Monitoring of Process Fouling Using First-Principles Modeling and Moving Horizon Estimation

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Overview

Objective:

Demonstrate online process fouling monitoring on a reactor using first-principles modeling and moving horizon estimation.

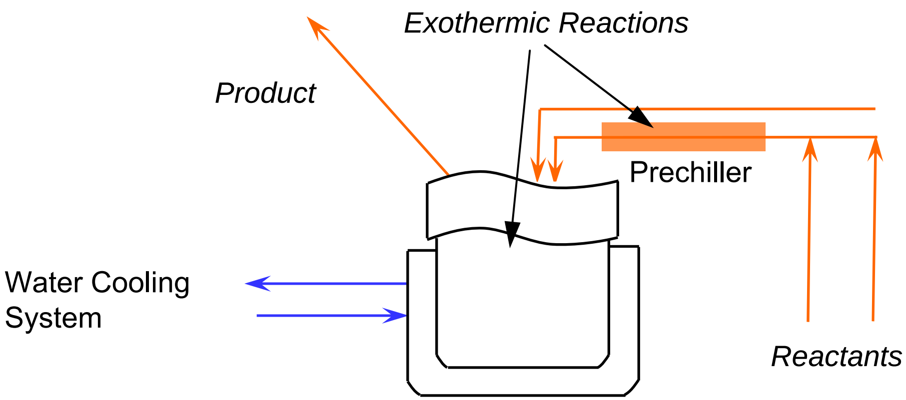
Outline:

- Fouling Monitor Motivation
- First-Principles Process Modeling
- Moving Horizon Estimation Background
- Online Fouling Monitor using MHE
- Results

Monitor completed during internship at ExxonMobil Chemical Company.

Fouling Monitor Motivation

Reactor Process



Temperature is maintained with active control.

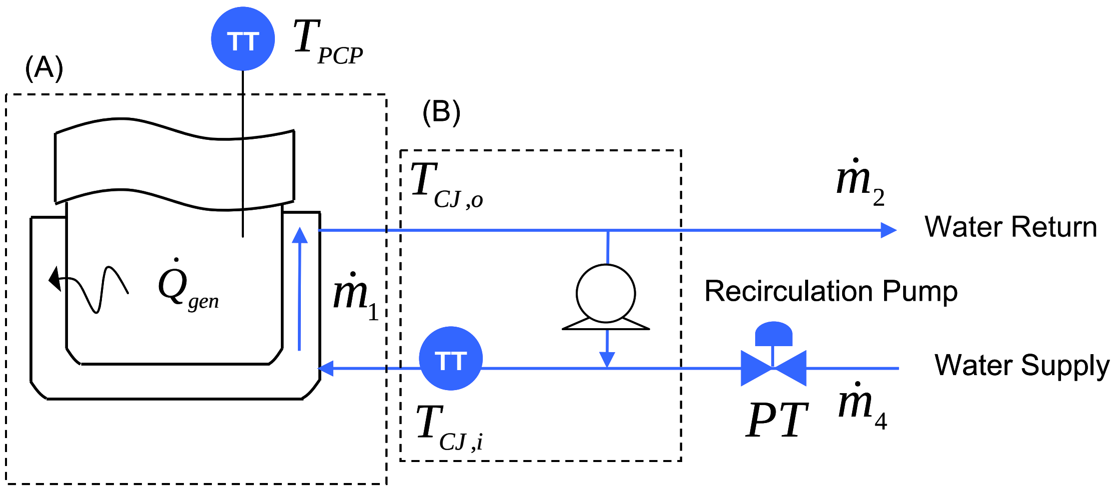
Fouling effects

- Fouling particles plug downstream.
- Reactor cleanings are performed based on a heuristic approach. A fouling monitor is needed to ensure cleaning is only performed when necessary.

