State Observers for Electrolyzers

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Summary

- Introduction
- Electrolyzer state estimation problem
- Electrolyzer mathematical model
- A prime on state estimation
- State observer design for electrolyzers
- Final comments

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- Our approach is based on advanced mathematical models based on the laws of physics.

  A much more complex study is being developed by the PhD student Franthiescolly Vieira de Carvalho supervised by Daniel F. Coutinho and co-supervised by me.

- Applications can be found in advanced model-based control/optimization methodologies and fault detection and isolation.

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Different type of faults in PEM electolyzer

Table 2 – Summary of different type of faults in PEM electrolyzer.

Type of fault	Affected components	Causes
Mechanical degradation	Membrane	Perforation by current collector; pinholes introduced during MEA manufacturing; swelling and shrinking; nonuniform water uptake or water starvation
Chemical degradation	Membrane	Radical attack; metal poisoning
Thermal degradation	Membrane	Thermal cycles; thermal stress
Dissolution of catalyst	Catalyst/catalyst layer	High operating potential; the formation of soluble iridium (III) complexes during OER (oxygen evolution reaction); bubble effect; current reversal in shut-down procedures
Passivation of support	Catalyst/catalyst layer	High potential and rich oxidation environment
Agglomeration of catalyst	Catalyst/catalyst layer	Sintering or increase in the crystal size; load and onoff cycle
Ionomer dissolution	Catalyst/catalyst layer	High current densities; chemical attack by radicals
Cation contamination	Catalyst/catalyst layer	Active site blocked by under potential deposition; the proton of ionomer replaced by external cations
Mechanical damage	Catalyst/catalyst layer	Nonuniform clamping pressure; improper membrane swelling
Hydrogen embrittlement	Bipolar plate	Hydrogen absorption of metal plates in cathode
Passivation	Bipolar plate	Oxide layer formation
Corrosion	Bipolar plate	Titanium oxidized, and then corroded by F^- ion; stainless steel corroded by acid
Chemical degradation	Current collector	Passivation and corrosion of metallic plate
Mechanical degradation	Current collector	Improper compression; hydrogen embrittlement

Kheirrouz, M., Melino, F., Ancona, M. A. *Fault detection and diagnosis methods for green hydrogen production: A review*. International Journal of Hydrogen Energy, 47, 27747-27774, 2022.

Approaches for dealing with faults in PEM electolyzer

Dash, B. M., Bouamama, B. O., Pekpe, K. M., Boukerdja, M. *Prior knowledge-infused self-supervised learning and explainable AI for fault detection and isolation in PEM electrolyzers*. Neurocomputing, 594, 127871, 2024.

Lebbal, M. E., Lecoeuche, S. *Identification and monitoring of a PEM electrolyser based on dynamical modelling*. International Journal of Hydrogen Energy, 34, 5992-5999, 2009.

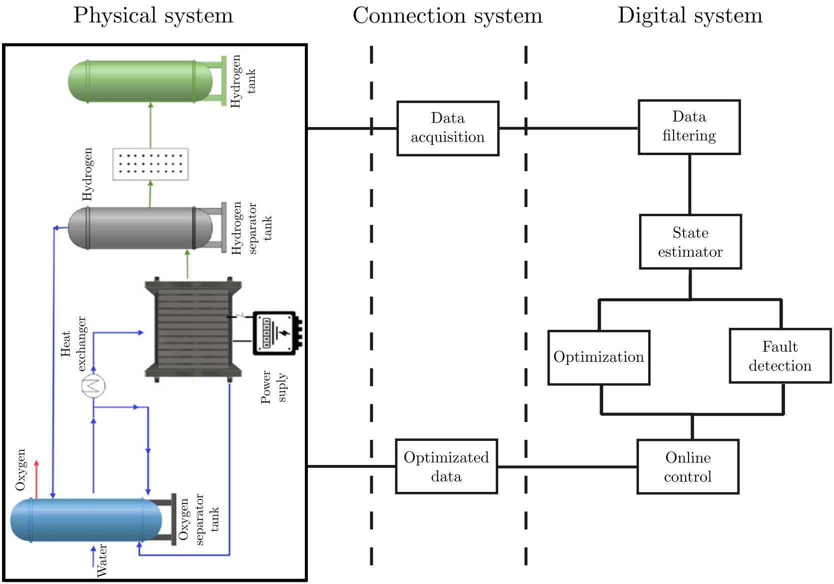
Folgado, F. J., González, I., Calderón, A. J. *Data acquisition and monitoring system framed in industrial internet of things for PEM hydrogen generators*. Internet of Things, 22, 100795, 2023.

