Nonlinear State Estimation Methods – Overview and Application to PET Polymerization

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Outline

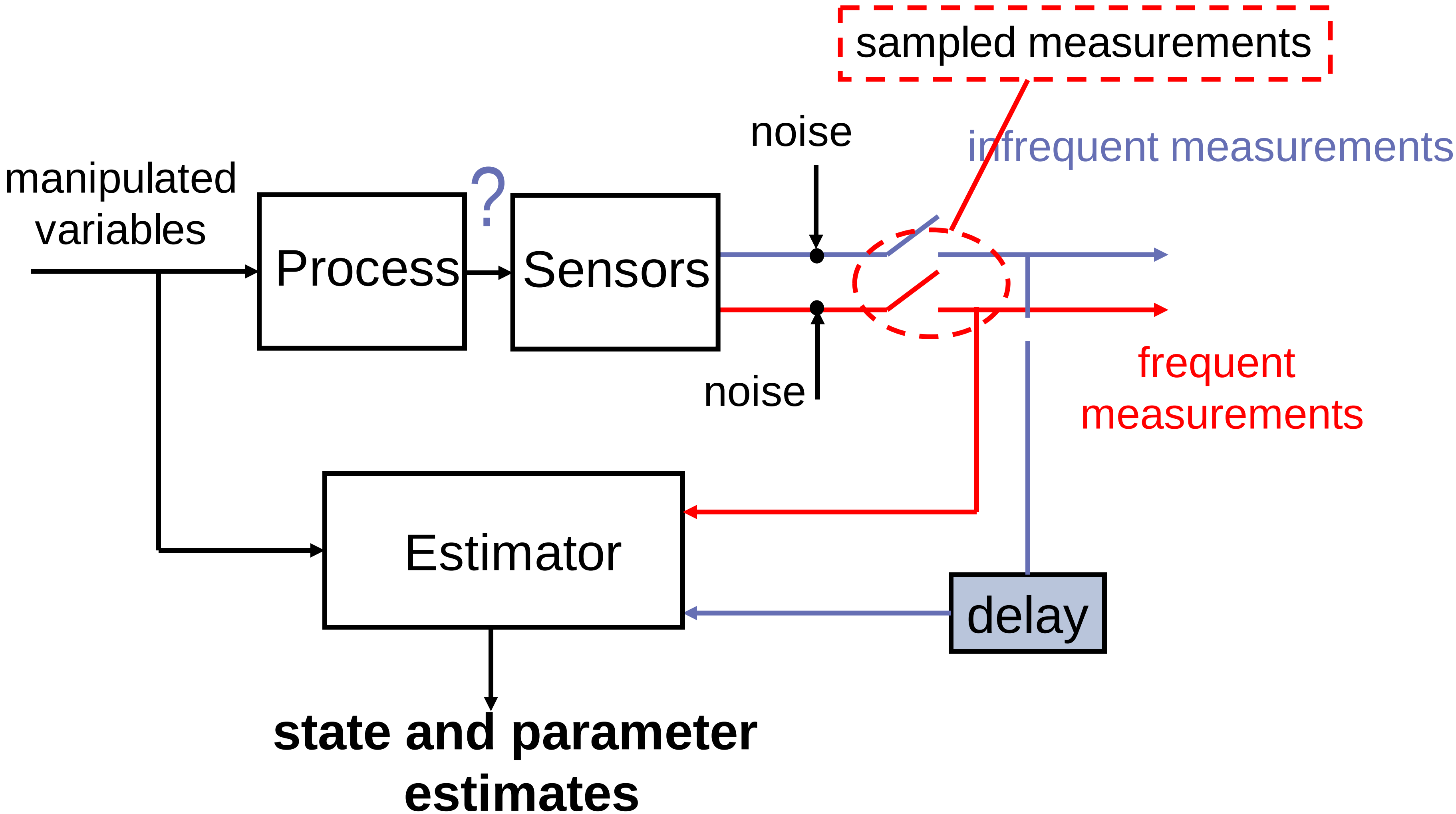
- Introduction
- Approaches to nonlinear state estimation
- Application to PET polycondensation
- Multirate estimation
- Conclusions

Introduction

- Important product qualities are not measureable online but they are needed for control purposes.
- Measurements are often available at different sampling intervals.
- Analytic measurements cause time delays.

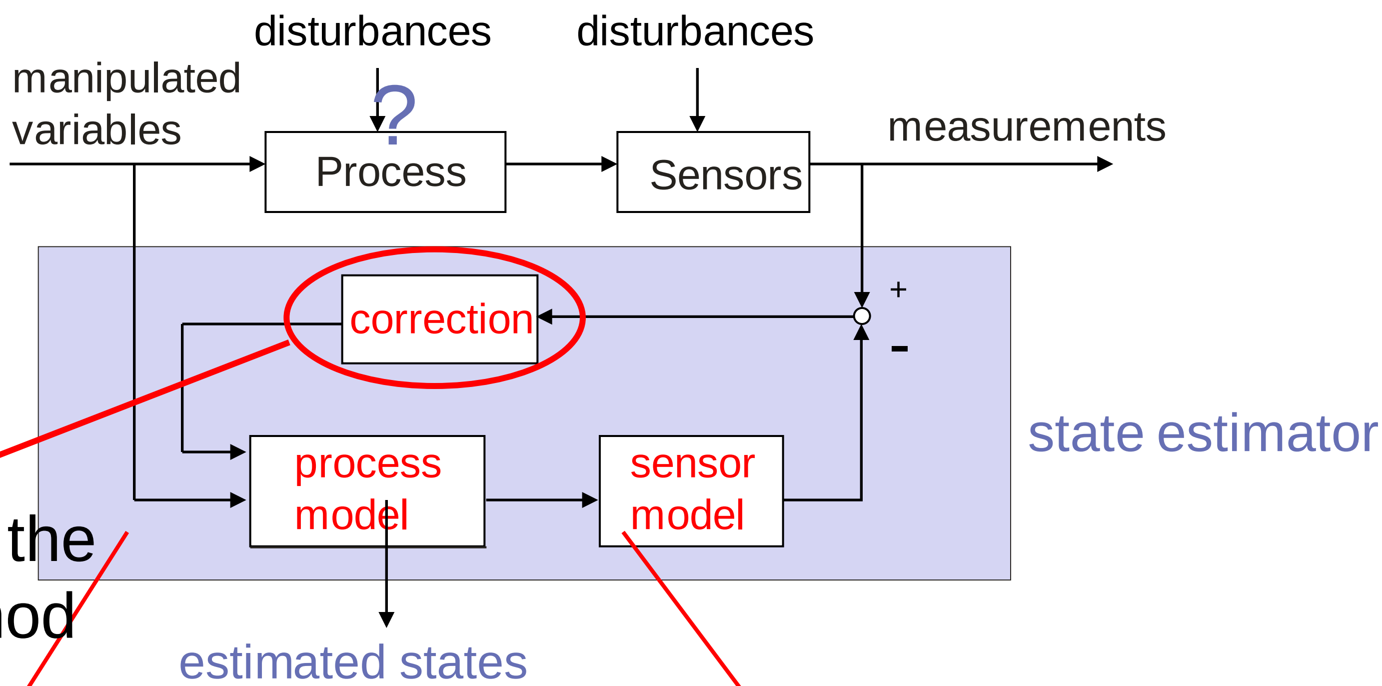
  ⇒ State estimation can provide additional online information.
- Numerous approaches are available: Which one should be applied?
- How can offline analyses be incorporated in state estimation?
  - Black Box Modelling (Neural Nets, …)
  - Extended approaches are necessary to consider measurements with different sampling intervals.