Images from generic heat exchanger fouling (Images Source: Maverick Inspection)

Reactor Model

Water Cooling System: Process Flow Diagram



State Variables

$\dot{m}_1$ $\quad k_v$

$\dot{m}_2$ $\quad T_{CJ,o}$

$\dot{m}_4$ $\quad T_{CJ,i}$

$\dot{m}_{4,lag}$

Measured Variables

$T_{CJ,i}$ $\quad PT$

T_{PCP}

Estimated Variable

UA_{CJ}

Energy Conservation

$$\text{(A)}\quad \rho V c_p \frac{dT_{CJ,o}}{dt} = \dot{m}_1 c_p \left(T_{CJ,i} - T_{CJ,o}\right) + UA_{CJ}\left(T_{PCP} - T_{CJ,o}\right)$$

$$\text{(B)}\quad \dot{m}_1 c_p \left(T_{CJ,o} - T_{CJ,i}\right) = \dot{m}_2 c_p T_{CJ,o} - \dot{m}_4 c_p T_{WRS} - W_p$$

Mass Conservation

$$\dot{m}_1 = \dot{m}_{4,lag} + \dot{m}_3$$

$$\dot{m}_2 = \dot{m}_1 - \dot{m}_3$$

Empirical Loss Coefficient

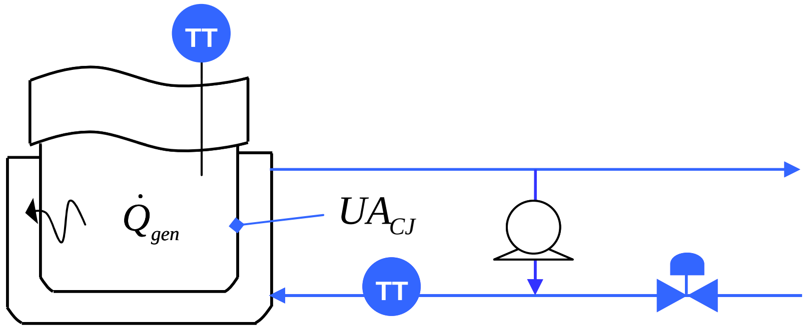
$$k_v = \alpha \cdot e^{(\beta \cdot \%\_rated\_travel)} + \delta$$

$$\dot{m}_4 = \rho k_v \sqrt{\frac{p_s - p_a}{\gamma_{H_2O}}}$$

Empirical Loss Coefficient

$$\tau \cdot \frac{d\dot{m}_{4,lag}}{dt} = -\dot{m}_{4,lag} + \dot{m}_4$$

Reactor Model



UA_{CJ} is the overall heat transfer coefficient across the reactor wall.

Operating experience suggested that the fouling thermally insulates the reactor from the cooling system

Model Justification and Assumptions

● **First-principles model:** ideal for a multimode process with future data expected to be outside training set.

● **SS energy balance:** describes the energy balance on process flows entering and exiting the system. No energy storage is expected since flow is incompressible.

● **Lagged mass flow:** accommodates the observed delay between inlet temperature and valve percent travel.

● **Adiabatic wall and lumped jacket temperature**

Key Challenges

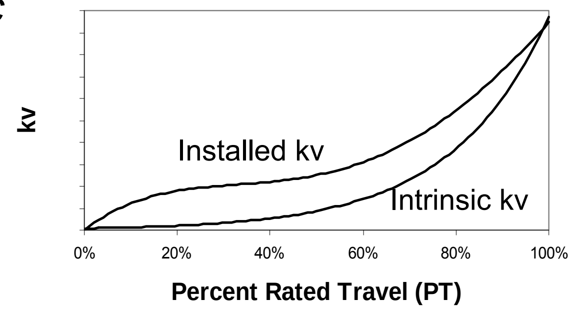
● **Correlated measurements:** All three measurements are correlated but offset in time due to the system dynamics – empirical fault detection methods often cite highly correlated data as a challenge.

● Used existing three measurements which were implemented for temperature control.

