First European Fuel Cell Technology & Applications Conference

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A Reduced Fuel Cell Stack Model for Control and Fault Diagnosis

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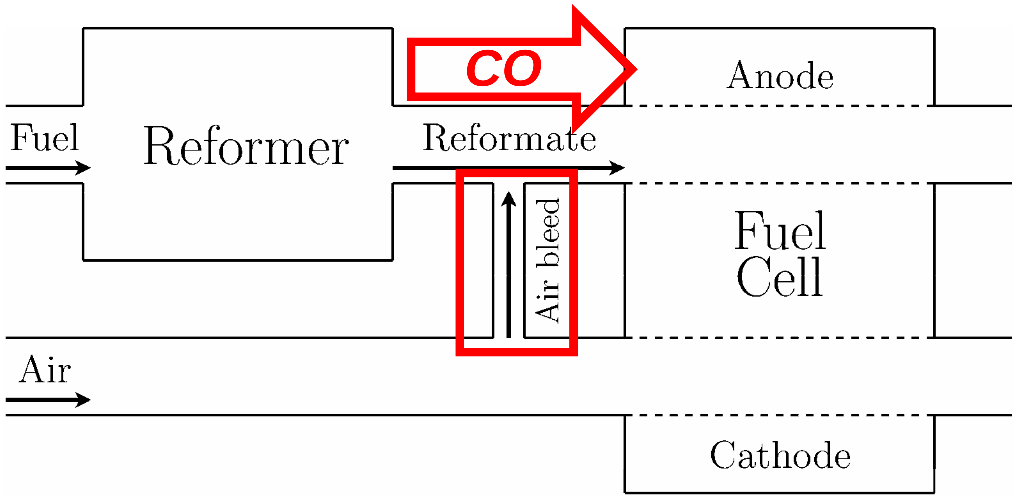
1 Introduction

Motivations:

- Hydrogen fuel cell systems are a promising alternative power source in transport applications.
- Hydrogen currently lacks good infrastructure for refueling, distribution and storage.
- On-board reforming appears to be a likely way for industrialization in the next decade.

- Fuel cell system considered :



- The great technical complexity of the fuel cell system entails a need of on-board model based control and fault diagnosis strategies.
- We present here a stack model suited for controllers and diagnosis algorithms.

2 Electro-chemical Model

Anode:

Hydrogen adsorption/desorption: $H_2 + 2M \underset{b_{fh}k_{fh}}{\overset{k_{fh}}{\rightleftarrows}} 2(M-H)$

Hydrogen electro-oxidation (Tafel reaction): $(M-H) \overset{k_{eh}}{\rightarrow} M + H^+ + e^-$

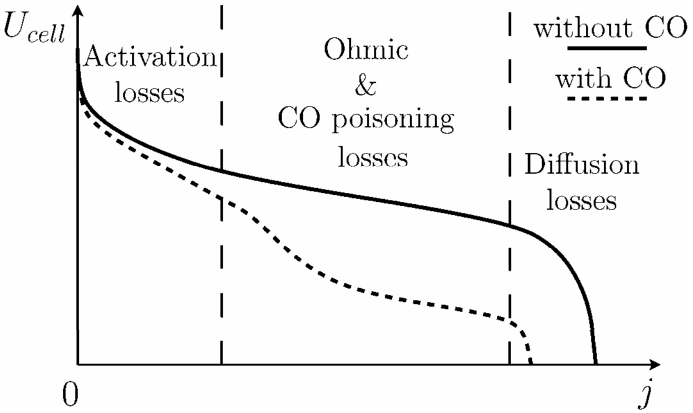
CO adsorption/desorption: $CO + M \underset{b_{fc}k_{fc}}{\overset{k_{fc}}{\rightleftarrows}} (M-CO)$

