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Control, Operator Support and Safety System of PVC-reactors

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In modern petrochemical plants the corporate and societal demands to plant safety and minimum environmental effects are high. These demands rise high performance requirements to the technical systems, specially the process control and safety systems including an effective operator support system with fault detection capability. The systems must have high reliability also against erroneous operations which may cause shutdown situations or quality deviations.

PVC producing plants have high inherent hazard potentials. The risk can be minimised to an acceptable level with an integrated and well structured system consisting of a highly reliable basic process control system, a supervisory control system, an operator support system and a high integrity protective system.

The PVC reaction studied in this paper is exothermic and non-linear, and open-loop unstable. This may cause stability problems with varying operational conditions. The size of modern PVC reactors is so big that two independent cooling systems are needed to keep the reaction under control. The parallel control of two such cooling systems is complicated. Many existing solutions have problems with oscillatory control and even stability problems, causing reduced safety margins. In this paper a system to solve the stability problem of parallel control is suggested. The philosophy of the solution is decoupling of the dynamic dependency of the parallel control loops. The system is as shown simulated on real process data, and it is installed on a Norsk Hydro PVC plant.

When a reaction comes out of control, or rather when it shows a tendency to do so, an operator support system is needed to give the process operator an early warning so he can overrule the automatic control before a shut down situation occurs. Here is described a system for monitoring the heat of reaction in the autoclave. The system consists of a model based estimator. The process model is based on first principles. There are uncertainties in some parameters, specially the heat transfer and the measurement of the cooler difference temperature. The operator support system performs state and parameter estimation as well as fault detection, based on an extended Kalman filter. The system is tested on-line. In this paper results of simulations and on line estimates are presented.

Keywords: *parallel control, fault detection, extended Kalman filter, process reliability*

1. The PVC Process

The polymerisation of VCM (vinyl chloride monomer) to PVC (polyvinyl chloride) is a chain reaction of free radical type:

$$n\,CH_2 = \underset{\displaystyle Cl}{\underset{|}{CH}} \rightarrow [CH_2 - \underset{\displaystyle Cl}{\underset{|}{CH}}]n$$

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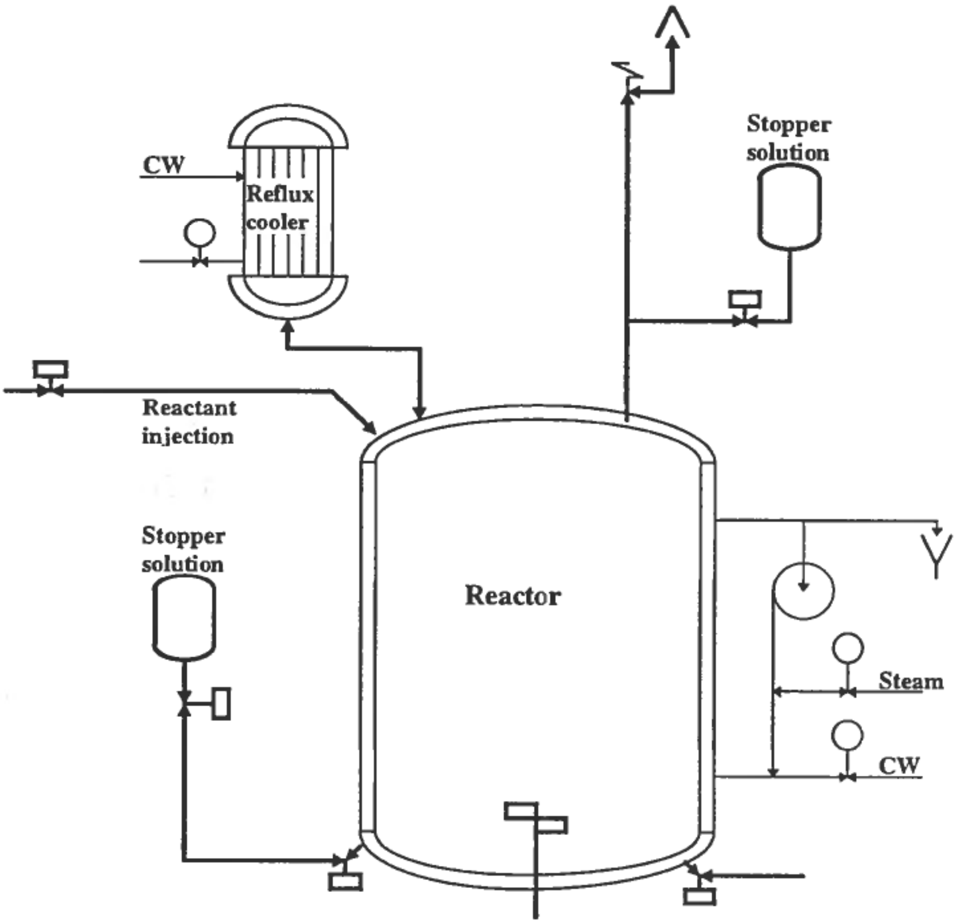

Figure 1. The PVC process.