Introduction: Application of State Estimation



Nonlinear State Estimation

- Basic principle of state estimation



depends on the design method

$$\dot{x} = f(x, u, t) \qquad y = h(x)$$

Approaches to Nonlinear State Estimation

- Process model is given as ODE-system or system of difference equations

$$\dot{\hat{x}} = f\left(\hat{x}, u, t, y\right) \qquad \hat{x}_{k+1} = F\left(\hat{x}_k, u_k, t_k, y_k\right)$$

$$\hat{y} = h\left(\hat{x}\right) \qquad \hat{y}_k = H\left(\hat{x}_k\right)$$

- The estimator must fulfill:
  - Simulation condition:
    if $x\left(t = t_0\right) = \hat{x}\left(t = t_0\right)$ then $x\left(t\right) = \hat{x}\left(t\right) \forall\, t > t_0$
  - Convergence condition:

$$\lim_{t \to \infty}\left(x\left(t\right) - \hat{x}\left(t\right)\right) = 0$$

for all inputs *u(t)* and for all inital errors.

Observability

- **Theory:**
  - Assume a linear system: $\dot{x} = Ax + Bu\,,\; y = Cx$ with $x \in \Re^n, y \in \Re^p$
  - The state variables of the system (A, C) can be divided into two groups:
    - **Observable states**:
      The error dynamics can be prescribed arbitrarily by choice of the observer gains and are independent of the states and the known inputs.
    - **Unobservable states**:
      the error dynamics are given by the (unobservable) eigenvalues of the system.
  - **Definition:** A linear system is said to be observable, if the matrix $Q = [C^T, A^T C^T, (A^T)^2 C^T, \dots (A^T)^{n\text{-}1} C^T]$ has rank *n*. In this case, all states are observable.

Observability of Nonlinear Systems

- **Theory:**
  - Assume a nonlinear system: $\dot{x} = f(x,u),\ y = h(x)$
  - **Definition:**
    A nonlinear system is said to be globally observable, if all initial states $x_0 \in X_0$ can be computed from observations of the output y(t) over an arbitrary interval of time. The states are then called observable.
  - **Definition:**
    A nonlinear system is said to be locally observable at $x_1 \in X_0$, if initial states $x_0 \in X_0$ in the neighborhood of x_1 are observable.

  - To check global observability a unique solution for the nonlinear observability map has to be found.
  - Local observability can be checked using the linearized model (see conditions for linear models).

State and Parameter Estimation

- Observers can be extended to the **estimation** of **unknown process parameters**.
- The parameters are assumed to be additional state variables with dummy dynamics.

$$\dot{\hat{x}} = f\left(\hat{x}, u, \hat{p}\right)$$

$$\dot{\hat{p}} = 0$$

- Observability in general becomes worse if more parameters must be estimated.
- The number of unknown parameters which can be estimated is restricted by the number of measurements!

Approaches to Nonlinear State Estimation

- **Gain Scheduled Observer (Luenberger observer with gains that depend on the estimated states and the inputs)**
  - **Observer equations:**

$$\dot{x} - \dot{\hat{x}} = \dot{\tilde{x}} = f(x,u) - f(\hat{x},u) - K(\hat{x},u)\left(y - h(\hat{x})\right)$$

$K(\hat{x},u)$ calculated by eigenvalue placement for linearized error dynamics

$$\lambda_i\left(I - \left(\left.\frac{\partial f}{\partial x}\right|_{\hat{x},u} - K\left.\frac{\partial h}{\partial x}\right|_{\hat{x},u}\right)\right) = \lambda_{i,\text{desired}}$$

  - Low effort for design
  - Performance and stability only are guaranteed close to a fixed (slowly varying) operating point.

Approaches to Nonlinear State Estimation

- **Sliding Mode Observer:**
  - For nonlinear systems of the form:

Measured nonlinearity

Bounded nonlinearities not measured

$$\dot{x} = Ax + \alpha(y,u) - E\Psi(x,u), \quad x(0) = x_0$$

$$\Psi(x,u) \in \Re^w \text{ with } \|\Psi(x,u)\| \leq \rho(u) \quad \forall \quad x \in \Re^n$$