Jarvinen, L, Puranen, P., Kosonen, A., Ruuskanen, V., Ahola, J., Kauranen, P., Hehemann, M. *Automized parametrization of PEM and alkaline water electrolyzer polarisation curves*. International Journal of Hydrogen Energy, 47, 31985-32003, 2022.

Hernández-Gómez, A., Ramirez, V., Guilbert, D., Saldivar, B. *Development of an adaptive static-dynamic electrical model based on input electrical energy for PEM water electrolysis*. International Journal of Hydrogen Energy, 45, 18817-18830, 2020.

and many more...

Advanced electrolyzer control/monitoring architecture



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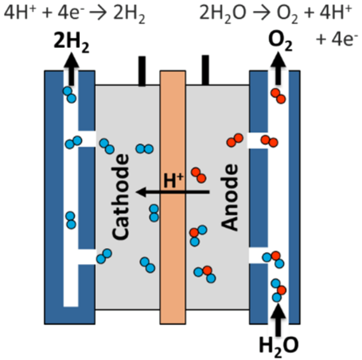
Electrolyzer state estimation problem

Given, at each time instant t, measurements of

- current
- tension

Estimate, at each time instant t, the

- Temperature
- Gradient of oxygen concentration
- Gradient of hydrogen concentration



https://www.energy.gov/eere/fuelcells/hydrogen-production-electrolysis

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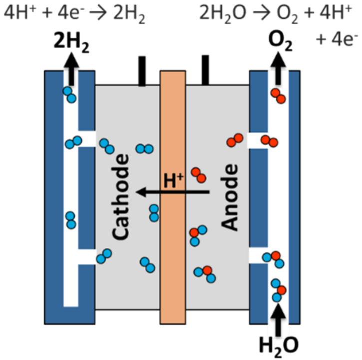

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Electrochemical reaction

- Operational voltage:

$$V = V_{Nernst} + V_{act} + V_{ohm} + V_{con}$$

- Equilibrium potential:

$$V_{Nernst} = E^0_{H_2} + \frac{RT}{2F} \ln \left(\frac{P^L_{H_2} \left(P_{O^L_2} \right)^{1/2}}{P^L_{H_2O}} \right)$$

- Activation overpotential:

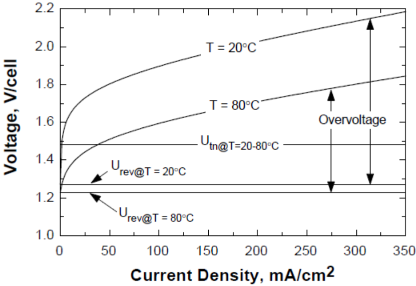
$$V_{act} = \frac{RT}{\alpha_{an}} \sinh^{-1} \left(\frac{i}{2 i_{0,an}} \right) + \frac{RT}{\alpha_{cat}} \sinh^{-1} \left(\frac{i}{2 i_{0,an}} \right)$$

- Ohmic overpotential

$$V_{ohm} = RI$$

- Concentration overpotential

$$V_{con} = \frac{RT}{4F} \ln(C_{O_2}/C_{O_2,o}) + \frac{RT}{2F} \ln(C_{H_2}/C_{H_2,o})$$



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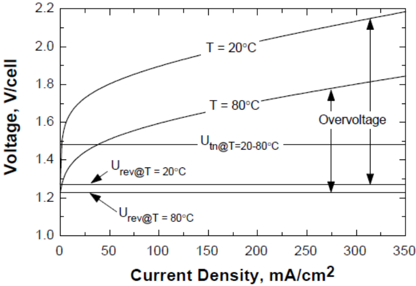

