Application: Fluid Catalytic Cracker (FCC)
Reactor model

\[
S_c H_{ra} \dot{T}_{ra} = S_c R_c (T_{rg} - T_{ra}) + S_{tf} R_{tf} (T_{tf} - T_{ra}) - \Delta H_{fv} R_{tf} - \Delta H_{cr} R_{tf} C_{tf}
\]

\[
C_{tf} = \frac{1}{1 + \frac{R_{tf}}{R_{cr}}}
\]

\[
R_{cr} = K_{cr} P_{ra} H_{ra}
\]

\[
C_{cat}^2 = \frac{100 P_{ra} H_{ra}}{R_c C_{rc}^{0.06}} k_{cc} \exp \left( - \frac{A_{cc}}{RT_{ra}} \right)
\]

\[
K_{cr} = \frac{k_{cr}}{C_{cat} C_{rc}^{0.15}} \exp \left( - \frac{A_{cr}}{RT_{ra}} \right)
\]

\[
H_{ra} \dot{C}_{sc} = R_c (C_{rc} - C_{sc}) + R_{cf}
\]

\[
R_{cf} = R_{cc} + R_{ad}
\]

\[
R_{ad} = F_{cf} R_{tf}
\]

\[
R_{cc} = K_{cc} P_{ra} H_{ra}
\]

\[
K_{cc} = \frac{k_{cc}}{C_{cat} C_{rc}^{0.06}} \exp \left( - \frac{A_{cc}}{RT_{ra}} \right)
\]
Regenerator model

\[ S_c H_{rg} \dot{T}_{rg} = S_c R_c (T_{ra} - T_{rg}) + S_a R_{ai} (T_{ai} - T_{rg}) + \Delta H_{rg} R_{cb} \]

\[ R_{cb} = \frac{R_{ai}}{242} (21 - O_{fg}) \quad O_{fg} = 21 \exp \left( \frac{-P_{rg} H_{rg}}{R_{ai} \left( \frac{1}{K_{od}} + \frac{1}{K_{or} C_{rc}} \right)} \right) \]

\[ K_{or} = \text{unknown function of } T_{rg}. \]

\[ K_{od} = 6.34 \times 10^{-9} R_{ai}^2 \]

\[ H_{rg} \dot{C}_{rc} = R_c (C_{sc} - C_{rc}) - R_{cb} \]
New form of the system

\[
\varphi (x; u) = \varphi \left( T_{rg}, T_{ra}, C_{rc}, C_{sc}, F_{cf}; R_{ai} \right) \\
= \left( T_{rg}, T_{ra}, C_{tf} \left( C_{rc}, T_{ra} \right), \frac{C_{sc}}{C_{rc}}, \frac{F_{cf}}{C_{rc}} \right) = \xi
\]

\[
\begin{align*}
\dot{x}_1 &= T_{rg} = \psi (x, \varphi (x_1), u) \\
\dot{x}_2 &= T_{ra} = a_3(t)x_3 + f_2(x_1, x_2) \\
\dot{x}_3 &\approx C_{rc} = a_4(t)x_4 \\
&\quad + f_3(x_1, x_2, x_3, \psi (x, \varphi (x_1), u), u, \dot{u}) \\
\dot{x}_4 &\approx C_{sc} = a_5(t)x_5 + f_4(x_1, x_2, x_3, x_4) \\
\dot{x}_5 &\approx F_{cf} = F(x)
\end{align*}
\]

Here, \(\psi = R_{cb}, \varphi = K_{or}\) and \(\pi (x) = T_{rg} = x_1\).
\[u = (R_{ai}, P_{ra})\]
Time dependent change of coordinates

\[ \frac{dx}{dt} = F(x, u) \]

Our **diffeomorphism** \( \xi = \varphi(x, u) \) depend on \( u \) supposed to be smooth, hence:

\[ \frac{d\xi}{dt} = D\varphi \left( \varphi_u^{-1}(\xi) \right) f \left( \varphi_u^{-1}(\xi), u \right) + \frac{\partial \varphi \left( \varphi_u^{-1}(\xi), u \right)}{\partial u} \dot{u} \]

\[ = F(\xi, u, \dot{u}) \]

\[ \begin{cases} 
\frac{d\hat{\xi}}{dt} = F(\hat{\xi}, u, \dot{u}) + PC^TR^{-1}(y - C\hat{\xi}) \\
\frac{dP}{dt} = F^*(\hat{\xi}, u, \dot{u}) P + PF^*(\hat{\xi}, u, \dot{u}) + Q_0 - PC^TR^{-1}CP 
\end{cases} \]
In the original coordinates