$$y = Cx \text{ and } \quad y \in \Re^m$$

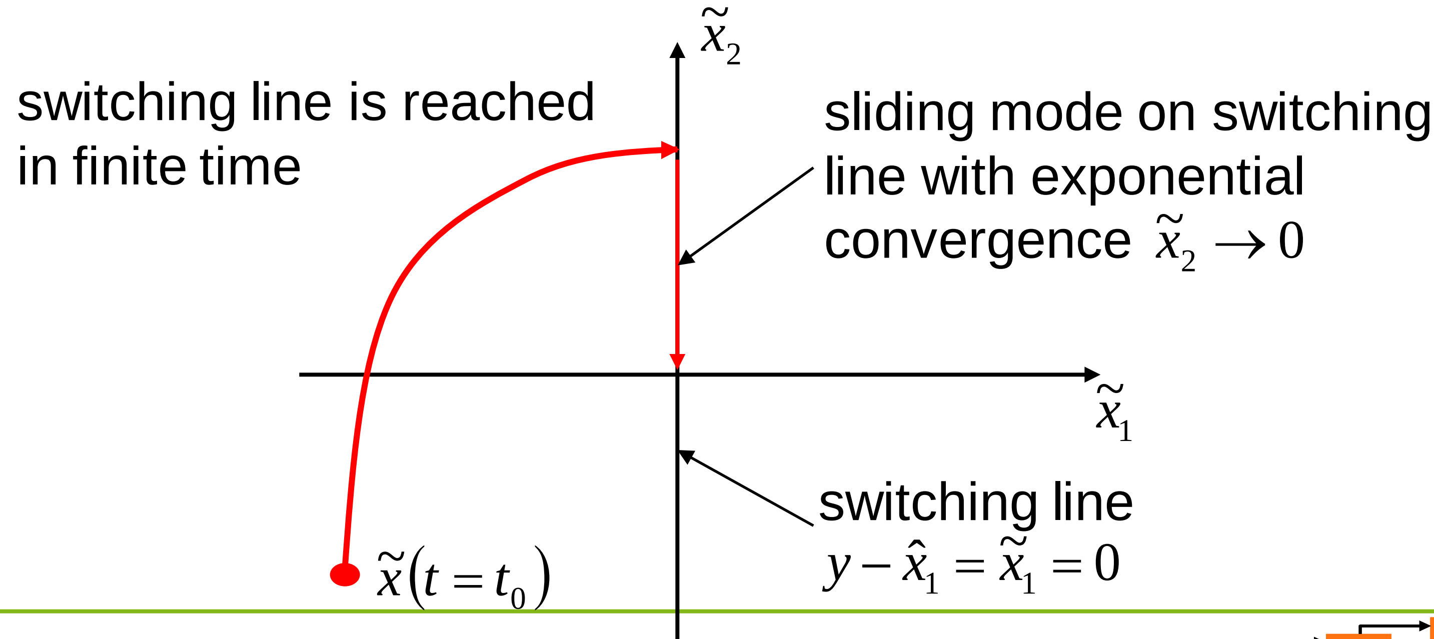
  - Number of measurements ≥ number of unmeasured nonlinearities $\Psi(x,u)$
  - Observer equation:

$$\dot{\hat{x}} = A\hat{x} + \alpha(y,u) + \rho(u)E\frac{D(y - C\hat{x})}{D\|y - C\hat{x}\|} + G(y - C\hat{x}), \quad \hat{x}(0) = x_0$$

  - P,D,G are weighting matrices which have to be determined in an iterative manner (an implicit Ljapunov equation has to be solved).

Sliding Mode Observer

- **Properties of the SMO:**
  - Large effort for design
  - Guaranteed global stability
  - Convergence in 2 steps:
    1. Movement to the switching plane: $y - C\hat{x} = 0$
    2. Sliding on the switching plane until the desired state is reached.



Extended Kalman Filter

- Extension of the model equations by stochastic errors (zero mean and given variance)

$$\dot{x} = f(x,u,t) + \xi$$
$$y = h(x) + \omega$$

- Filter minimizes the variance of the estimation error:

$$E\left\{(x-\hat{x})^T (x-\hat{x})\right\} = E\left\{\tilde{x}^T \tilde{x}\right\} \rightarrow \text{Min}$$

- For nonlinear time discrete (sampled) systems the solution is a 2-step-algorithm:
  - Correction of the predicted states and estimated covariance matrix $P = E\left\{(x_i - \hat{x}_i)(x_i - \hat{x}_i)^T\right\} = E\left\{\tilde{x}_i \tilde{x}_i^T\right\}$ after a new measurement was obtained
  - Prediction of the states and the covariance matrix of the estimation error up to the next time step by nonlinear forward simulation

EKF Algorithm

- Notation: Estimated state at $t=t_{k+1}$ based on measurements up to $t=t_k$

  $\hat{x}_{k+1,k}$
- Correction:

$$K_k = P_{k,k-1} H_{k,k-1}^T \left(H_{k,k-1} P_{k,k-1} H_{k,k-1}^T + R \right)^{-1}$$

$$\hat{x}_{k,k} = \hat{x}_{k,k-1} + K_k \left(y_k - h\left(\hat{x}_{k,k-1}\right)\right)$$

$$P_{k,k} = \left(I - K_k H_{k,k-1} \right) P_{k,k-1}$$

- Prediction:

$$\hat{x}_{k,k+1} = F\left(\hat{x}_{k,k}, u_k\right)$$

$$P_{k,k+1} = A_{k,k} P_{k,k} A_{k,k}^T + Q \quad \text{with} \quad A_{k,k} = \left.\frac{\partial f}{\partial x}\right|_{\hat{x}_{k,k}} \quad \text{and} \quad H_{k,k-1} = \left.\frac{\partial h}{\partial x}\right|_{\hat{x}_{k,k-1}}$$

- Constraints on states and disturbances cannot be considered.
- Only (at best) local stability!
- The critical part is the update of the covariance matrix based on the linearized state equations.

Batch Estimation

- Suppose k values of the process inputs and of the measured variables are available. Then the estimation of the corresponding states can be formulated as an optimization problem:

$$\min_{\hat{\xi}_j, \hat{\varphi}_j} \left(\Psi_k = \hat{\xi}_{0,k}^T P_0^{-1} \hat{\xi}_{0,k} + \sum_{j=1}^{k-1} \hat{\xi}_{j,k}^T Q^{-1} \hat{\xi}_{j,k} + \sum_{j=1}^{k} \hat{\varphi}_{j,k}^T R^{-1} \hat{\varphi}_{j,k} \right)$$

Subject to

$$\hat{x}_{0,k} = \hat{x}_{0,0} + \hat{\xi}_{0,k}$$

$$\hat{x}_{j,k} = F\left(\hat{x}_{j-1,k}, u_{j-1}\right) + \hat{\xi}_{j,k} \qquad j = 1, \ldots, k-1$$

$$y_j = h\left(\hat{x}_{j,k}\right) + \hat{\varphi}_{j,k} \qquad j = 1, \ldots, k$$

- In this formulation, there are no assumptions on the statistics of the errors.
- No linearization is performed!
- Nonlinear optimization problem!
- Computational effort increases with k → reduce to a finite horizon!

