

On-line Estimation of Reactor Key Performance Indicators: An Industrial Case Study

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Abstract

On-line monitoring of key performance indicators of chemical processes is a crucial factor for fast operator response to abnormal operating conditions and for the long term optimization of the process operating point. While the scientific background for the design of such estimation algorithms has been well developed, the realization in the industrial environment is hardly documented. In this paper, the design and the implementation of on-line key performance indicators for a industrial Ketene reactor are described. The benefits of the on-line performance estimation were an additional 5% of productivity potential.

Keywords: performance indicators, soft sensors, on-line estimation

1 Introduction

The increasing competition on the global market requires ongoing improvements of the economic efficiency. While the widespread use of distributed control system has simplified the fundamental process operation, the presentation of the process state to human operators is still in form of simple measurement readings such as temperature, pressure, and flow rate. An on-line calculation and presentation of the real process performance indicators is barely found in the chemical industry, but has found some acceptance in the petrochemical area. In the following sections, the industrial implementation of such key performance indicators is described considering as example a Ketene process.

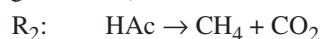
2 The Ketene process

2.1 The Ketene process

Ketene is an important raw material for the synthesis of a large variety of active agents for life science industries. Ketene is produced in large tubular reactors at high temperature and low pressure by cracking acetic acid under catalyst addition (Figure 1):



The yield of the process is limited by a number of side reactions which may produce undesired products such as carbon, carbon monoxide, or carbon dioxide (Meingast and Mugdan, 1924):



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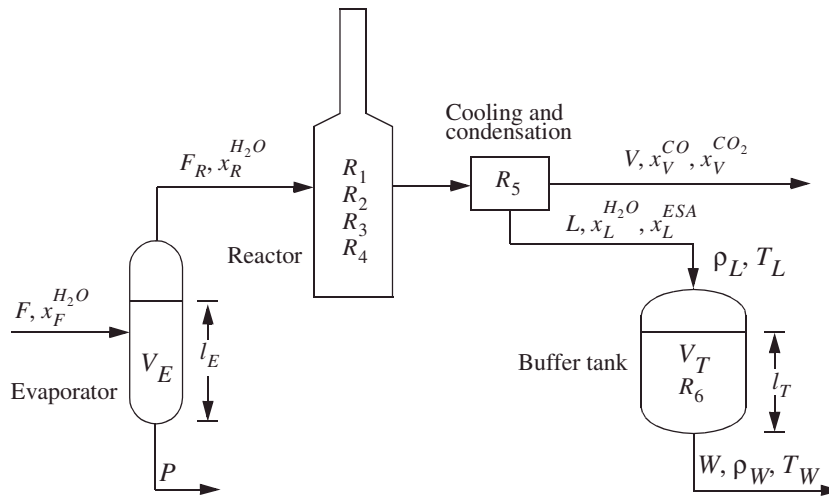
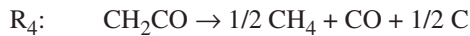
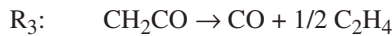
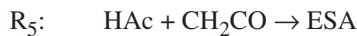


Fig. 1: Schematics of the ketene reactor

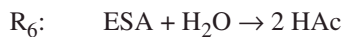


Since the rate of the side reactions R_2 - R_4 depends on the operating conditions (e.g. reactor temperature, catalyst feed rate, water content in feed) an optimal operating point must be maintained.

Further, in order to limit the amount of back reaction, the stream leaving the reactor is quickly cooled down. The water and unreacted acetic acid contained in the product stream is condensed and fed into a tank. In the quenching section, a small amount of ketene reacts to acetic acid anhydride (ESA):



In the buffer tank, ESA is hydrolysed to acetic acid:



Other reactions have been identified, but are of less importance to the process mass and energy balances.