To start the reaction, a solution of VCM and several components is heated above a threshold temperature and an initiating agent is added. Thereafter the reaction is self sustained and exothermic.

Fig. 1 shows a PVC production system. The process is batch, starting with injection of a number of component after a recipe to give the desired quality. In order to give enough cooling effect, two cooling systems are installed—a jacket cooling system on the autoclave walls, and a reflux condenser cooler on the top. These two cooling systems are both controlled from the autoclave solution temperature. A problem is to find a control structure to exploit both sources of cooling.

The process heat of reaction is according to the following Arrhenius equation:

$$R_x = e^{(a-b/T)},$$

where R_x is heat of reaction, a and b positive constants and T_{So} is solution temperature. The rate of change with temperature increase is:

$$\frac{\partial R_x}{\partial T_{So}} = e^{-(a-b/T_{So})} \cdot \frac{b}{T_{So}^2} > 0$$

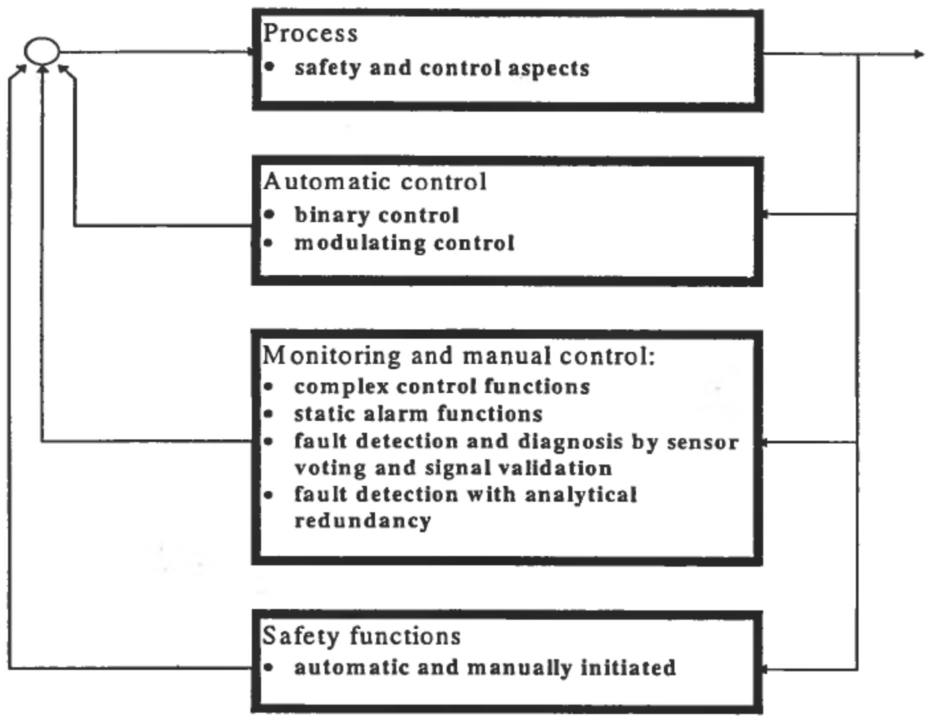

Figure 2. Control, monitoring and safety system.

This is a source of open-loop instability.

Due to failures or inaccuracies—in component injection (particularly initiator injection), in instrumentation, control or operation—the process may get out of control, and the temperature may increase until the reaction must be stopped by stopper solution injection or released through safety valves.

To get high safety, availability and product quality, the process has a control, monitoring and safety structure as illustrated in Fig. 2. The structure includes:

- Automatic control, binary and modulating.
- Monitoring, operator support and manual control.
- Safety functions, totally automatic or manually initiated.

Each of the indicated function blocks are designed to give high safety, availability and quality.

The non-linear heat-balance equations for the PVC reactor system are described below:

Heat balance for solution in autoclave:

$$C_{PSo}\frac{dT_{so}m_{so}}{dt} = R_x + A_2U_2(T_s - T_{so}) + A_{1re}U_{1re}(T_{sre} - T_{so})$$

Heat balance for steel in autoclave:

$$m_sC_{Ps}\frac{dT_s}{dt} = A_1U_1(T_v - T_s) - A_2U_2(T_s - T_{so})$$

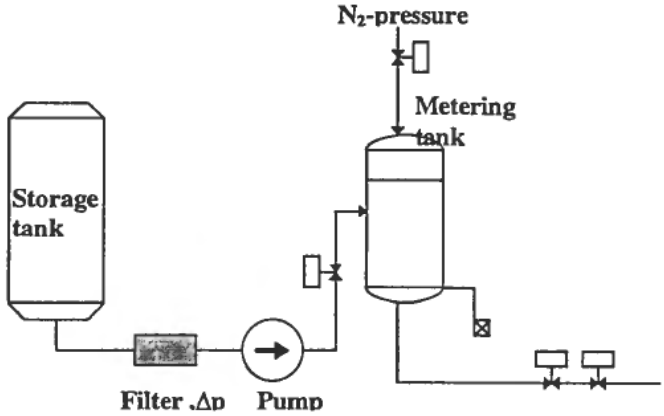

Figure 3. Injection system with high availability.