Moving Horizon State Estimation

- Further motivation for a deterministic observer based on numerical optimization:
  - Possiblity of imposing constraints on states and disturbances
- **Moving Horizon Estimator (MHE):**
  - Takes measurements over a finite horizon in the past into account
  - No approximation of the nonlinear system within this horizon
  - Model: Discrete-time nonlinear system

$$x_{k+1} = F(x_k, u_k) + \xi_k$$
$$y_k = h(x_k) + \varphi_k$$

Moving Horizon State Estimator

- The Moving Horizon Estimator can be formulated as:

Minimize the error

$$\min_{\hat{\xi}_{k-N-1,k},\ldots,\hat{\xi}_{k-1,k},\hat{\varphi}_{k-N,k},\ldots,\hat{\varphi}_{k,k}} \Psi_k^N = \hat{\xi}_{k-N-1,k}^T \mathbf{P}_{k-N}^{-1} \hat{\xi}_{k-N-1,k} + \sum_{j=k-N}^{k-1} \hat{\xi}_{j,k}^T \mathbf{Q}_k^{-1} \hat{\xi}_{j,k} + \sum_{j=k-N}^{k-1} \hat{\varphi}_{j,k}^T \mathbf{R}_k^{-1} \hat{\varphi}_{j,k}$$

$$s.t.: \quad \hat{\mathbf{x}}_{j+1,k} = \mathbf{F}\left(\hat{\mathbf{x}}_{j,k}, \mathbf{u}_j\right) + \hat{\xi}_{j,k} \qquad j = k-N,\ldots,k-1$$

$$\hat{\mathbf{x}}_{k-N,k} = \hat{\mathbf{x}}_{k-N,k-N-1} + \hat{\xi}_{k-N-1,k}, \qquad \mathbf{y}_j = \mathbf{h}\left(\hat{\mathbf{x}}_{j,k}\right) + \hat{\varphi}_{j,k}$$

Model equations

$$\xi_{\min} \le \hat{\xi}_{k,k} \le \xi_{\max}, \qquad \varphi_{\min} \le \hat{\varphi}_{k,k} \le \varphi_{\max}, \qquad \mathbf{x}_{\min} \le \hat{\mathbf{x}}_{k,k} \le \mathbf{x}_{\max}$$

Physical or other constraints

Constrained Extended Kalman Filter (CEKF)

- For a horizon of N=0 the MHE becomes the Constrained EKF
- CEKF equations:

$$\min_{\hat{\xi}_{k-1,k},\hat{\varphi}_{k,k}} \left(\Psi_k^0 = \hat{\xi}_{k-1,k}^T P_k^{-1} \hat{\xi}_{k-1,k} + \hat{\varphi}_{k,k}^T R^{-1} \hat{\varphi}_{k,k} \right)$$

subject to

$$\left.\begin{aligned} \hat{x}_{k,k} &= \hat{x}_{k,k-1} + \hat{\xi}_{k-1,k} \\ y_k &= h\left(\hat{x}_{k,k}\right) + \hat{\varphi}_{k,k} \end{aligned}\right\} \text{ equal. constr.}$$

$$\hat{x}_{k,k+1} = F\left(\hat{x}_{k,k}, u_k\right)$$

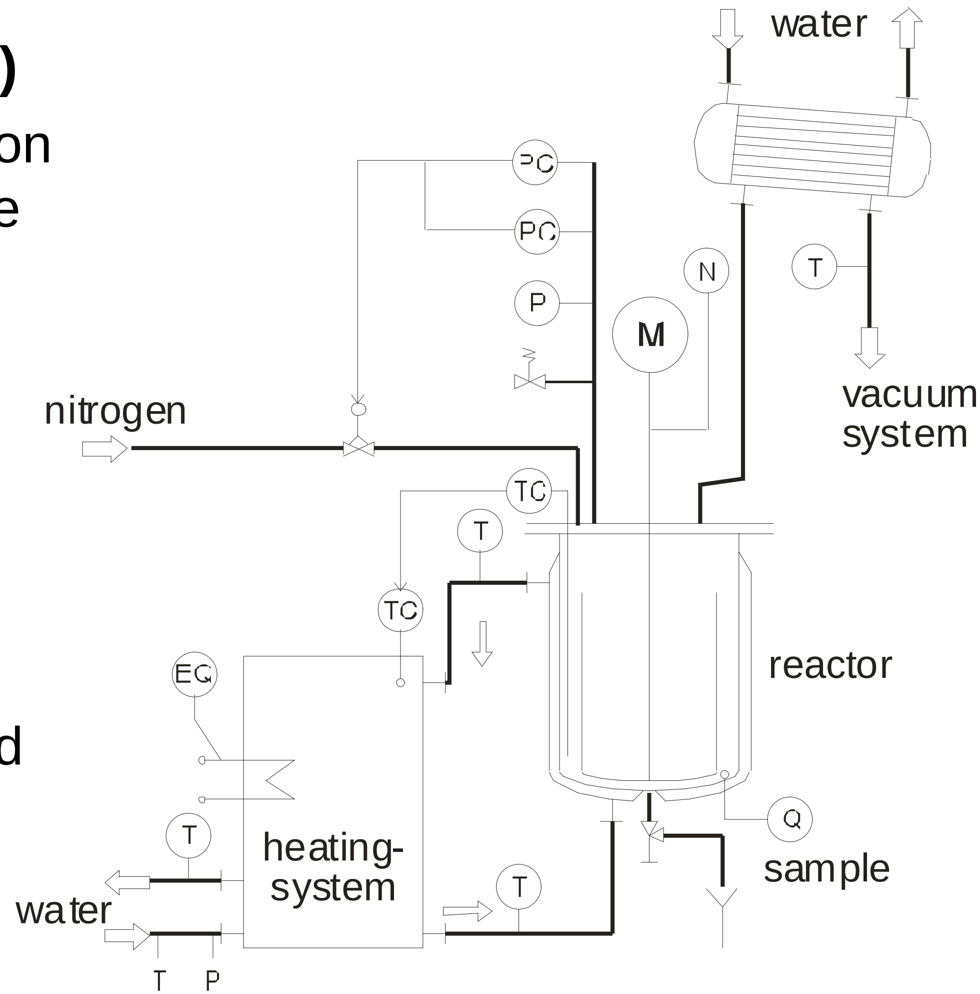
$$P_{k,k+1} = A_{k,k} P_{k,k} A_{k,k}^T + Q \quad \text{with} \quad A_{k,k} = \left.\frac{\partial f}{\partial x}\right|_{\hat{x}_{k,k}} \quad \text{and } H_{k,k-1} = \left.\frac{\partial h}{\partial x}\right|_{\hat{x}_{k,k-1}}$$