● **Model mismatch and unmeasured parameters:** pump flow, valve coefficient model

Reactor Model - System Identification

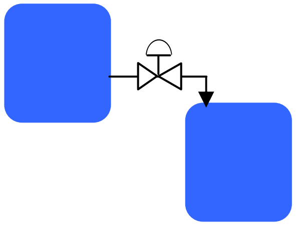
Valve Loss Coefficient Model: Intrinsic vs. Installed Characteristic



Equipment: Valtek Mark One Equal Percentage Valve

Available Measurement: Valve Percent Rated Travel (PT)

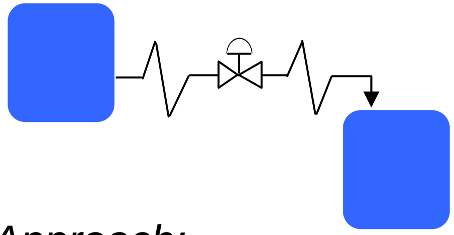
Intrinsic Characteristic Model



- Model regressed from manufacturer-provided data
- Assumes no pipe loss between reservoirs upstream or downstream of the valve.

$$k_v = 0.0762 \cdot e^{(4.18 \cdot PT)}$$

Installed Characteristic Model



- Unique to each specific process design.
- Valve characteristic curve may approach the linear characteristic curve in the field. In this case the curve is flatter in the region of operation.

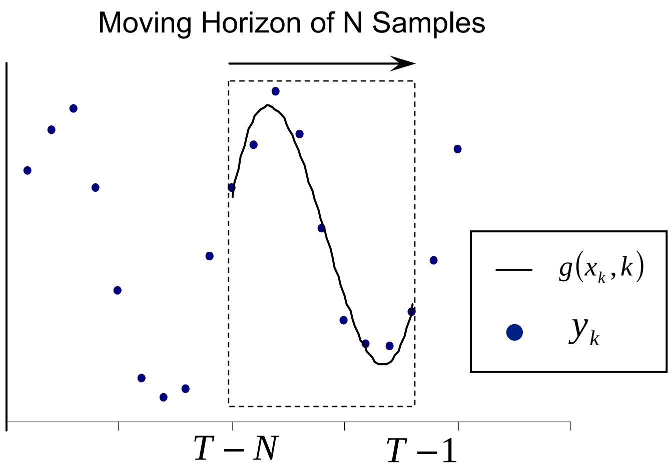
$$k_v = 0.0762 \cdot e^{(3 \cdot PT)} - 0.015$$

Approach:

Iterated dynamic simulations with varying parameters based on process knowledge.

Reduced model mismatch noise from ~ 100% of nominal to 11% of nominal

Moving Horizon Estimation Background



Moving horizon estimation (MHE) produces an approximation to the maximum a posteriori estimate of the state.

$$\arg \max_{(x_0, x_1, \ldots, x_T)} p\left(x_0, x_1, \ldots, x_T \mid y_0, y_1, \ldots, y_{T-1}\right)$$

Reference Rawlings (2002) for details of the derivation.

General Optimization form for Sequential Quadratic Programming

$$\min_{x_{T-N}, \{w_k\}_{k=T-N}^{T-1}} \hat{\Phi}_{\mathrm{T}}\left(x_{T-N}, \{w_k\}\right)$$

$$\text{s.t.} \quad x_{k+1} = f\left(x_k, u_k, k\right) + w_k$$

$$y_k = g\left(x_k, k\right) + v_k$$

$$\hat{\Phi}_{\mathrm{T}}\left(x_{T-N}, \{w_k\}\right) = \sum_{k=T-N}^{T-1} \left\| w_k \right\|_{Q^{-1}}^2 + \left\| v_k \right\|_{R^{-1}}^2 + \underbrace{\left\| x_{T-N} - \hat{x}_{T-N} \right\|_{\prod_{T-N}^{-1}}^2}_{\text{Arrival Cost}}$$

Weighting Matrices: Q and R represent the covariance on the model and measurement noise. These matrices can be used as tuning parameters in MHE to incorporate knowledge of uncertainty.

Arrival cost: can be computationally expensive to calculate accurately. In practice some algorithms neglect the arrival cost or use extended Kalman filtering (EKF) to approximate it.