Heat balance for cooling water in autoclave:

$$\mathrm{m_v} C_{Pv}\frac{dT_v}{dt} = q_v C_{Pv}(T_{vi} - T_v) - A_1 U_1 (T_v - T_s)$$

Heat balance for steel, reflux condenser:

$$\mathrm{C_{Psre}} m_{sre}\frac{dT_{sre}}{dt} = A_{2re} U_{2re}(T_{vre} - T_{sre}) - A_{1re} U_{1re}(T_{sre} - T_{so})$$

Heat balance for water, reflux condenser:

$$\mathrm{C_{Pv}} m_{vre}\frac{dT_{vre}}{dt} = q_{vre} C_{Pv}(T_{vir} - T_{vre}) - A_{2re} U_{2re}(T_{vre} - T_{sre})$$

The variables are shown in Table 1 below.

m_{so}	Mass of solution in autoclave	$\mathrm{m_v}$	Water around autoclave
C_{PSo}	Heat capacity of solution in autoclave	$\mathrm{C_{Psre}}$	Heat, capacity condenser steel
T_{so}	Temperature of solution	m_{sre}	Mass of condenser
R_x	Heat of reaction	Q_{vre}	Cooling water to reflux
m_s	Mass of steel in autoclave, except refl. cooler	T_{sre}	Temperature, condenser steel
C_{Ps}	Heat capacity steel	m_{vre}	Mass of water in reflux
T_s	Temperature of steel	Q_{vre}	Cooling water to reflux
A_1	Outside autoclave area	T_{sre}	Temperature, condenser steel
U_1	Heat transfer through A1	m_{vre}	Mass of water in reflux
A_2	Inside autoclave area	T_{vre}	Temperature of water in reflux
U_2	Heat transfer through A2	A_{1re}	Contact area, reflux/gas
C_{Pv}	Heat capacity of water	U_{1re}	Heat transfer through A1re
T_v	Temperature of water	A_{2re}	Contact area, water/reflux
T_{vi}	Temp. inlet cooling water	U_{2re}	Heat transfer through A2re
q_v	Flow cooling water	T_{vrir}	Inlet reflux cooling water temp.

Table 1. Model variables.

There are great uncertainties in several of these variables:

$\mathrm{R_x}$: Varying from charge to charge due to component injection and temperature control imprecision.

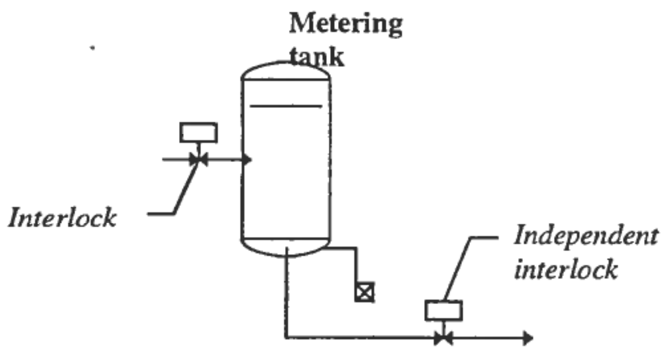

Figure 4. Injection system with high safety.

U_{2re}, U_2: These heat transfer coefficients are difficult to compute from thermodynamical and chemical engineering relations. In a precise model these must be estimated on-line.

m_s, T_s: The effective mass and temperature of steel taking part in the temperature variations is difficult to compute.

m_{su} Varying at start-up, and changing during the run.

T_{vi}–T_v: This small temperature difference is measured with high relative inaccuracy (bias).

2. Automatic control

2.1. *Binary control*

The binary control functions are designed to give high process safety and availability. A design for high availability is illustrated in Fig. 3. This is a system for injection of a solution to control the reaction level. To get high availability on demand, a metering tank connected to a N_2 pressure source is used. The injection to the autoclave is therefore independent of the pump, which may have a high failure tendency. The filter, pump and metering tank are monitored by appropriate instrumentation. There is start inhibit on the weight of solution in the metering tank.

Fig. 4 illustrates an injection system with high safety. The injection is controlled by timers, weight and independent interlock functions. These functions are in the control system. In addition safety functions for this are in the safety system.