plus additional constraints on errors and states

- Quadratic problem for linear measurement function

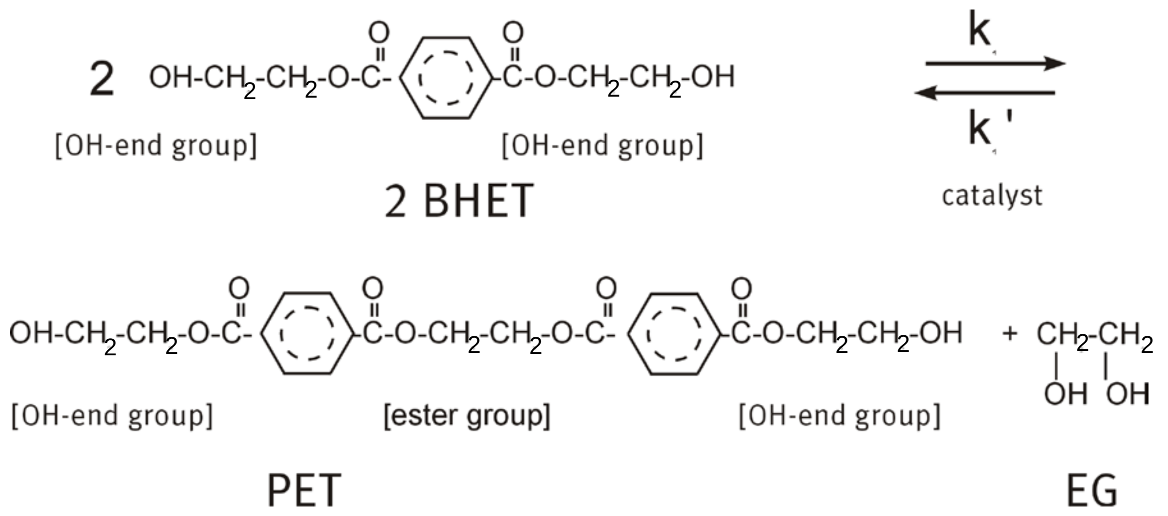
Case-Study: Polycondensation of PET

- **Polycondensation of polyethylenterephtalate (PET)**
  - The mass transfer of a reaction byproduct from the melt to the gas phase determines the progress of the poly-condensation process.
  - No measurements of mass transfer coefficients under industrial process conditions available
  - Process realized in a jacketed 10 l stainless steel reactor controlled by a DCS (Contronic-P, ABB)



PET Polycondensation

- Batch process, polymerization in the melt
- Main chemical reaction:



- The reverse reaction is 8 times faster than the forward reaction
- The removal of ethyleneglycol (EG) determines the speed of the polymerization

PET Polycondensation

- Main and side reactions:
  - -[OH] + -[OH] $\rightleftarrows$ -[E]- + EG (polymerisation)
  - -[E]- $\longrightarrow$ -[COOH] + -[$CO_2C_2H_3$] (thermal degradation)
  - -[COOH] + EG $\rightleftarrows$ -[OH] + H_2O
  - -[COOH] + -[OH] $\rightleftarrows$ -[E]- + H_2O
  - -[OH] $\longrightarrow$ -[COOH] + CH_3CHO
  - -[$CO_2C_2H_3$] + -[OH] $\longrightarrow$ -[E]- + CH_3CHO

- Mathematical modelling yields a system of differential equations for the concentrations of hydroxy group -[OH], ethylene glycol EG, carboxyl group -[COOH], acetaldehyde CH_3CHO, vinyl group -[$CO_2C_2H_3$], ester group -[E] and water H_2O

Model Reduction

- Model of 7^{th} order too complex, several unknown mass transfer parameters
- Simplification by:
  - Neglecting the side reactions
  - Estimation of the thermal degradation by steady state assumption as this reaction has slow dynamics compared to the main reaction
- Resulting model of 3^{rd} order includes dynamics of
  - Concentrations of hydroxygroup **-[OH**] and ethylene glycol **EG** and
  - A parameter which characterizes the mass transfer of EG: βa

Estimation Problem

- **Available data:**

  Measurements of

  - temperature
  - stirrer torque
  - stirrer speed
  - pressure

- **Problems:**
  - Online measurement of the degree of polymerisation not possible
  - Removal of the volatile reaction-product ethylene glycol crucial, but no infomation on the mass transfer coefficient is available

- **Solution**
  - Computation of the degree of polymerisation based on available process data
  - Design of an estimator based on a simple reaction model for
    - concentration of the most important end groups
    - mass transfer coefficient for the removal of ethylene glycol

Example: PET-Poly-Condensation

- Computation of the degree of polymerization
  Inputs: Temperature, stirrer torque, stirrer speed

  a) Semi-empirical model

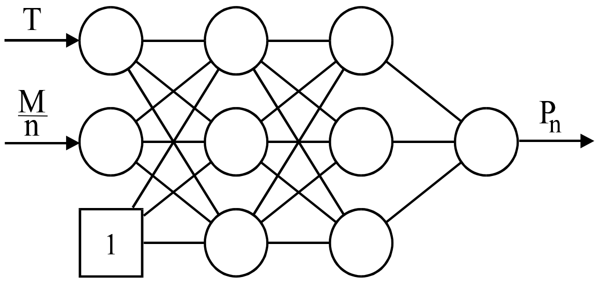
$$P_n = C_1 \cdot \left(\frac{M}{n^a} \exp\left(\frac{-7000}{T} \right) \right)^{C_2}$$