Moving Horizon Estimation Background

Alternative Formulations of MHE Objective Function

$$\min_{d} \phi = \left\| \frac{y_s - y_m}{y_m} \right\|_{Q_y}^2 + \left\| d - \hat{d} \right\|_{Q_d}^2 \qquad s.t. \quad f\left(\dot{x}, x, u, d\right) = 0$$

$$y_s = g(x, u, d)$$

$$h(x, d) \geq 0$$

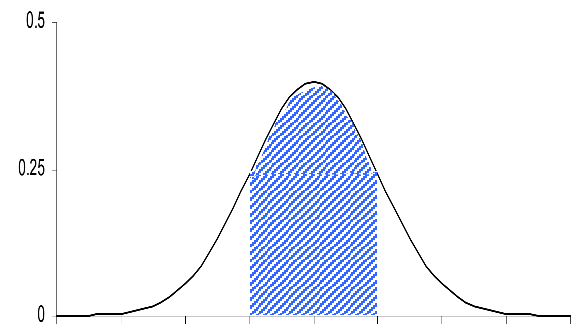
Inequality constraints are incorporated with the DAE model and discretized.

Differences between EKF and MHE:

● Constraint handling in MHE incorporates process knowledge and allows truncated Gaussian distributions on estimated states.

●EKF takes one Newton step while MHE iterates until tolerance is met.

● MHE can require greater computational power but may perform better for highly nonlinear systems.

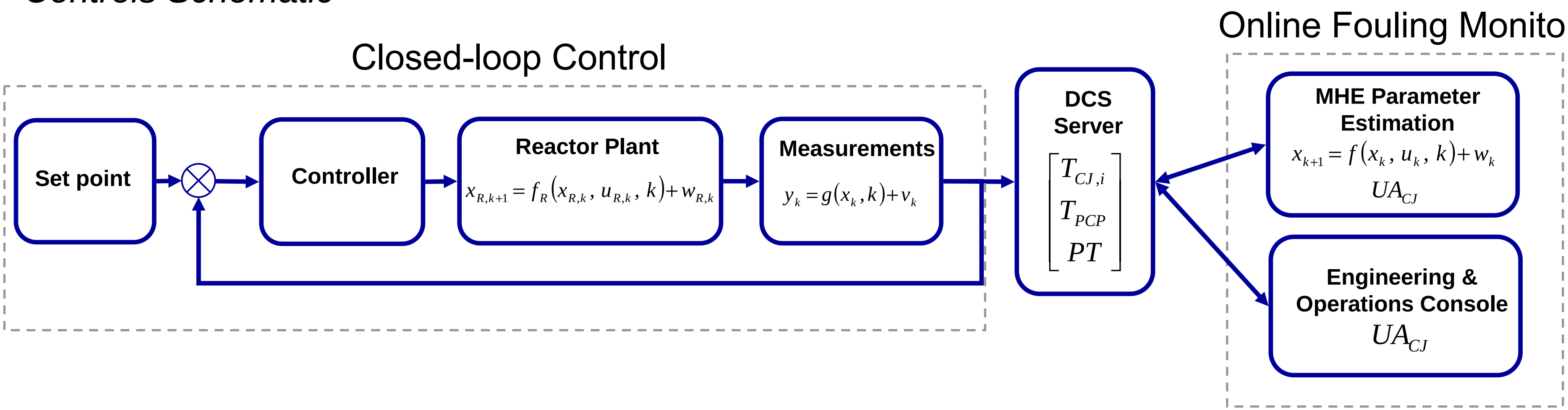


Background research

Recent applications of MHE include an industrial chemical reactor (Hedengren, 2007), chemical vapor deposition (Grover, 2008), and a bioprocess (Buchen, 2006).