2.2. *Modulating control*

The goals of the modulating control system for the PVC reactors system was formulated as:

- Robust control. The controller performance should be acceptable when parameters varies within normal limits. Parameter variations must be expected both in process and instrumentation, and this might cause stability problems when controlling the non-linear, open loop unstable process.
- The controller should have a structure which easily could be implemented on a standard process control system, and should be very easy to parameterize when process or operational conditions were changed. It is considered to be a great safety advantage that the controller is implemented in the standard process control platform.

With acceptable controller performance is meant stability margins and temperature deviations within limits that do not cause quality problems or reduced safety margins. Hence a parallel control with modified PID-structure was preferred.

A predictive controller might offer better performance in terms of reaction rate and economical aspect. Such a structure, however, is more cumbersome to make in a robust implementation. Hence this might be considered as an add-on possibility at a later stage when the process runs "acceptable" on a robust, "simple-structure" controller.

For a root-locus analysis of the system, a linearisation of the equations has to be made. For a state space representation of the system we use the state space vector:

$$x^T = (\Delta T_{so}, \Delta T_s, \Delta T_v, \Delta T_{re}, \Delta T_{vre}),$$

where Δ indicates deviation from working point.

The control action vector is:

$$u^T = (\Delta q_v, \Delta q_{vre})$$

If we write the system on matrix form:

$$\dot{x} = Ax + Bu$$
$$y = Cx$$

The matrices are given by:

$$A = \begin{bmatrix} a_{11} & 0{\cdot}0003076 & 0 & 0{\cdot}0001465 & 0 \\ 0{\cdot}0019091 & -0{\cdot}009655 & 0{\cdot}007745 & 0 & 0 \\ 0 & 0{\cdot}025357 & -\left(\dfrac{q_v}{4000} + 0{\cdot}025357\right) & 0 & 0 \\ 0{\cdot}0667 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0{\cdot}011904 & -\left(\dfrac{q_{vre}}{1000} + 0{\cdot}011904\right) \end{bmatrix}$$

Where coefficient a_{11} equals:

$$a_{11} = \left(\frac{1}{3M_{so}} \exp\left(a - \frac{8429{\cdot}86}{273 + T_{so}}\right) \frac{8429{\cdot}86}{(T_{so} + 273)^2} - \frac{105}{3M_{so}} - \frac{50}{3M_{so}}\right)$$

The matrices B and C equals:

$$B = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ \dfrac{1}{4000}(T_{vi} - T_v) & 0 \\ 0 & 0 \\ 0 & 0{\cdot}001(T_{vir} - T_{vre}) \end{bmatrix} \quad C = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

A linearisation around a typical point of operation gave the following corresponding time constants: 27sec, 132sec, 181sec, 560sec and 650sec.

For the jacket cooling a conventional PID controller was used and tuned after a root locus analysis.

The principles for the reflux cooler was:

- The reflux cooler should be put into action when the heat produced could not be removed by jacket cooling alone.

- Because of product quality considerations it was desired not to use the reflux cooler until it was necessary, i.e. until a certain extent of reaction was reached.
- Reflux cooling rate should be reasonably stable and hence not interact too much with the jacket cooling and give stability problems.
- Max. reflux cooling should be available when needed to give as high control margin as possible to the jacket cooling.
- A jacket cooling limit was defined. Reflux cooling is put into action by a hysteresis characteristics when this limit is exceeded.

Two alternative controller systems were tried for the reflux cooling:

- A proportional controller
- An integral controller with hysteresis as shown in Fig. 5 below.

Typical results with the two controller systems is shown below for batches of appr. 6 hrs.

As the Figs. 6 and 7 show, the hysteresis structure gives the best stability. In addition it gives more max. duty to the reflux cooler, leaving more freedom to the jacket cooling. In practice with varying parameters and the wish of high stability margin, the hysteresis controller is expected to be far better than proportional control. Fig. 8 shows the solution temperature with hysteresis controller.

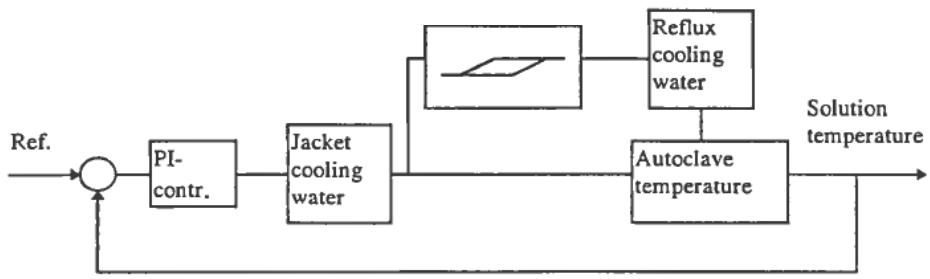

Figure 5. Hysteresis controller.