2.2 Performance indicators

In order to optimize and track the reactor performance, an on-line estimation of the following key performance indicators was desired by the process operator:

$$\text{Acid conversion} \quad C = \frac{F_{\text{HAc}}^{\text{in}} - F_{\text{HAc}}^{\text{out}}}{F_{\text{HAc}}^{\text{in}}} \quad (1)$$

$$\text{Selectivity} \quad S = \frac{F_{\text{CH}_2\text{CO}}^{\text{out}} \frac{w_{\text{HAc}}}{w_{\text{CH}_2\text{CO}}}}{F_{\text{HAc}}^{\text{in}} - F_{\text{HAc}}^{\text{out}}} \quad (2)$$

$$\text{Yield} \quad Y = \frac{F_{CH_2CO}^{out} \frac{w_{HAc}}{w_{CH_2CO}}}{F_{HAc}^{in}} \quad (3)$$

Other project targets were reliable operation of the estimation algorithms and the sensors, low maintenance cost, implementation in the control system, and sufficiently fast response to changes of process conditions.

3 Process model

3.1 Mass balance

Since the performance indicators can not be measured directly, they must be inferred from the measurement signals and the process mass balance. The steady state component balance equation for the process can be given in terms of feed to reactor F_R , the ketene gas V , and liquid flow L_W leaving the buffer tank:

$$\begin{aligned} Fx_{HAc}^F - r_1 &= Vx_{HAc}^V + Lx_{HAc}^L \\ Fx_{H_2O}^F + r_1 &= Vx_{H_2O}^V + Lx_{H_2O}^L \\ Fx_{CH_2CO}^F + r_1 - (r_3 + r_4) &= Vx_{CH_2CO}^V + Lx_{CH_2CO}^L \\ Fx_{CO_2}^F + r_2 &= Vx_{CO_2}^V + Lx_{CO_2}^L \\ Fx_{CO}^F + r_3 + r_4 &= Vx_{CO}^V + Lx_{CO}^L \\ r_5 &= (Vx_V^{ESA} + F_L x_L^{ESA}) (w_{HAc}^{HAc} / w_{ESA}^{ESA}) \end{aligned} \quad (4)$$

The CO and CO₂ composition in the feed and in the liquid flow L are below significance. Further, if the outlet temperature of the gas stream leaving the coolers is sufficiently low and spray forming does not occur in the condensation, the water flow in the gas phase is a factor 100 and the HAc is a factor 50 smaller than in the liquid phase. Consequently, neglecting all other reactions apart from R₁-R₅, the mass balance can be reduced to:

$$\begin{aligned} Fx_{H_2O}^F + r_1 &= Lx_{H_2O}^L \\ r_2 &= Vx_{CO_2}^V \\ (r_3 + r_4) &= Vx_{CO}^V \\ r_5 &= F_L x_L^{ESA} \frac{w_{HAc}^{HAc}}{w_{ESA}^{ESA}} \end{aligned} \quad (5)$$

3.2 Calculation of the performance indicators

The performance indicators (1)-(3) can be written in terms of the reaction rates r_1 - r_5 :

$$\text{Acid conversion} \quad C = \frac{r_1}{Fx_{HAc}^F} \quad (6)$$

$$\text{Selectivity} \quad S = \frac{r_1 - r_2 - (r_3 + r_4) - r_5}{r_1} \quad (7)$$

$$\text{Yield} \quad Y = \frac{r_1 - r_2 - (r_3 + r_4) - r_5}{F_R x_R^{HAc}} \quad (8)$$

4 Design of the estimation algorithm

4.1 Measuring set

It was shown before, that the calculation of the performance indicators can be reduced to an estimation of the reaction rates r_1 - r_5 and to the reactor feed rate and feed composition. If perfect measuring devices for the signals given below would be available, the rate of reactions could be accurately determined according to the balance equations (5):

- Feed rate to reactor, water content in reactor feed
- Liquid and vapor flow rate after the cooling zone
- CO and CO₂ concentration in the product stream
- ESA concentration in liquid flow leaving the condensate

It is rather typical for chemical and petrochemical plants, that hundreds of sensors are installed, but the sensors required for more advanced dynamic estimation or control applications are missing. In case of this case study, none of the measurement signals given above was available at project start. Further, due to corrosion and fouling neither the vapour flow rate V nor the liquid flow rate L can be measured.