Online Fouling Monitor Using MHE

Controls Schematic



Online Fouling Monitor Performance

Typical Execution Time per Run: 1 second

Service Factor > 98% since August 2008

Horizon Length: 10

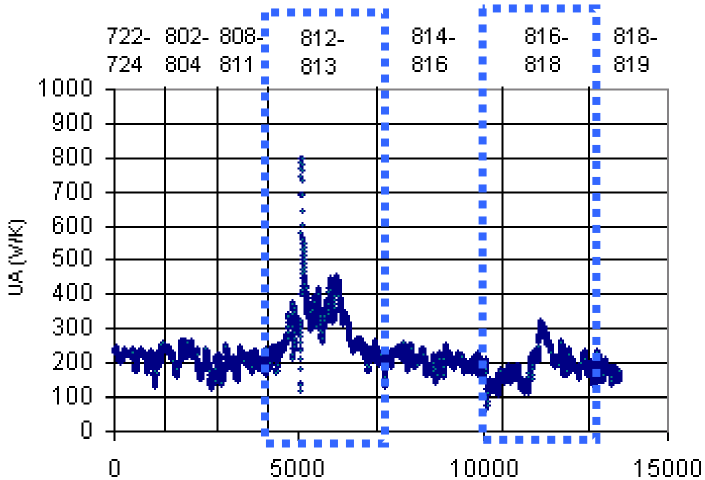
Constraints: UA_{CJ} > 30 W/m^2K

Number of state variables	1532
Number of total equations	1530
Number of slack variables	0
Degrees of Freedom	2

Current online monitor solves three models simultaneously for use in model refinement. The number of states can be reduced by 1/3 for future operation.

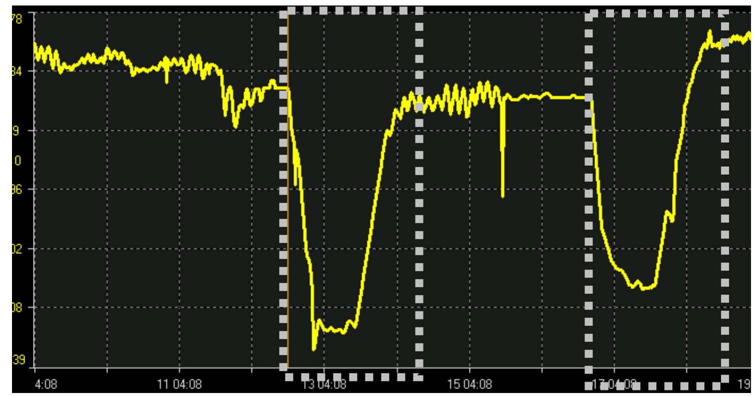
Results: Estimated UA in July-August 08

Unfiltered UA: Process Aberrations Included

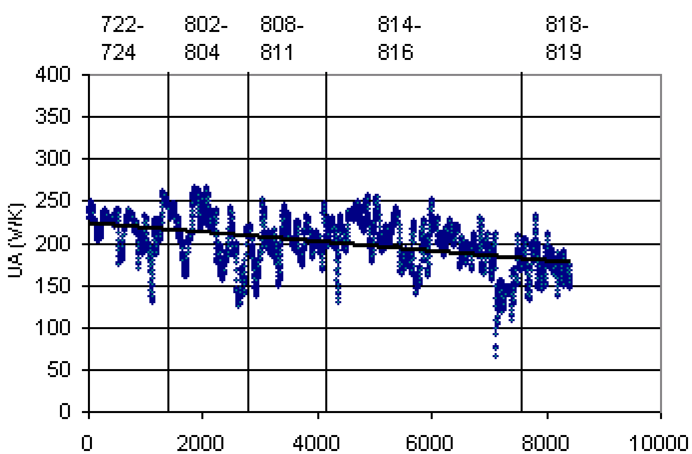


Process Aberration Flow Rate Plot

Donor level decrease by ~ 3-4x during transition



Unfiltered UA: Process Aberrations Removed



UA_{AVG} = 222 200 175

- Results from July-August data are promising:

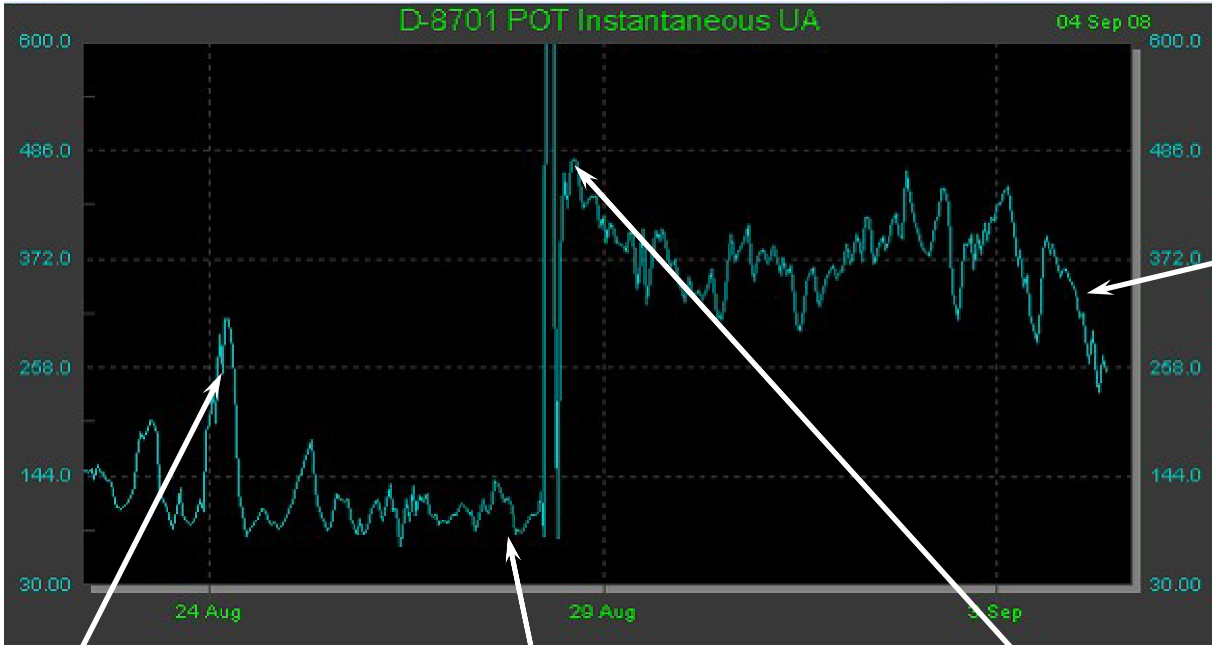
Mean UA decreased by 21% from July 22 - August 19. Standard deviation over a few days is ~ 11% of nominal value.

- UA should be ignored during transitions – error increases due to low temperature difference across wall.

Flow → Heat Generation → Wall Temp Delta

Results: Estimated UA in September 08

Estimated UA at Reactor Cleanout



1 Week Following Cleanout

Steady during first week and begins to decrease afterwards likely due to fouling increase.

Model mismatch

Temporary deviations from the UA trend often occur during process grade transitions. Model is not expected to match data during transitions.

1 ½ Month of Fouling Coalescence

Average UA decreased from ~ 250 to 110 from July 22 – Aug 28. Data taken from July 22 after process began to run steadily.

Reactor Cleanout

Average UA increased ~ 360% immediately following cleanout. Spike above 600 is bad data – during cleanout process conditions violate model.

Results

Project Status

Phase	Description	Status
1	Develop a reliable online estimation model to predict level of long-term fouling within reactor. Validated with past data.	✓
2	Create operator display for online fouling monitor	✓
3	Validate monitor online over several months with real-time process data.	✓
4	Develop a consistent UA limit for fault detection	In process
5	Develop automated reactor cleanout control to prevent unnecessary cleanouts and minimize time length of clean out.	Future plan

Conclusions

- Developed a first-principles model with sufficient accuracy to characterize gradual drift in reactor wall fouling.
- Demonstrated an online application of MHE with low execution time and high reliability.
- Improved operating knowledge of the fouling process.

Future Work

- Investigating Bayesian estimation techniques capable of characterizing multimode processes.
- Applications to offline system identification of first-principles modeling and fault detection for chemical processes.

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Questions?