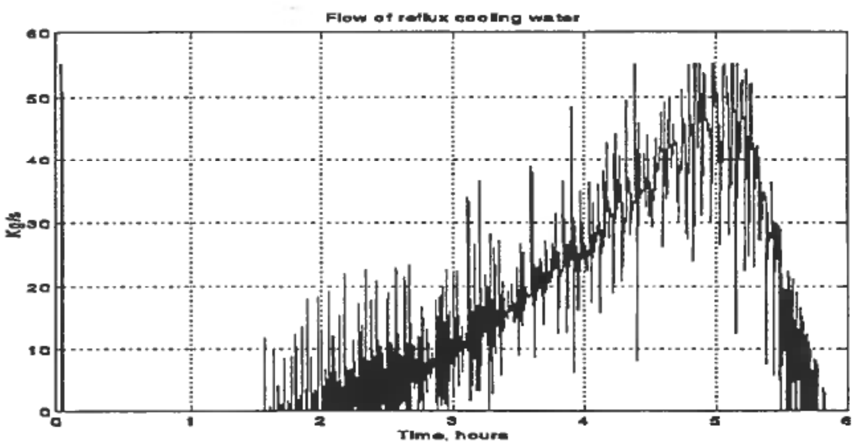

Figure 6. P-control of reflux cooling.

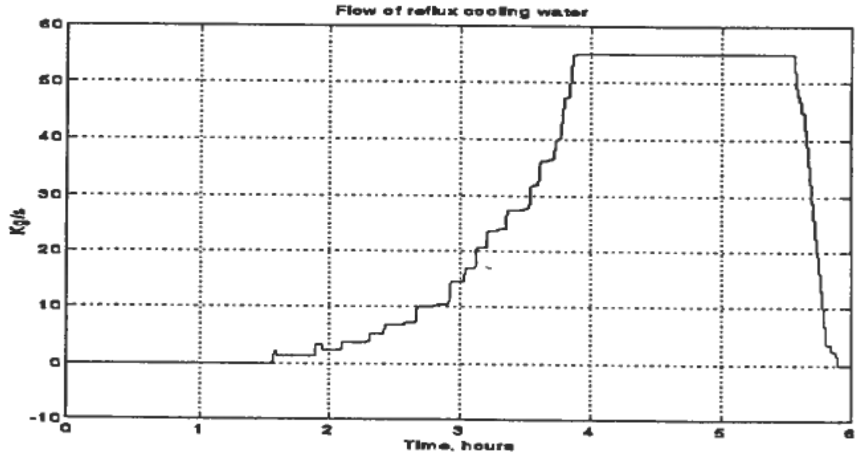

Figure 7. Hysteresis controller for reflux cooling.

3. Monitoring operator support and manual control

In this functional block the following functions illustrated in Fig. 2 are implemented: Static alarm functions, voting, signal validation and complex control functions. In addition advanced fault detection is implemented.

3.1. *Analaytical redundancy*

For model based fault detection or analytical redundancy, use of four methods are often reported over the last five–six years (Chen, J. *et al* 1995, Patton and Kangethe 1989, Chow and Willsky 1989, Isermann 1989)

- Unknown Input Observer
- Eigenstructure approach
- Chow-Willsky Parity Space approach.
- Identification based approach.

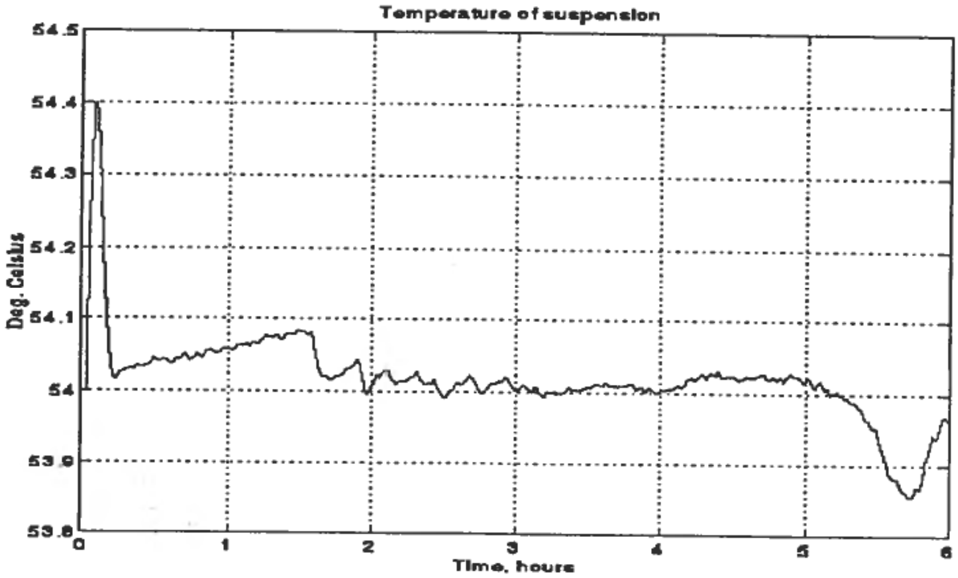

Figure 8. Solution temperature with hysteresis reflux controller.