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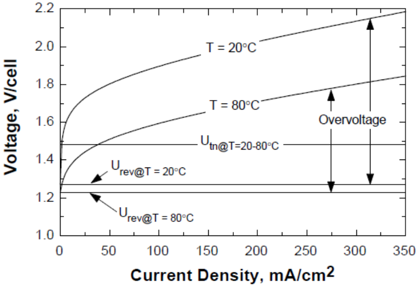

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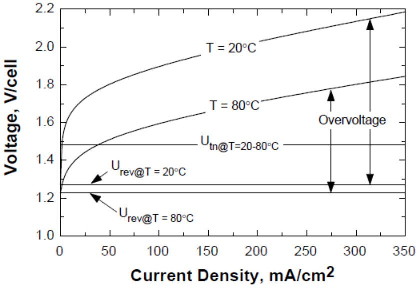

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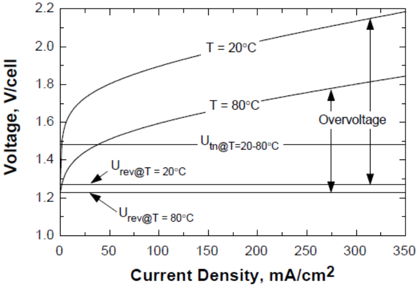


Mass and energy balances

- Anode side:

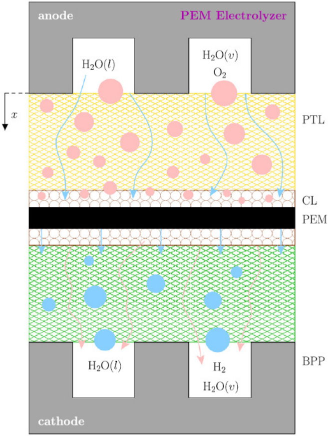
$$\begin{cases} \partial_t C_{O_2}(t,z) = D_{O_2}\partial_{zz}C_{O_2}(t,z) + S_{O_2}(t), \\ \partial_z C_{O_2}(t,0) = 0, \\ \partial_z C_{O_2}(t,r_a) = -\frac{RT}{D_{O_2}}\frac{i}{4F}(t) \end{cases}$$

- Cathode side:

$$\begin{cases} \partial_t C_{H_2}(t,z) = D_{H_2}\partial_{zz}C_{H_2}(t,z) + S_{H_2}(t), \\ \partial_z C_{H_2}(t,0) = 0, \\ \partial_z C_{H_2}(t,r_c) = -\frac{RT}{D_{H_2}}\frac{i}{2F}(t) \end{cases}$$

- Average temperature:

$$\rho_{av}c_p\frac{dT}{dt}(t) = h_{cell}(T_{amb}(t) - T(t)) + (V(t) - U_{tn})i(t)$$



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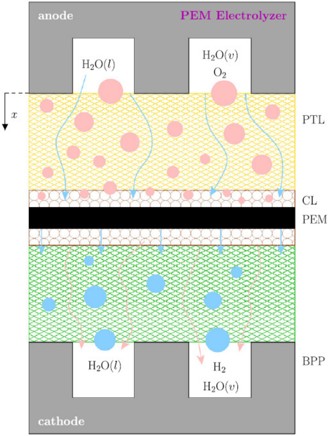

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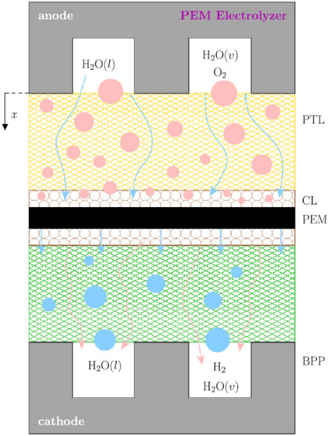

