer states are correctly initialized. The reaction yield should be maximized and the temperatures should be below the safety limit, see Fig. 9 and 10. To test the disturbance rejection property of the EKF and the MPC controller, there is a ramp increase in inlet concentration of both reactants of total 5% during $t = 60 - 100$ s. The increase in inlet concentrations will increase the

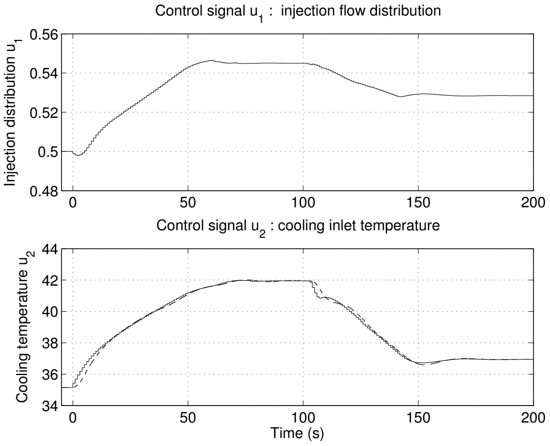

Fig. 10 Control signals for the OPR. Lower plot: The reference signal from the MPC (solid) and the actual temperature of the water from the cooling system (dashed).

amount of reaction heat released inside the reactor, thus increasing the risk of violating the temperature safety constraint.

During the first 50 seconds u_1 increases from 0.5 to 0.54, redistributing reactant flow from the second to the first injection point. This changes temporarily the stoichiometric balance, which causes the drop in reaction yield during the first 70 s. The flow time from the second injection point to the reactor outlet is around 15 s, which explains the time delay from the change in u_1 to the change in reaction yield. Meanwhile, the temperatures inside the reactor increase when the cooling temperature u_2 is increased. After $t = 50$ s, the temperatures after the two injection points have reached the safety constraint $T_{max} = 90°\mathrm{C}$. To maximize the yield, the temperatures are thereafter kept just below the constraint level. Note that the temperature constraint imposes the main limitation on reactor performance.

During the ramp disturbance the EKF estimates the increasing inlet concentrations with the disturbance states. The MPC controller uses that information to ensure that the temperature constraints are not violated by decreasing u_2 and u_1, i.e. redistributing reactant to the second injection point, see Fig. 10. In the lower plot of Fig. 9, the norm of the estimation error vector $e = x - \hat{x}$ is plotted. When the ramp disturbances start, the error increases up to 40. As the inlet concentrations reach their new steady-state value, the norm of the estimation error converges to zero within 40 s.

6. CONCLUSIONS

The concept and process operation of the Open Plate Reactor has been presented. The combination of good mixing and high heat transfer capacity makes the OPR very suitable for exothermic reactions and process intensification. The flexible configuration with reactor plates, cooling plates, multiple injections and internal sensors give increased possibilities for improved process control.

A utility system that provides the OPR with cooling water has been presented and experimentally verified with a mid-ranging control structure. The mid-ranging control largely increases the operating range for the utility system and increase performance for large setpoint changes or disturbances.

An MPC controller has been designed, which uses the injection flow distribution and the cooling inlet temperature to maximize the reaction yield while considering temperature constraints. An extended Kalman filter uses the temperature measurements for state, disturbance and parameter estimation, e.g. the unknown concentrations inside the reactor and in the reactor feed. The simulations show that very good reaction yield can be achieved, while the reactor temperature does not violate the safety constraints. The disturbance and parameter estimation in the EKF increases the robustness of the process control system. By reducing the impact from external disturbances, the risk of unnecessary shutdowns is decreased.

7. ACKNOWLEDGMENTS

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8. REFERENCES

Allison, B. J. and A. J. Isaksson (1998): "Design and performance of mid-ranging controllers." *Journal of Process Control*, **8**, pp. 469–474.

Åström, K. J. and T. Hägglund (1995): *PID Controllers: Theory, Design, and Tuning.* Instrument Society of America, Research Triangle Park, North Carolina.

Dochain, D. (2003): "State and parameter estimation in chemical and biochemical processes: a tutorial." *Journal of Process Control*, **13**, pp. 801–818.

Haugwitz, S. and P. Hagander (2004a): "Mid-ranging control of the cooling temperature for an open plate reactor." In *Proceedings of Nordic Process Control Workshop.*

Haugwitz, S. and P. Hagander (2004b): "Temperature control of a utility system for an open plate reactor." In *Proceedings of Reglermöte.*

Maciejowski, J. M. (2002): *Predictive Control with Constraints.* Pearson Education Limited.

Morud, J. and S. Skogestad (1996): "Dynamic behaviour of integrated plants." *Journal of Process Control*, **6**, pp. 145–156.

Pannocchia, G. and J. Rawlings (2003): "Disturbance models for offset-free model predictive control." *AIChE Journal*, **49**, pp. 426–437.

Petitjean, R. (1994): *Total hydronic balancing.* Tour and Andersson.