State Estimation in Fermentation of Lignocellulosic Ethanol. Focus on the Use of pH Measurements

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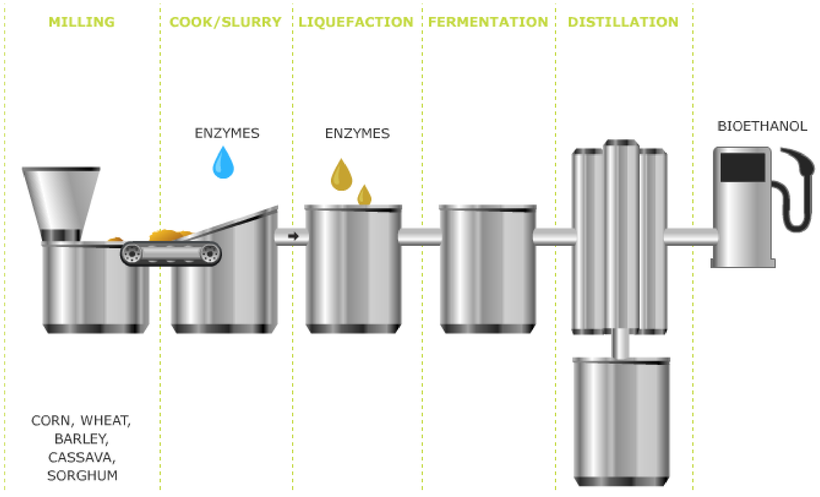
Introduction. Monitoring of biochemical processes is essential for fault-diagnosis, control and optimisation. Lack of appropriate sensors and inherent non-linearity are some of the main obstacles to monitoring in biochemical processes The continuous-discrete extended Kalman filter (CD-EKF) is an appropriate tool for state estimation in biochemical processes. The non-linearity of the model can be efficiently tackled by the CD-EKF since the sensitivity of the dynamic model is updated at each sampling time via ODE integration. The focus of this contribution is specifically on the use of pH as this is a variable that correlates well with the yeast catabolism (CO_2 is co-produced with ethanol, leading to acidification of the medium) and that can be easily measured online.

PROCESS DESCRIPTION



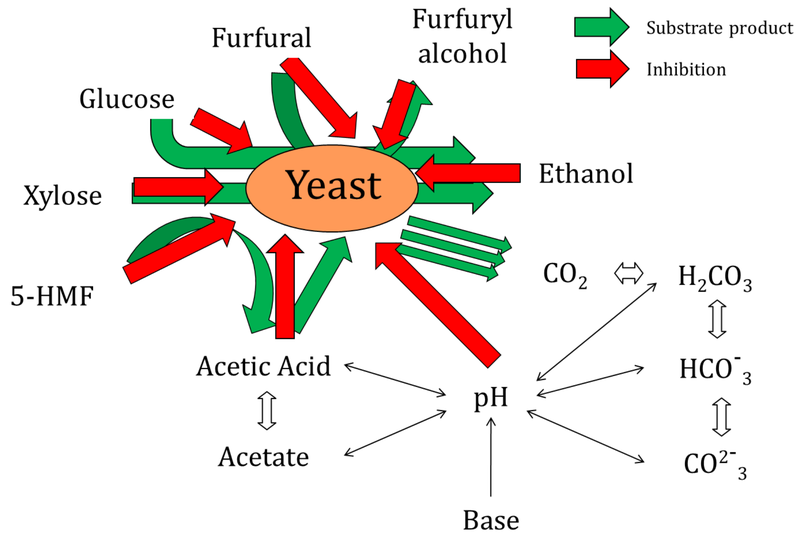
Presence of inhibitors from the hydrolysis stage, e.g. furfural, acetic acid, 5-hydroxymethylfurfural (5-HMF)

Production of a commodity (cost is the most important factor)

The presence of organic acids impacts pH

The yeast metabolism changes with pH

Possible contamination by lactic acid bacteria (LAB)



CONTINUOUS-DISCRETE EXTENDED KALMAN FILTER (CD-EKF)

Plant model

$$x_{k+1} = x_k + \int_{t_k}^{t_{k+1}} f\left(x(\tau), u_k, d_k\right) d\tau + w_k$$

$$y_k = G(x_k) + \nu_k, \quad \nu_k \in \mathrm{N}_{iid}(0, R_\nu)$$

Measurement update

Error $e_k = y_k - C_k \hat{x}_{k|k-1}$

Gain $K_{f,k} = P_{k|k-1} C_k{}^T \left[C_k P_{k|k-1} C_k{}^T + R_\nu\right]^{-1}$

State estimate $\hat{x}_{k|k} = \hat{x}_{k|k-1} + K_{f,k} e_k$

Covariance $P_{k|k} = P_{k|k-1} - K_{f,k}\left[C_k P_{k|k-1} C_k{}^T + R_\nu\right]^{-1} K_{f,k}^T$

One step-ahead prediction

$$\hat{x}_{k+1|k} = \hat{x}_{k|k} + \int_{t_k}^{t_{k+1}} f\left(x(\tau), u_k, d_k\right) d\tau$$

$$\overline{A}_k = I + \int_{t_k}^{t_{k+1}} \frac{\partial f}{dx}\left(x(\tau), u_k, d_k\right) S_{\hat{x}_{k|k}} \, d\tau$$

$$P_{k+1|k} = \overline{A}_k P_{k|k} \overline{A}_k^T + R_w$$

Configuration	Measurements	Sampling rate (min)
1 -Online fast-sampling measurements	M, pH	20
2 -Offline slow-sampling measurements	M, Glu, Xyl, Eth	240
3 - Combination of measurements	M, Glu, Xyl, Eth, pH	240