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Dynamic model

- Defining the operator

$$\mathscr{A}(t)\begin{pmatrix}\varphi_1\\ \varphi_2\\ \varphi_3\end{pmatrix}=\begin{pmatrix}D_{O_2}\varphi_1''\\ D_{H_2}\varphi_2''\\ -\frac{h_{cell}}{\rho_{av}c_p}\end{pmatrix},\quad \forall(\varphi_1,\varphi_2,\varphi_3)\in \mathrm{Dom}(\mathscr{A}(t)),$$

$$\mathrm{Dom}(\mathscr{A}(t))=\Big\{(\varphi_1,\varphi_2,\varphi_3)\in (H^2(0,r))^2\times\mathbb{R}|\ \varphi_1'(0)=\varphi_2'=0,\varphi_1'(r)=-\frac{RT}{D_{O_2}}\frac{i}{4F},$$
$$\varphi_2'(r)=-\frac{RT}{D_{H_2}}\frac{i}{2F}\Big\}.$$

Then, the system can be written into the following abstract equation:

$$\dot{x}(t)=\mathscr{A}(t)x(t)+S(t),$$
$$x(0)=x_0,$$

with $S=(S_{O_2},\, S_{H_2},\, h_{cell}/(\rho_{av}c_p)(T_{amb}(t)+(V(t)-U_{tn}))i(t))$.

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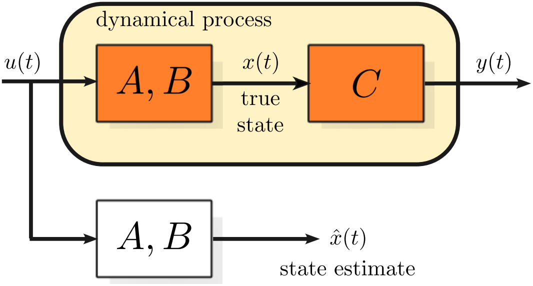
A prime on state estimation

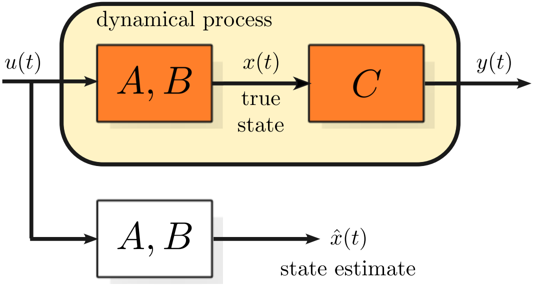
At each time t construct an estimate of the state by only measuring the output $y(t)$ and input $u(t)$.

- **Open-loop observer:** Build an artificial copy of the system, fed in parallel by with the same input signal $u(t)$



- The copy is a numerical simulator reproducing the behavior of the real system

Open-loop observer



- The dynamics of the real system and of the numerical copy are

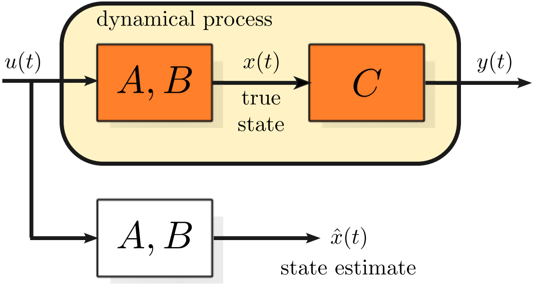
$$\dot{x}(t) = Ax(t) + Bu(t) \qquad \text{(True process)}$$
$$\dot{\hat{x}}(t) = A\hat{x}(t) + Bu(t) \qquad \text{(Numerical copy)}$$

- The dynamics of the estimation error $\tilde{x}(t) = x(t) - \hat{x}(t)$ is

$$\dot{\tilde{x}}(t) = Ax(t) + Bu(t) - A\hat{x}(t) + Bu(t) = A\tilde{x}(t)$$

and then $x(t) = \mathrm{e}^{At}x(0)$.

Open-loop observer

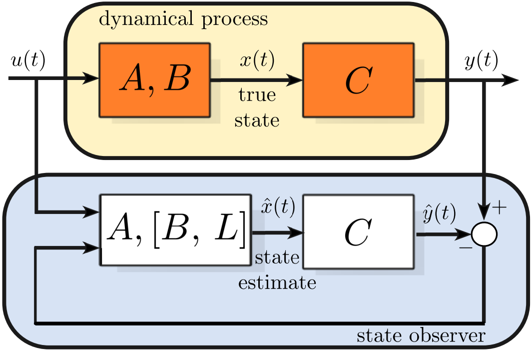


The estimation error is $x(t) = \mathrm{e}^{At}x(0)$. This is not ideal, because

- The dynamics of the estimation error are fixed by the eigenvalues of A and cannot be modified.
- The estimation error vanishes asymptotically if and only if A is asymptotically stable

Note that we are not exploiting $y(t)$ to compute the state estimate $\hat{x}(t)$!