  Parameters C_1, C_2 and a calculated by nonlinear regression from data of analysis of samples

  b) **Neural net**

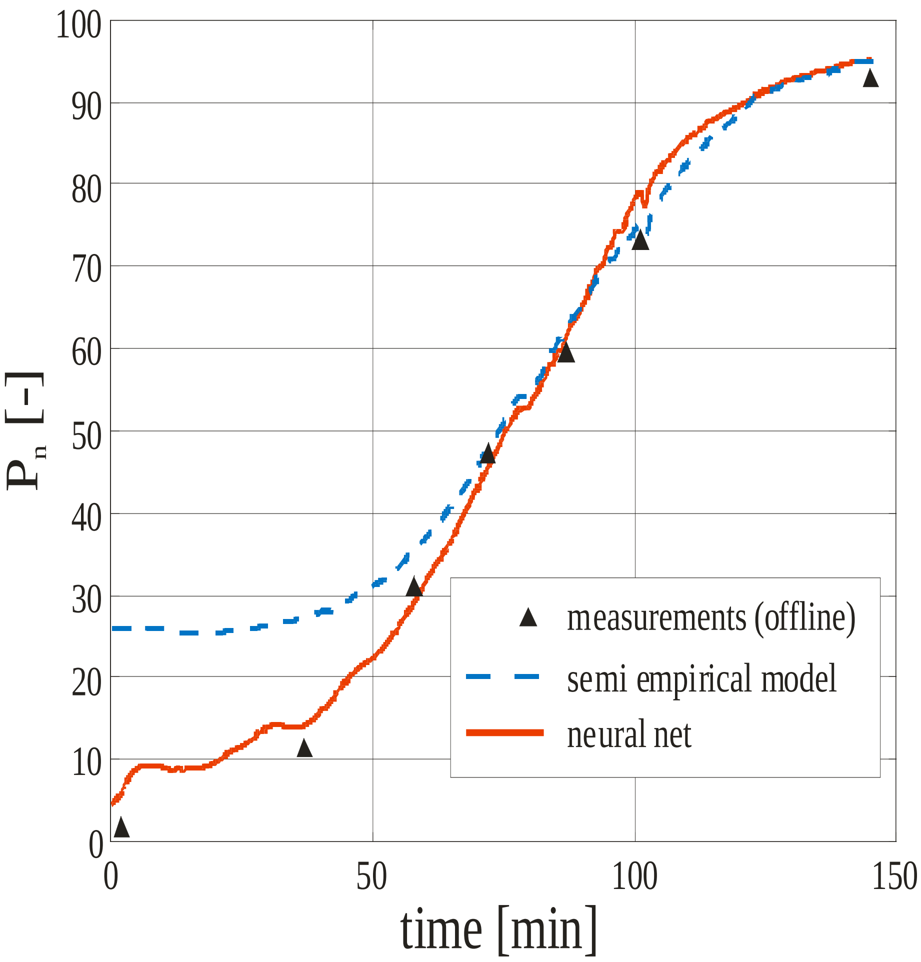
  Inputs: Ratio of stirrer torque and stirrer speed, temperature

  Output: Degree of polymerisation



  Training data: Laboratory analysis of samples

Estimation of the Degree of Polymerization



PET Polycondensation Model

- **Simplified model:**

$$\dot{x}_{EG} = -\beta a(x_{EG} - x_{EG}^{*}) + \frac{1}{2}\left[x_{OH}^{2} - 8x_{EG}\left[x_{E,\max} - \frac{1}{2}x_{OH}\right]\right]$$

$$\dot{x}_{OH} = -k_1 x_{OH}^{2} + 8x_{EG}\left[x_{E,\max} - \frac{1}{2}x_{OH}\right]$$

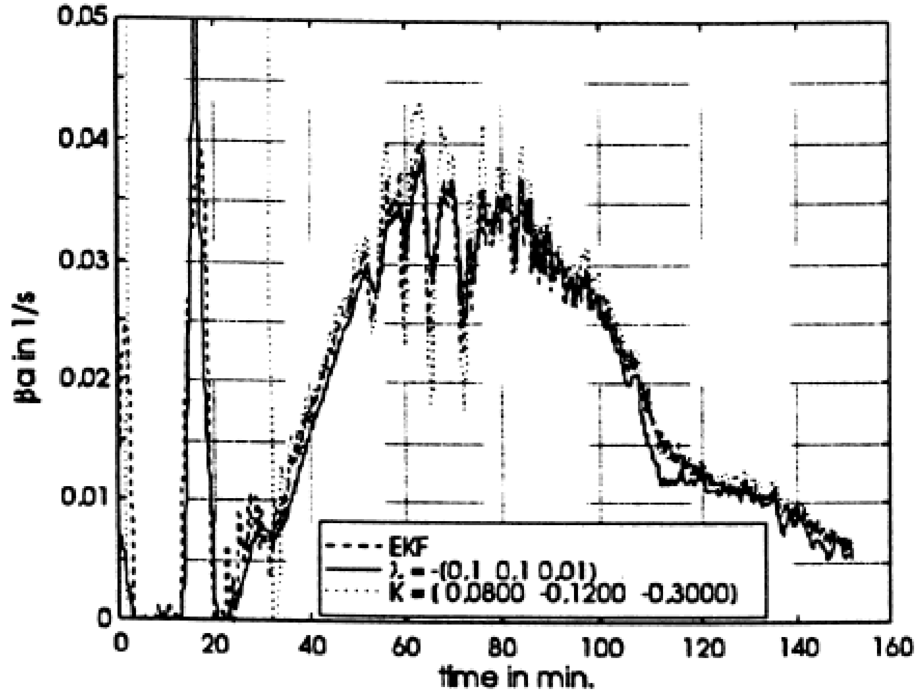
$$\dot{\beta a} = 0$$

Measurement equation: $y = x_{OH}$ where $x_{OH} = f\left(P_n, M_{EG}, M_E\right)$

- **Goal:** Estimation of the mass transfer coefficient in order to find dependencies on process conditions (stirrer speed, temperature)

Thesis by Paul Appelhaus

Results after careful tuning



EKF Parameters:

$$\underline{Q} = \frac{1}{\hat{x}_2}\begin{bmatrix} 0.001 & 0 & 0 \\ 0 & 0.0005 & 0 \\ 0 & -0.01 & 0.06 \end{bmatrix}$$