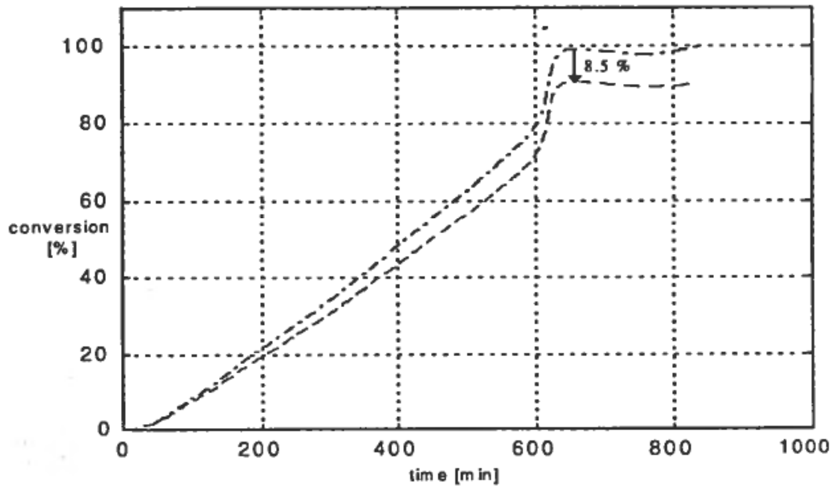

Figure 9. Comparison of reaction conversion estimated with Kalman filtering and calculation based on heat removal from autoclave.

The three first mentioned methods are based on linear (or regime linearised) models. This is not appropriate here with strongly varying operational conditions. Identification is difficult since the transformation between failures and corresponding offsets might be difficult.

Instead an extended Kalman filter was used, where the failures were estimated. The non-linear model and a continuous-discrete filter was used. There is need for an early warning and detection of the critical failure run-away. To find a fast estimate model

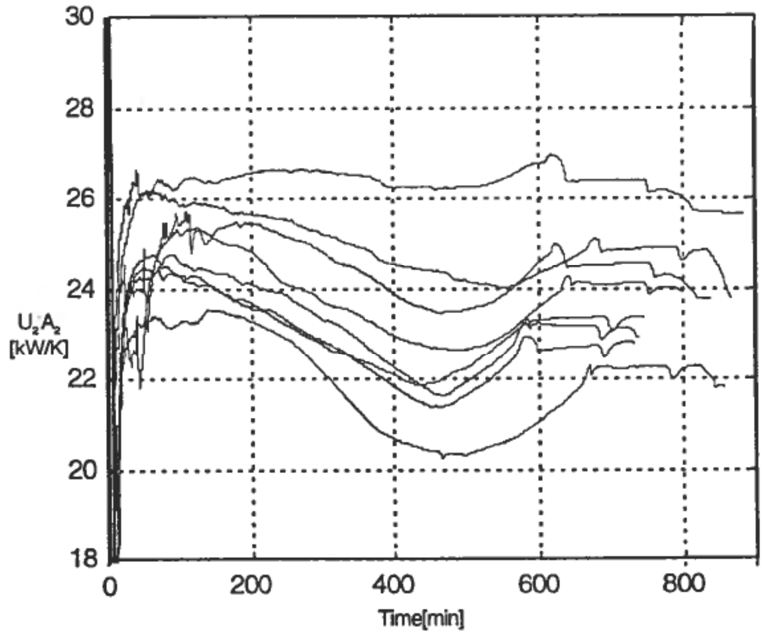

Figure 10. Variation in heat transfer coefficient.