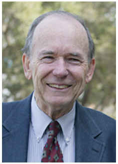
Luenberger observer



- **Luenberger observer:** Correct the estimation equation with a feedback from the estimation error $y(t) - \hat{y}(t)$

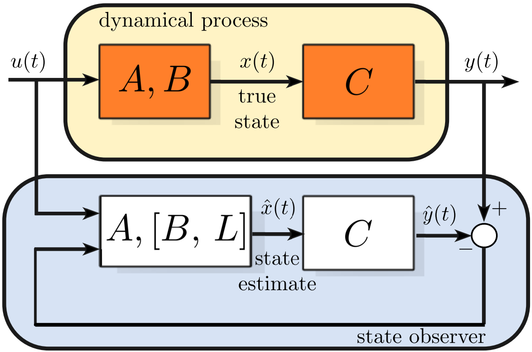
$$\dot{\hat{x}}(t) = A\hat{x}(t) + Bu(t) + \underbrace{L(y(t) - \hat{y}(t))}_{\text{feedback on estimation error}}$$

where L is the observer gain



David G. Luenberger (1937-)

Luenberger observer



- The dynamics of the state estimation error $\tilde{x}(t) = x(t) - \hat{x}(t)$ is

$$\dot{\tilde{x}}(t) = Ax(t) + Bu(t)A\hat{x}(t) + Bu(t) - L(y(t) - \hat{y}(t)) = (A - LC)\tilde{x}(t)$$

Eigenvalue assignment of state observer

Theorem

If the pair (A, C) is observable, then the eigenvalues of $(A - LC)$ can be placed arbitrarily.

Proof:

- If the pair (A, C) is completely observable, the dual system (A', C', B', D') is completely reachable.
- Then we can design a compensator K for the dual system and place the eigenvalues of $(A' + C'K)$ arbitrarily.
- The eigenvalues of $(A' + C'K)$ are the same of its transpose $(A + K'C)$.
- Define $L = -K'$. The proof is complete.

```
MATLAB
» L = acker(A',C',P)';
» L = place(A',C',P)';
```

Example of observer design

- We want to design a state observer for the continuous-time system in state-space form

$$\dot{x}(t) = \begin{pmatrix} -1 & 0 \\ 1 & -1 \end{pmatrix} x(t) + \begin{pmatrix} 2 \\ 0 \end{pmatrix} u(t),$$
$$y(t) = \begin{pmatrix} 0 & \frac{1}{2} \end{pmatrix} x(t).$$

- We want to place the poler of the observer in $\{-4, -4\}$.
- Let $L = (\ell_1, \ \ell_2)$ be the unknown observer gain.
- Write the generic state estimation matrix

$$A - LC = \begin{pmatrix} -1 & 0 \\ 1 & -1 \end{pmatrix} - \begin{pmatrix} \ell_1 \\ \ell_2 \end{pmatrix} \begin{pmatrix} 0 & \frac{1}{2} \end{pmatrix} = \begin{pmatrix} -1 & -\frac{1}{2}\ell_1 \\ 1 & -1 - \frac{1}{2}\ell_2 \end{pmatrix}$$

Example of observer design (cont'd)

- The characteristic polynomial of the observer is

$$\det(\lambda I - A + LC) = \lambda^2 + \left(2 + \frac{1}{2}\ell_2\right)\lambda + \frac{1}{2}\ell_2 + \frac{1}{2}\ell_1 + 1.$$