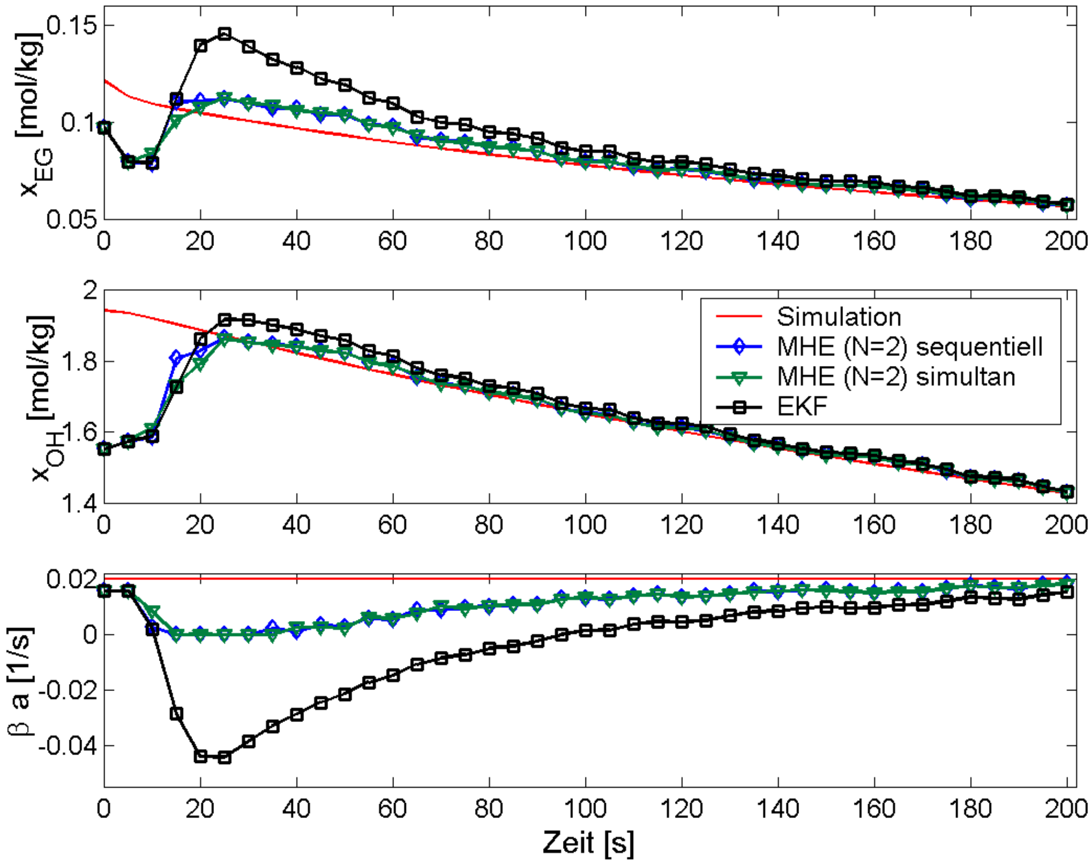
$$\underline{P}_0 = c_p \cdot r(0) \cdot \mathrm{diag}\left(\hat{x}_{10}, \hat{x}_{20}, (\widehat{\beta \cdot a})_0\right)$$

$$r = c_r \cdot \hat{x}_2^{-1}$$

$$c_r = 1$$
$$c_p = 0.5$$

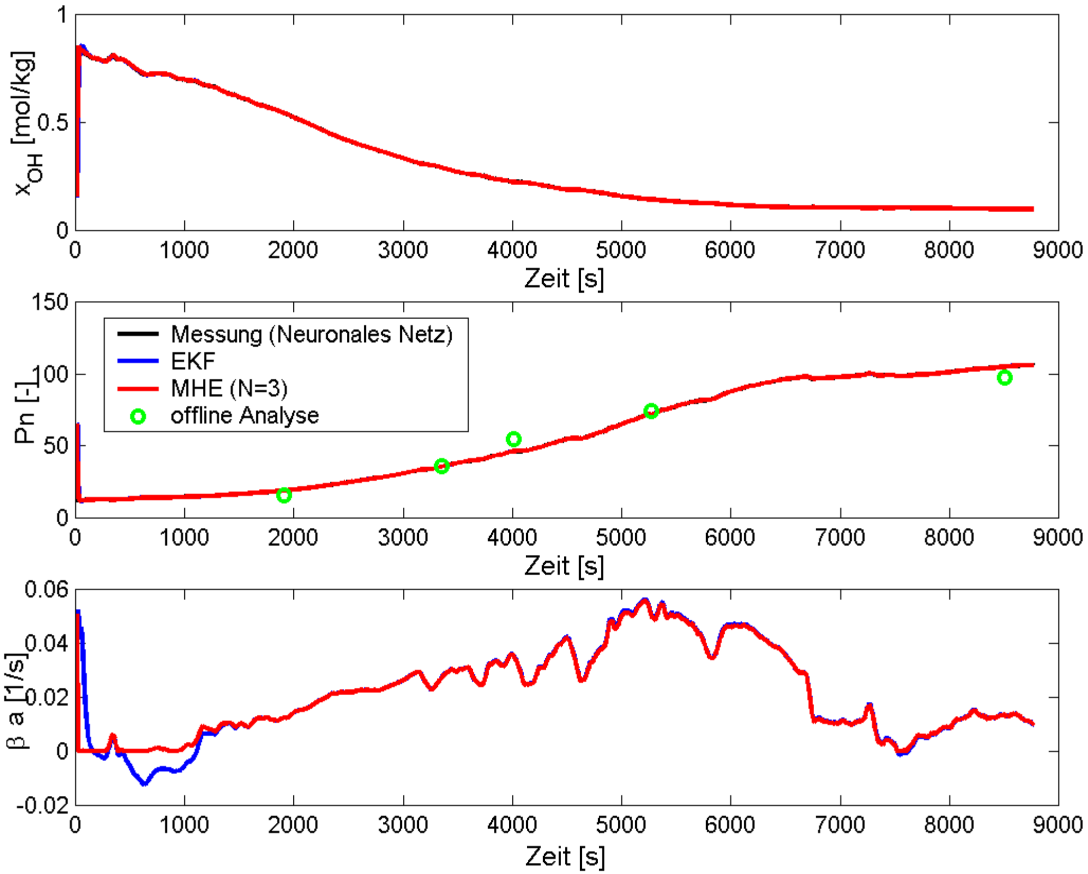
Comparison EKF-MHE, Simulation

- 20 % initial error in all states
- Constraints:
  $x_{EG} \geq 0$, $x_{OH} \geq 0$, $\beta a \geq 0$
- better convergence of the MHE