4.2 Outline of the estimator design

A sketch of the main building blocks of the estimator is given in figure 2. In order to keep the cost for additional sensors at a minimum level, reactor feed flow rate and composition, as well as the liquid flow rate L and composition are estimated using standard flow, level and density measuring devices. Since the holdup of the gas phase is very small, the process dynamics is dominated by liquid phase holdups. Therefore the dynamics of the evaporator and the buffer tank were incorporated into the estimator design using extended Kalman filter techniques (Gelb 1994).

Reactor feed flow rate and water content. The following equations give some insight into the online calculations performed by the first Kalman filter. Please note that the feed composition to the reactor is not observable, since only the water concentration in the

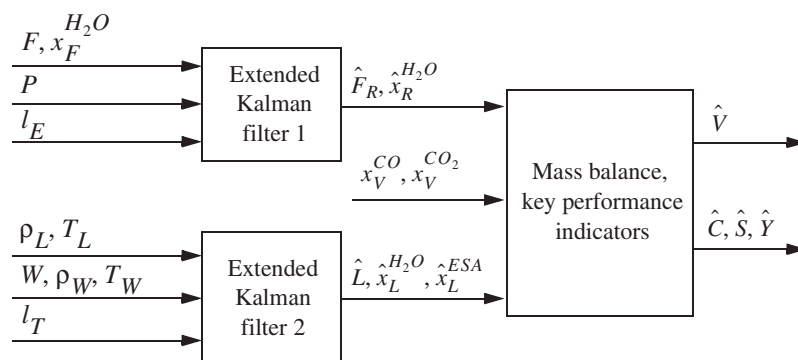


Fig. 2: Main signal flow in the estimator

evaporator feed is inferred from the liquid density. In the estimation algorithm, the differential equations for the evaporator holdup and the water content are integrated with the Euler method using a fixed step size t_s :

Error between the volume estimated and predicted:

$$e_E(t) = V_E(t) - \hat{V}_E(t) = [l_E(t)A_E + V_E^0] - \hat{M}_E(t)/\rho_E \quad (9)$$

Vapour-liquid equilibrium for the acetic acid/water mixture in evaporator 702:

$$\hat{x}_R^{H_2O} = \frac{\alpha \hat{x}_E^{H_2O}}{(\alpha - 1) \hat{x}_E^{H_2O} + 1} = \frac{2.25 \hat{x}_E^{H_2O}}{1.25 \hat{x}_E^{H_2O} + 1} \quad (10)$$

State update for mass in evaporator 702:

$$\begin{aligned} \hat{M}_E(t + t_s) &= \left[\hat{M}_E(t) + \frac{d\hat{M}_E(t)}{dt} t_s \right] + k_1 e_E(t) \\ &= \hat{M}_E(t) + (F(t) - P(t) - F_R(t)) t_s + k_1 e_E(t) \end{aligned} \quad (11)$$

Update of flow rate to reactor:

$$\hat{F}_R(t + t_s) = \hat{F}_R(t) + k_2 e_{M702}(t) \quad (12)$$

Prediction of water content in evaporator:

$$\begin{aligned} \hat{x}_E^{H_2O}(t + t_s) &= \hat{x}_E^{H_2O}(t) + \frac{d\hat{x}_E^{H_2O}(t)}{dt} t_s \\ &= \hat{x}_E^{H_2O}(t) + \left(\frac{F(t)}{M_E(t)} (x_F^{H_2O}(t) - \hat{x}_E^{H_2O}(t)) - \frac{F_R(t)}{M_E(t)} (\hat{x}_R^{H_2O} - x_E^{H_2O}(t)) \right) t_s \end{aligned} \quad (13)$$

Liquid flow rate and composition. The design of the second Kalman filter is far more involved, as it takes into account the ESA hydrolysis (R_6). This reaction causes a small difference in liquid density (temperature compensated) between the liquid flow L and the waste stream W. This difference is sufficient for a slow adjustment of the ESA concentration within the filter.