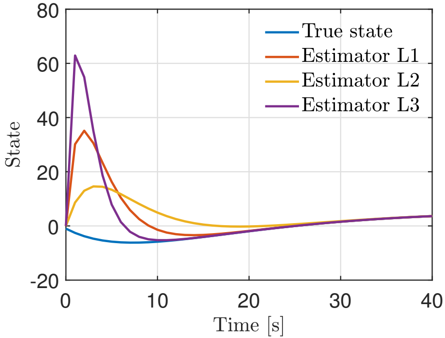
- Impose the polynomial equals the desired one $(\lambda + 4)^2 = \lambda^2 + 8\lambda + 16$.
- Solve the linear system of equations in ℓ_1, ℓ_2 and get

$$\ell_1 = 18, \quad \ell_2 = 12.$$

- The resulting Luenberger observer is

$$\dot{\hat{x}}(t) = \begin{pmatrix} -1 & -9 \\ 1 & -7 \end{pmatrix} \hat{x}(t) + \begin{pmatrix} 2 \\ 0 \end{pmatrix} u(t) + \begin{pmatrix} 18 \\ 12 \end{pmatrix} y(t)$$

Example of observer design (simulations)



Comparison of different observer gains

Response from initial conditions

$x(0) = \begin{pmatrix} -1 \\ 1 \end{pmatrix}, \ \hat{x}(0) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \ \text{for } u(t) = 0.1$

A fast observer often implies large estimation errors in the transient

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- It seems that the a Luenberger observer design cannot be directly applied into our problem.

- Note that we are not measuring an state directly, and therefore we would have

$$\dot{x}(t) = \mathscr{A}(t)x(t) + S(t) + \underbrace{L \begin{pmatrix} I(t) \\ V(t) - \hat{V}(t) \end{pmatrix}}_{\text{injection terms}},$$

There is no feedback on the estimation error!

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Exploring the temperature dynamics and the operational voltage

- Recall that the temperature dynamics and the operational voltage are given by

$$\begin{aligned}\rho_{av} c_p \frac{dT}{dt}(t) =& h_{cell}(T_{amb}(t) - T(t)) + (V(t) - U_{tn}) i(t),\\ V(t) =& V_{Nernst}(t) + V_{act}(t) + V_{ohm}(t) + V_{con}(t)\end{aligned}$$

- The goal of is to obtain an inversion of the function V with respect to the concentrations.
- First, we simplify the average temperature to derive an expression for T only in terms of time, ambient temperature and current:

$$\rho_{av} c_p \frac{dT}{dt}(t) = \chi(t) T(t) + \boldsymbol{\omega(t)}$$

The terms in ω are obtained by substituting T by T_{amb} and c_{co_2} and c_{H_2O} by their relations with the current.

- Then, it holds that

$$T(t) = T(0) \mathrm{e}^{\frac{1}{\rho^{av} c_p} \int_0^t \chi(\tau) d\tau} + \frac{1}{\rho^{av} cp} \int_0^t \mathrm{e}^{\frac{1}{\rho^{av} c_p} \int_0^{t-\tau} \chi(s) ds} \omega(\tau) d\tau$$

Exploring the temperature dynamics and the operational voltage

- Substituting $\check{T}(t) \triangleq T(t, i(t), T_{amb}(t))$ into the operational voltage equation, we obtain

$$\check{V}(t) \triangleq V(t, \check{T}(t), C_{H_2}, i(t)) \triangleq g(t, C_{H_2}, i(t)).$$

- As long as g is a bijection with respect to C_{H_2}, uniformly in i, one could invert it to obtain the concentration as a function of the measurements $(V(t), i(t))$:

$$C_{H_2}(t, r) = h_1(t, V(t), i(t)).$$

- A similar procedure can be applied to obtain $C_{O_2}(t, r) = h_2(t, V(t), i(t))$.