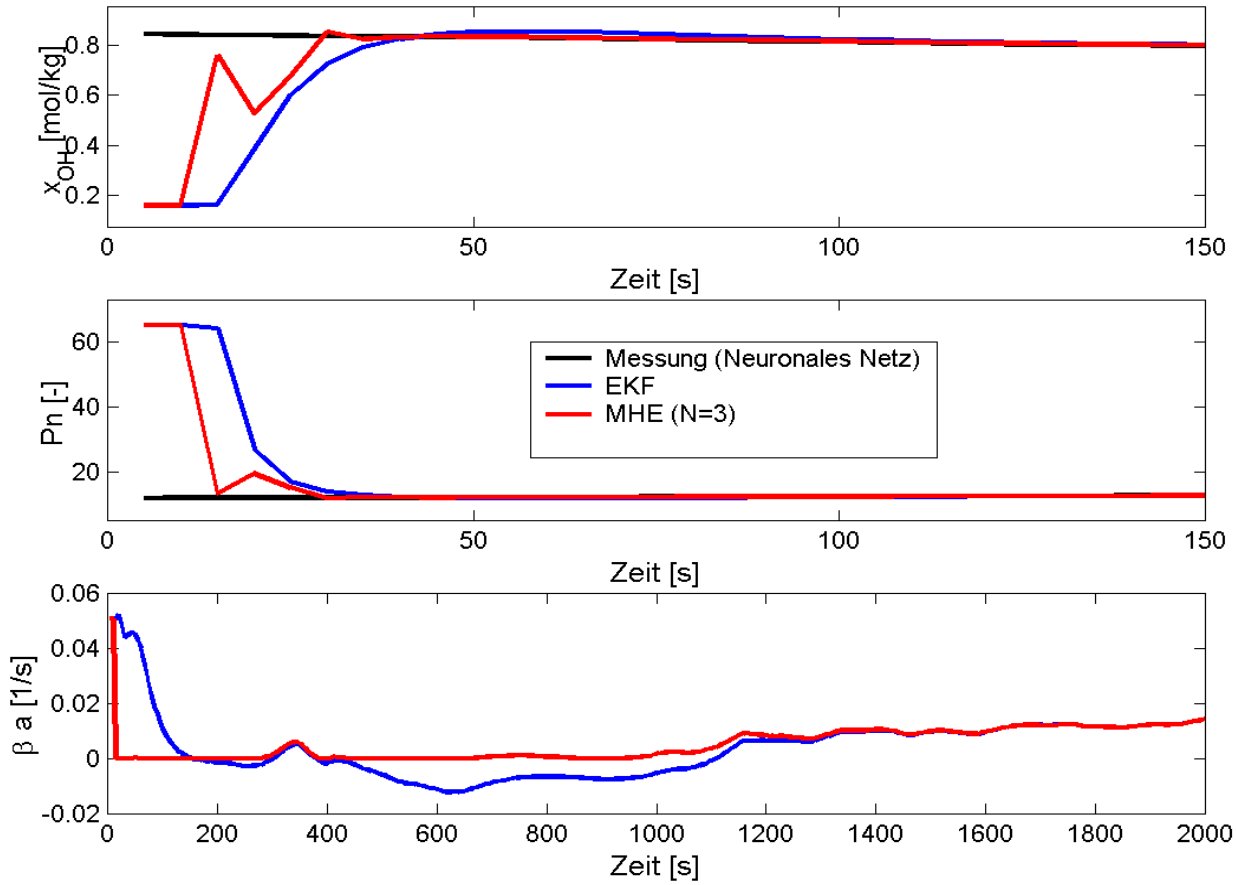
Comparison EKF-MHE

- MHE (N=3), experimental data
  - constraints
    $x_{EG} \geq 0$, $x_{OH} \geq 0$,
    $\beta a \geq 0$



Results PET Polycondensation

- Comparison EKF - MHE (N=3), experimental data

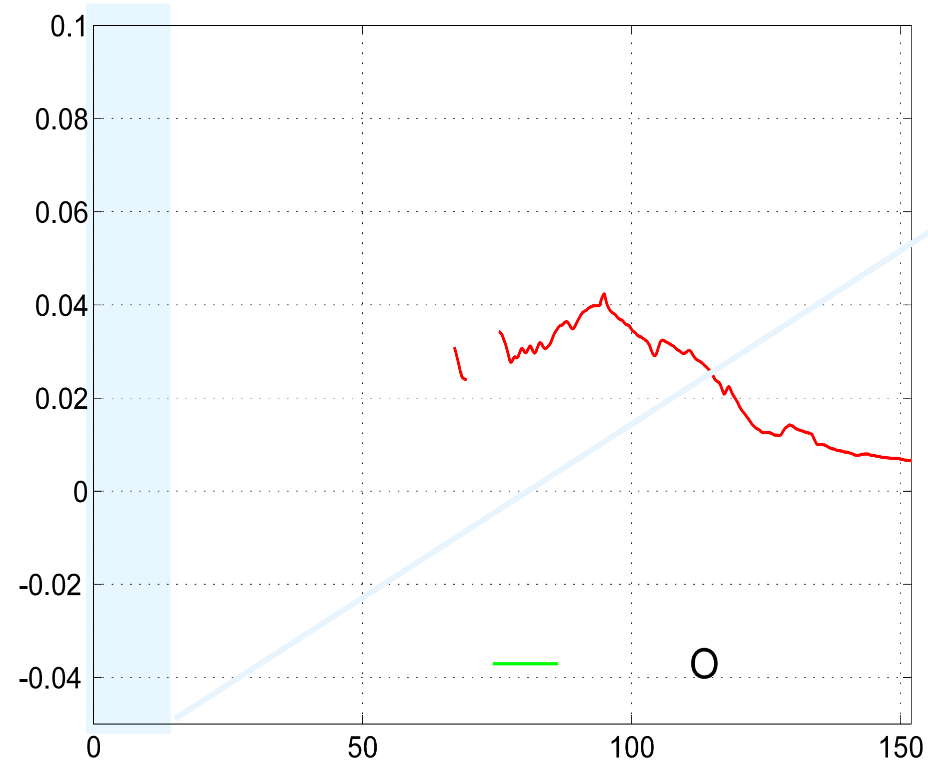


Estimation of the Mass Transfer Coefficient

- Different estimation methods gave similar results.
- Additional information about the process is provided.
- Estimation results enabled to improve process operation.

⇒ Development of improved trajectories of stirrer speed and reaction temperature

- Result: reduction of batch time by 10-15 %



Summary EKF vs. MHE vs. CEKF

- EKF:
  - Simple
  - Often good results
  - Tuning is not straightforward, requires insight and trial-and-error
  - Instability may occur
- MHE:
  - Uses full nonlinear model $\Rightarrow$ better convergence
  - Constraints on states and disturbances can be imposed
  - Numerically demanding
  - Tuning also an issue
- CEKF:
  - Good compromise between performance and effort