RESULTS. CASE STUDY WITH CONTAMINATION

The filter was tested by simulating lactic acid bacteria contamination in the reactor (accounting for 0.2% w/w of the yeast biomass in the inoculum)

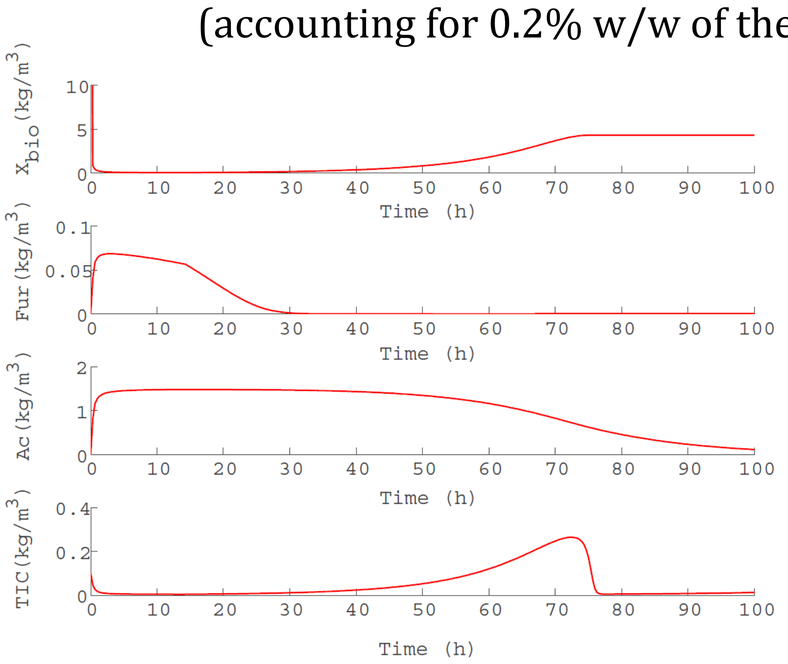


Figure 1. Simulation of the process with LAB contamination. Selection of key states.

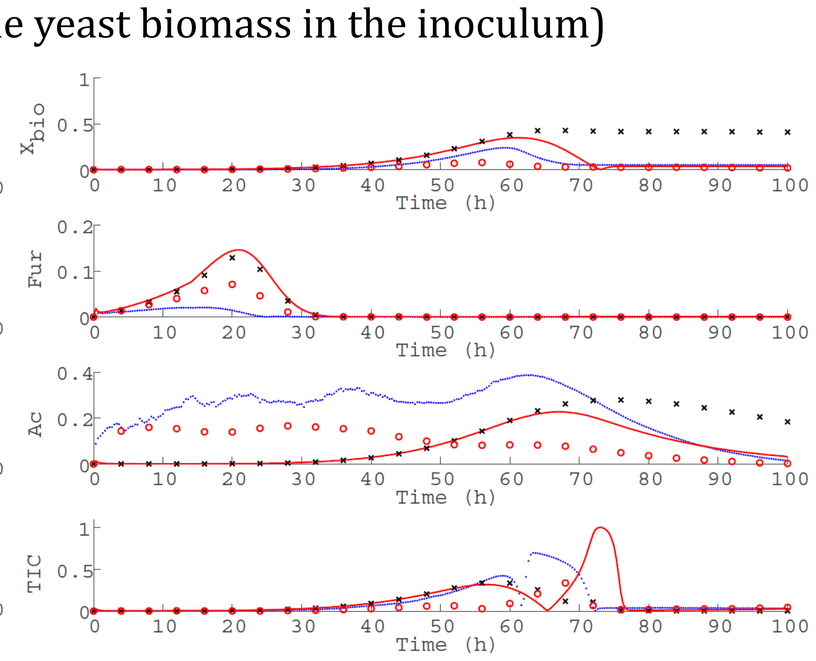


Figure 2. Absolute normalized prediction error for pure simulation (line), configuration 1 (dots), configuration 2 (crosses) and configuration 3 (empty circles)

Table. Estimation statistics: the mean is given for the absolute estimation error on selected states based on the normalized data.

Variable→ Configuration ↓	X_{bio} $\mu\cdot10^3$	Fur $\mu\cdot10^3$	Ac $\mu\cdot10^3$	TIC $\mu\cdot10^3$
Simulation	96.0	21.9	77.7	181
1	62.0	2.90	232	173
2	239	19.3	123	117
3	27.2	10.9	89.0	66.9

- Conf. 1 and 2 present a severe bias, in particular for cell biomass and acetate
- Cell biomass is accurately estimated by conf. 3
- Acetate estimation is probably hindered by the presence of lactic acid

Conclusions

The CD-EKF was proven as a suitable tool for monitoring of biochemical processes. Providing pH helps improving the prediction of the filter when comparing several configurations. The use of pH is of great interest for such processes since it is a ubiquitous measurement in biochemical processes.

References:
Price, J. Nordblad, M., Woodley, J.M., Huusom, J.K. Biotechnology Progress,, 31(2) 585-595, 2014

Acknowledgements:
This work is partially financed by BIOPRO funded by the European Regional Development Fund (ERDF), Region Zealand (Denmark) and BIOPRO partners.