Mass balance and key performance indicators. The calculation of the performance indicators based on the Kalman filter estimates is straightforward. These calculations include the CO and CO₂ concentration in the Ketene gas, which will be discussed in the next section.

5 CO/CO₂ sensor

A laser operated spectrometer measures the CO/CO₂ concentrations using their characteristic stretching frequencies. To avoid loss of beam transmittancy by fouling, the optical window-system is purged with nitrogen. Calibration of the spectrometer affords specific attention and was achieved in two steps:

- Calibration with pure calibration gas
- Cross-checking the consistency of the spectrometer output by data reconciliation, using overall plant-redundancy (Dempf and List 1998, Belsim 2002).

6 Implementation

After installation of the CO/CO₂ sensor during a plant maintenance period, the estimation algorithms were decomposed in basic arithmetic operations and fully implemented in the control system. This approach requires more engineering effort, but eliminates maintenance cost and trouble caused by interfaces between a PC and the distributed control sys-

tem. After an initial observation period, some fine tuning of the filter parameters k , and an adjustment of a density measuring device, the key performance indicators were commissioned and placed at the disposal of the plant operating staff.

7 Practical experiences

Since the process is always operating close to steady state, usually the key performance indicators show some fluctuation around their long term average. In figure 3, however, a significant drop of the selectivity is shown. It was caused by a failure of the steam supply to the evaporator. The reduction of the reactor feed increased the residence time which favoured the cracking reactions R_3 and R_4 . An additional 5% of productivity potential hidden under process noise was exploited, even at the plants advanced life-cycle.

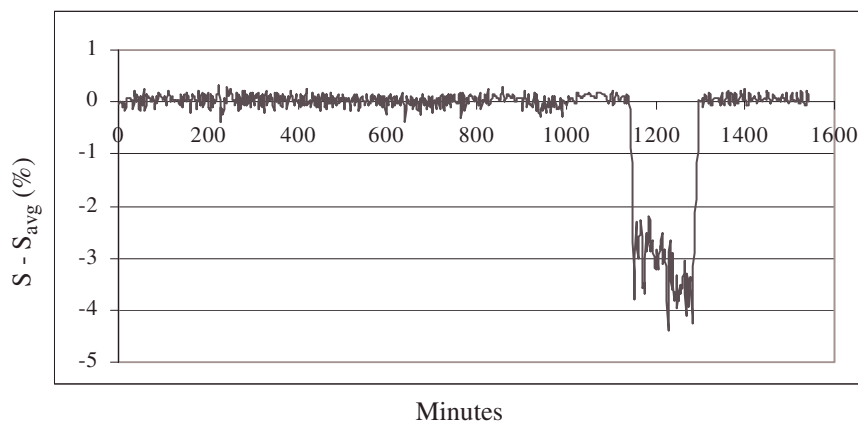


Fig. 3: Estimated selectivity S over 25 day period.

8 Conclusions

The step from estimation theory into industrial operation is by no means simple. Successful implementations are based on an interdisciplinary cooperation between experts for sensor technology, control systems, algorithm design, and chemists. Further, even the most advanced estimator design can not always rely on “standard” measuring devices only. Since for many projects the on-line composition analysis is a limiting factor, each stage of development of such sensors will have a significant impact on the acceptance and application of these techniques. Typically, the payback period for such projects is rather short as the improved insight into the process allows tracking of the optimal operating point.

9 References

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