Since \( C\varphi_u(x) = Cx \), equations are those of a modified extended Kalman filter

\[
\begin{align*}
\frac{d\hat{x}}{dt} &= f(\hat{x}, u) + pC^TR^{-1}(y - C\hat{x}) \\
\frac{dp}{dt} &= f^*(\hat{x}, u)p + pf^*(\hat{x}, u)^T + q_\theta(\hat{x}) \\
&\quad -ph^*(\hat{x}, u)^TR^{-1}h^*(\hat{x}, u)p \\
&\quad + D_{\psi_u}(\hat{x})D_{\psi_u}^2 \cdot \left(ph^*(\hat{x}, u)^TR^{-1}(h(\hat{x}, u) - y)\right)p \\
&\quad + pD_{\psi_u}^2 \cdot \left(ph^*(\hat{x}, u)^TR^{-1}(h(\hat{x}, u) - y)\right)D_{\psi_u}^{-1}(\hat{x})^T
\end{align*}
\]

where \( q_\theta(\hat{x}) = D\varphi_u(\hat{x})^{-1}Q_\theta\left(D\varphi_u(\hat{x})^{-1}\right)^T \)

The two last lines (transposed) correspond to the change of coordinate.
We use a second order system to estimate $K_{or}$

\[
\frac{d^3 K_{or}}{dt^3} = 0
\]

We use three parallel extended Kalman filters such that

- $\theta_0 = 3$ (starting value for each observer)
- $\theta_{HG} = 2$ (minimal value of $\theta$ ensuring high-gain)
- Time between two consecutive initializations: 2 hours
At last,
\[
\xi = \left( T_{rg}, R_{cb}, \dot{K}_{or}, \ddot{K}_{or}, T_{ra}, C_{tf}, \frac{C_{sc}}{C_{rc}}, \frac{F_{cf}}{C_{rc}} \right)
\]
and
\[
\Delta^{-1} = \text{diag} \left( 1, \theta, \theta^2, \theta^3, 1, \theta, \theta^2, \theta^3 \right)
\]
with \( Q_\theta = \theta^2 \Delta^{-1} Q \Delta^{-1} \)
and \( R_\theta = \left( C \Delta^{-1} C' \right) R \left( C \Delta^{-1} C' \right) \)
Colored noise (Ornstein–Uhlenbeck process) on both measured variables $T_{rg}$ and $T_{ra}$.

$$K_{or} = 1.16 \times 10^{-5} \exp \left( \frac{A_{or}}{R \left( \frac{1}{866.7} - \frac{1}{T_{rg}} \right)} \right)$$
Constants of the model

Reactor operating conditions
\[ H_{ra} = 1.85 \times 10^{-4}, \quad P_{ra} = 211.7, \]
Feed properties
\[ R_{tf} = 41, \quad T_{tf} = 492.8, \quad S_{tf} = 3140, \]
Cat. recirculation
\[ R_c = 290, \quad S_c = 1047, \]
Heat constants
\[ \Delta H_{cr} = 4.65 \times 10^5, \quad \Delta H_{fr} = 1.7410^5, \]
\[ \Delta H_{rg} = 3.02 \times 10^7, \quad R = 8.314 \]
\[ k_{cr} = 8.31 \times 10^{-2}, \quad A_{cr} = 6.28 \times 10^4, \]
\[ k_{cc} = 2.66 \times 10^{-4}, \quad A_{cc} = 4.18 \times 10^4 \]
Regenerator operating conditions
\[ H_{rg} = 1.53 \times 10^5, \quad P_{rg} = 254.4, \]
Air properties
\[ R_{ai} = 26, \quad T_{ai} = 394, \quad S_{ai} = 1130 \]
\[ A_{or} = 1.47 \times 10^5 \]
Simulation using Matlab/Simulink

to be continued...
Observer: Parameter estimation

Norm of the gain

$F_{cf}$

Actual process

Observer
Identification: state estimation

$T_{ra}$

$T_{rg}$

Reactor

Regenerator

$C_{sc}$

$C_{rc}$

actual process
observer
Identification of unknown function

actual process
observer