Electrolyzer Luenberger observer

- Now, a Luenberger state observer can be designed:

$$\dot{\hat{x}}(t) = \tilde{A}(t)\hat{x}(t) + S(t) + L\begin{pmatrix} C_{O_2}(t,1) - \hat{C}_{O_2}(t,1) \\ C_{H_2}(t,1) - \hat{C}_{H_2}(t,1) \end{pmatrix}$$

- Error dynamics

$$\dot{\tilde{x}}(t) = \tilde{A}(t)\tilde{x}(t) + L\tilde{y}(t)$$

Desired error dynamics

- Using the observer gains, we want to map the error dynamics into the following exponentially stable system

$$\dot{\tilde{w}}(t) = \mathfrak{A}\tilde{w}(t)$$

  with

$$\mathfrak{A}\begin{pmatrix}\varphi_1\\ \varphi_2\end{pmatrix} = \begin{pmatrix} D_{H_2}\varphi_1'' + \lambda_1\varphi_1 \\ D_{O_2}\varphi_2'' + \lambda_2\varphi_2\end{pmatrix}, \quad \forall(\varphi_1,\varphi_2)\in \mathrm{Dom}(\mathfrak{A}),$$

$$\mathrm{Dom}(\mathfrak{A}) = \Big\{(\varphi_1,\varphi_2)\in (H^2(0,r))^2; \varphi_1(0)=\varphi_2(0)=0,\ \varphi_1'(r) = -\frac{1}{2}\varphi_1(r), \\ \varphi_2'(r) = -\frac{1}{2}\varphi_2(r)\Big\}.$$

- λ_1, λ_2 is a free parameter to be chosen, which determines the **convergence rate** of the observer state to the real system.
- If

$$0 < \lambda_1\frac{D_{H_2}}{4} \quad 0 < \lambda_2\frac{D_{O_2}}{4}$$

  then for any initial condition $\tilde{w}_0 \in L^2(0,r)$, the $\tilde{w}$-system is exponentially stable.

Gains design

- Using the backstepping approach it is possible to obtain an explicit expression for the gains:

$$
\begin{aligned}
l_1 =& \frac{-\lambda_1 r_1}{2\sqrt{\lambda_1(r_1^2-1)}}\left(I_1(\sqrt{\lambda_1(r_1^2-1)}) - \frac{2\lambda_1}{\sqrt{\lambda_1(r_1^2-1)}} I_2(\sqrt{\lambda_1(r_1^2-1)})\right), \\
l_2 =& \frac{-\lambda_2 r_2}{2\sqrt{\lambda_2(r_2^2-1)}}\left(I_1(\sqrt{\lambda_1(r_2^2-1)}) - \frac{2\lambda_1}{\sqrt{\lambda_1(r_2^2-1)}} I_2(\sqrt{\lambda_1(r_2^2-1)})\right), \\
l_{10} =& \frac{1}{2}(3-\lambda_1), \qquad l_{20} = \frac{1}{2}(3-\lambda_2)
\end{aligned}
$$

Summary of the algorithm

1 - Given λ_1, λ_2, compute, in an off line fashion, the observer gains::

$$l_1 = \frac{-\lambda_1 r_1}{2\sqrt{\lambda_1(r_1^2-1)}}\left(I_1(\sqrt{\lambda_1(r_1^2-1)}) - \frac{2\lambda_1}{\sqrt{\lambda_1(r_1^2-1)}} I_2(\sqrt{\lambda_1(r_1^2-1)})\right),$$

$$l_2 = \frac{-\lambda_2 r_2}{2\sqrt{\lambda_2(r_2^2-1)}}\left(I_1(\sqrt{\lambda_1(r_2^2-1)}) - \frac{2\lambda_1}{\sqrt{\lambda_1(r_2^2-1)}} I_2(\sqrt{\lambda_1(r_2^2-1)})\right),$$

$$l_{10} = \frac{1}{2}(3-\lambda_1), \qquad l_{20} = \frac{1}{2}(3-\lambda_2)$$

Then, online do:

2 - Measure V and i;

3 - Compute the observed states by solving the differential equations;

Summary

- Introduction
- Electrolyzer state estimation problem
- Electrolyzer mathematical model
- A prime on state estimation
- State observer design for electrolyzers
- **Final comments**

Final comments

- The observer is characterized by only two tuning parameters – thereby making calibration significantly simpler than KF-based estimators, for example.
- The internal average temperature can be monitored in an open-loop framework.
- Some simplifications were necessary for the proposed design.
- Directions for future work include the design of an observer for the hydrodynamics of the plant.

Muchas gracias!

Obrigado!