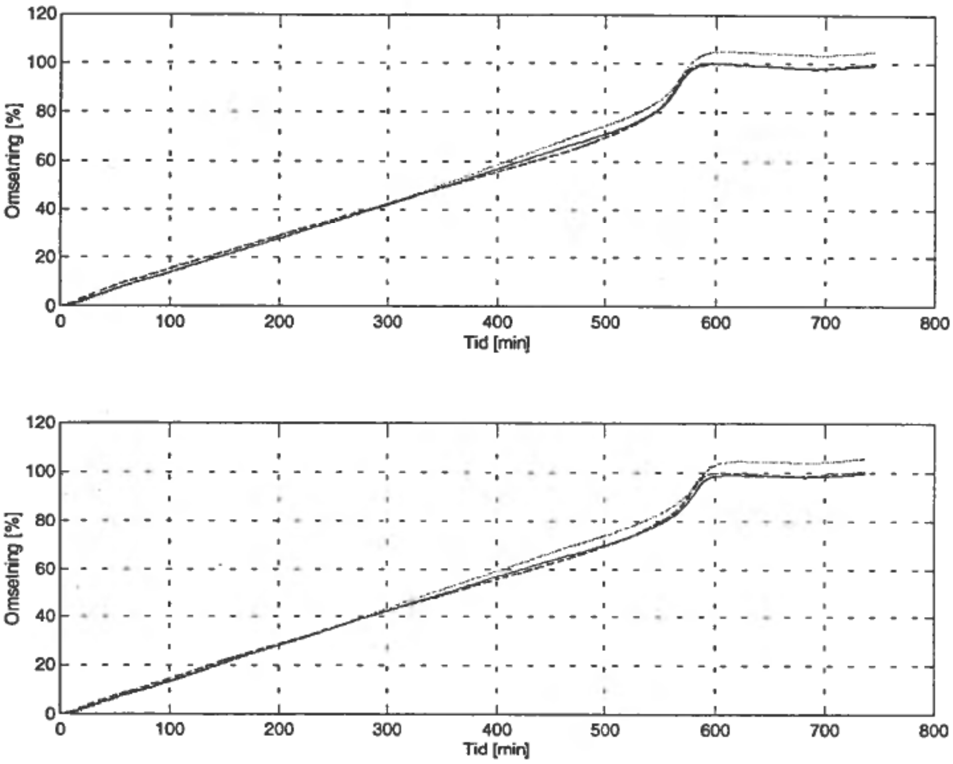

Figure 11. Two examples of: Comparison of conversion estimated with Kalman filter and calculated from heat removal.

based estimation of the heat of reaction was tried. The heat of reaction was modelled as:

$$\frac{dR_x}{dt} = 0 + w_{Rx}$$

In Fig. 9 is shown a run with estimator. The computed degree of reaction is shown. This is compared to a calculation based on the heat removal from the autoclave. There is a failure of app. 10%. The conclusion is that the estimate is inconsistent, and this inconsistency is due to model failures. The most uncertain parameter is the heat coefficient U_2A_2, as shown for several runes in Fig. 10.

It was then decided to try to estimate also this parameter in the filter, with the equation:

$$\frac{dA_2U_2}{dt} = 0 + w_{A2U2},$$

where w_{A2U2} is white noise.

Fig. 11 shows the conversion estimated from this extended Kalman filter which is compared to conversion calculation based on heat removal. The upper curves in the two examples are with constant A_2U_2. The two lower curves in each figure are with estimated A_2U_2 and computed conversion from heat removal. The consistence is now good.

In Fig. 12 a runaway situation is simulated. The R_x-estimate is compared to a heat of reaction calculation based on heat loss. This shows that the model based estimator responds much faster than the loss of heat calculation.

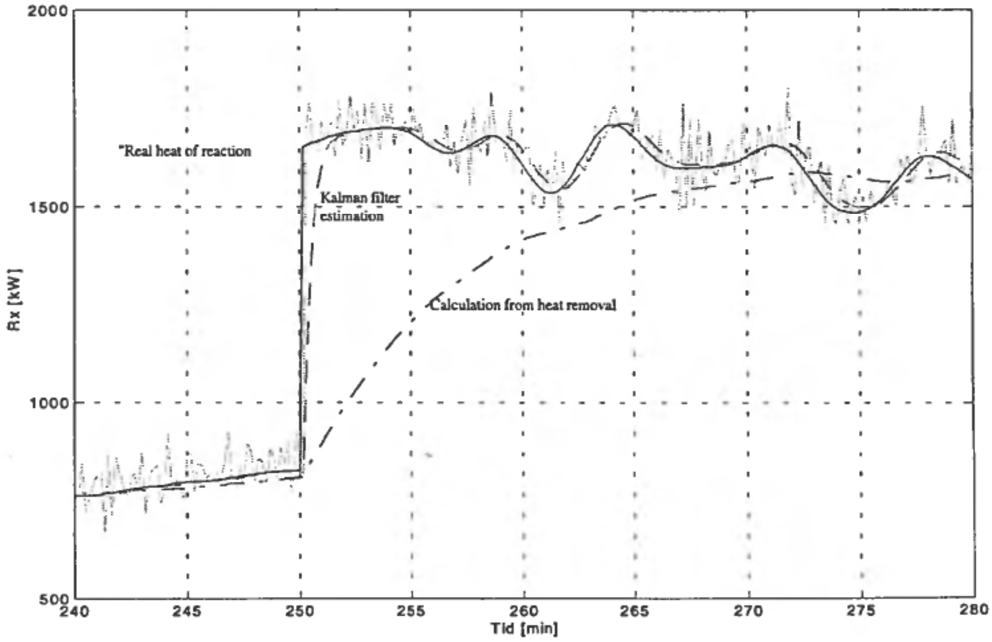

Figure 12. Kalman filter estimate compared to heat removal calculation.

4. Safety functions

Quantitative safety goals for the reactor system was set after corporate criteria. To see if these criteria were met, a fault tree analysis was performed. In such an analysis one has to estimate the reliability of the process, the instrumentation, the distributed control system and the instrument and mechanical safety systems. In addition the reliability of manual operations have to be calculated. Fig. 13 shows an example.

DCS or ISS failures:	Failure data are available from PDS-study (Reliability Protection Handbook 1989). ISS: Instrument Safety System, DCS: Distributed Control System.
Instrument failures:	Failure data are available from generic data banks, f. ex. OREDA (OREDA, 1992). These generic data must be compared to the plant application; maintenance, operation, process experience…
Operator failure:	These failure data must be obtained from careful studies of the operator work situation, the MMI…
Monitoring:	The quality of the monitoring system in the actual situations is important to failure probabilities.
Failure detection:	The design of the system with respect to detection of failures is important for the failure probabilities.

The presented fault tree is for a manually operated safety function. This is selected to show that manual operations also can be appropriate in safety situations. In the moderator addition the operator has to do several additions of moderator solution in order to control the reactor activity level. There is no clear model between action and result, and the operation has to be done in several steps by careful examination of the monitoring system. The manual control is more reliable than automatic control in this situation.

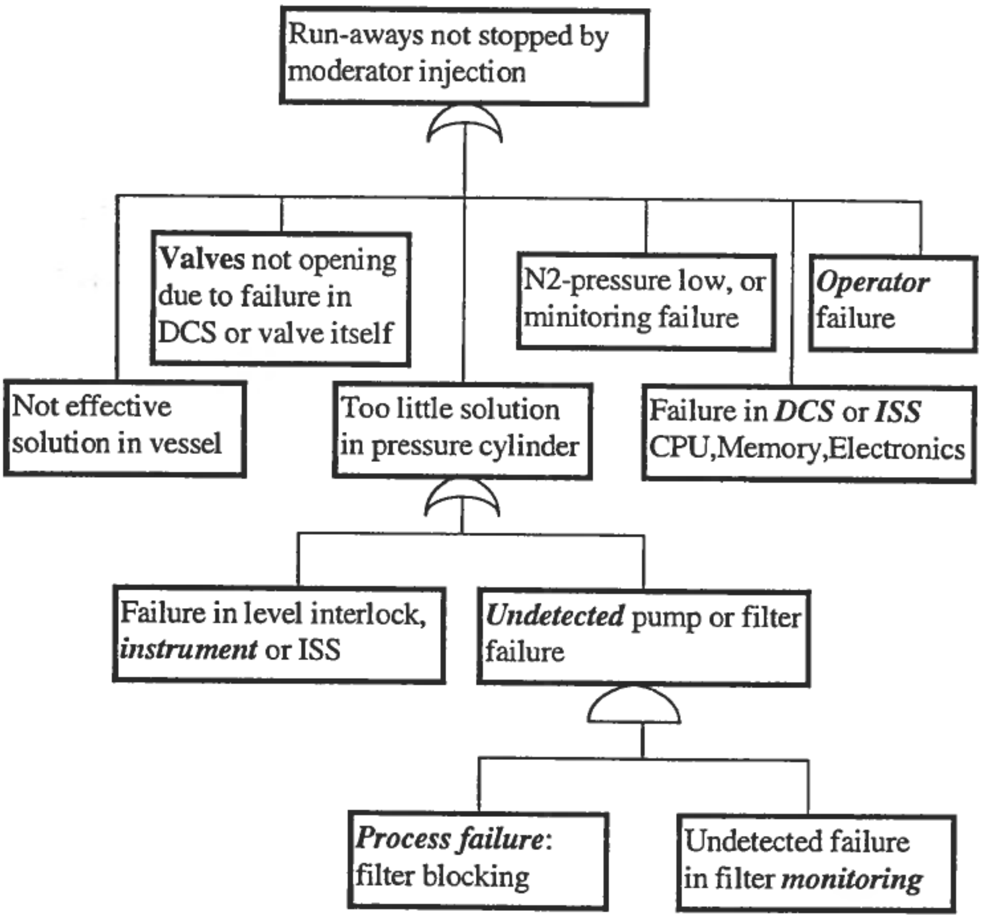

Figure 13. Example of fault tree from reliability analysis.

Of course most of the safety functions are totally automatic, many with possibility for additional initialisation from the operator. The philosophy is a high degree of redundancy to reduce the failure probability and diversity to reduce the amount of common mode failures:

- Mechanical and instrument based safety systems.
- Safety valves, duplicated stopper injection systems and blow down tank facility.
- A DCS and a separated, fault tolerant ISS.
- Safety philosophy also included in automatic control, monitoring and manual control as depicted in Fig. 2.

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