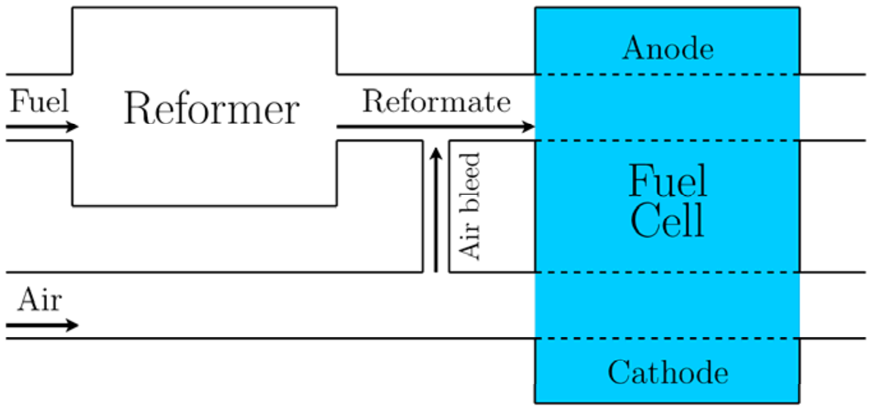
CO electro-oxidation (water-gas-shift): $H_2O + (M-CO) \overset{k_{ec}}{\rightarrow} M + 2H^+ + 2e^- + CO_2$

Oxygen (air bleed) adsorption/desorption: $O_2 + 2M \underset{b_{foa}k_{foa}}{\overset{k_{foa}}{\rightleftarrows}} 2(M-O)$

CO oxidation (CO removal): $(M-CO) + (M-O) \overset{k_{oc}}{\rightarrow} 2M + CO_2$

Hydrogen oxidation (chemical losses): $2(M-H) + (M-O) \overset{k_{oh}}{\rightarrow} 3M + H_2O$





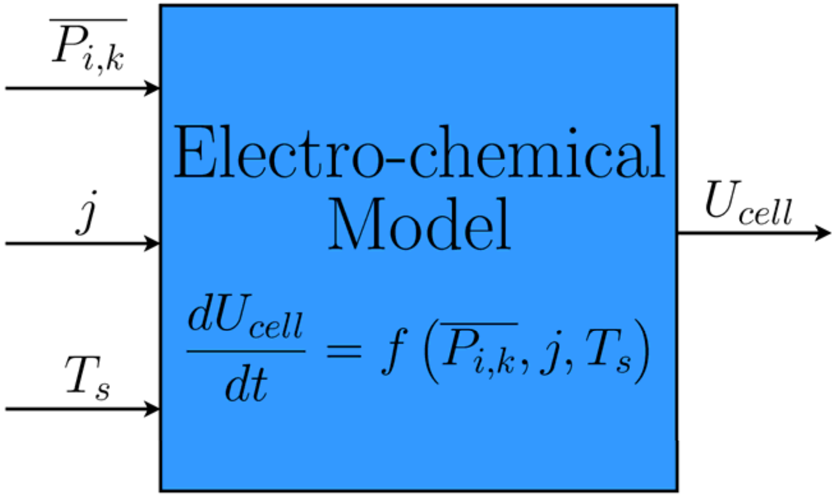
Cathode:

Oxygen adsorption/desorption: $O_2 + 2M \underset{b_{foc}k_{foc}}{\overset{k_{foc}}{\rightleftarrows}} 2(M-O)$

Oxygen electro-reduction: $(M-O) + 2H^+ + 2e^- \overset{k_{eo}}{\rightarrow} M + H_2O$

Assumptions:

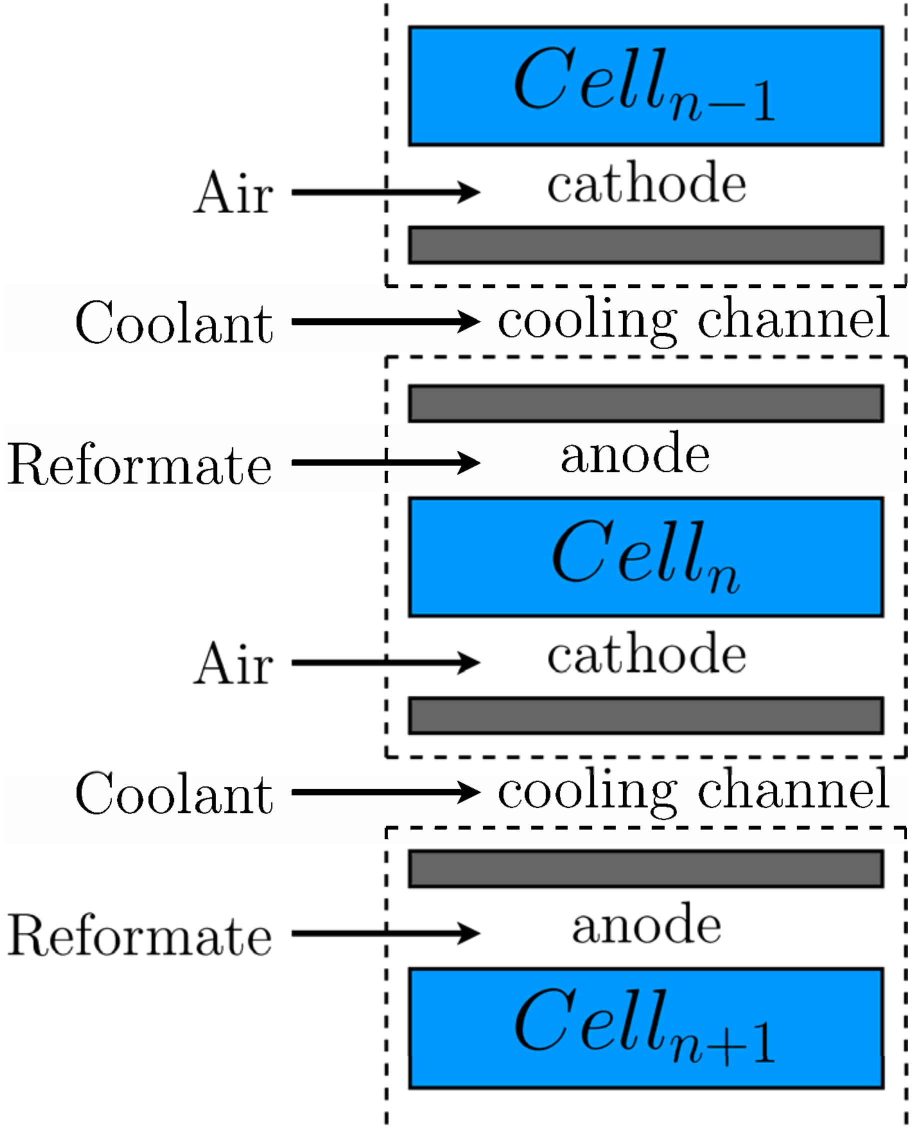
- Reaction rates depend on the electrode coverages of catalyst by the reactants
- Electro-catalysis phenomenon is described by the Butler-Volmer equation
- Kinetics coefficients are functions of the stack temperature via the Arrhenius law
- Cell voltage is computed as the difference between the Nernst potential and the overpotentials : $U_{cell} = E_r - \eta_a - \eta_c - \eta_{ohm}$



With:

- $\overline{P_{i,k}}$: mean partial pressure of species i in the electrode $k \in \{a, c\}$
- j: current density in the cell/stack
- T_s: stack temperature
- U_{cell}: cell voltage

3 Thermal Model


$Cell_{n-1}$
Air
cathode
Coolant
cooling channel
Reformate
anode
$Cell_n$
Air
cathode
Coolant
cooling channel
Reformate
anode
$Cell_{n+1}$

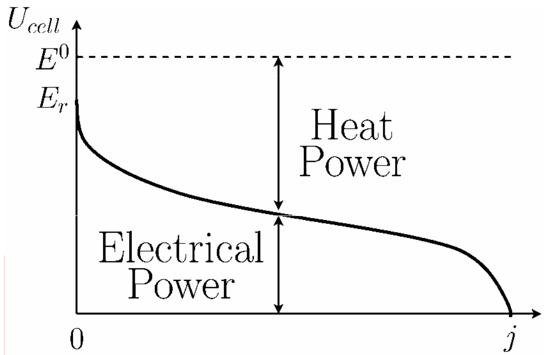
Assumptions:

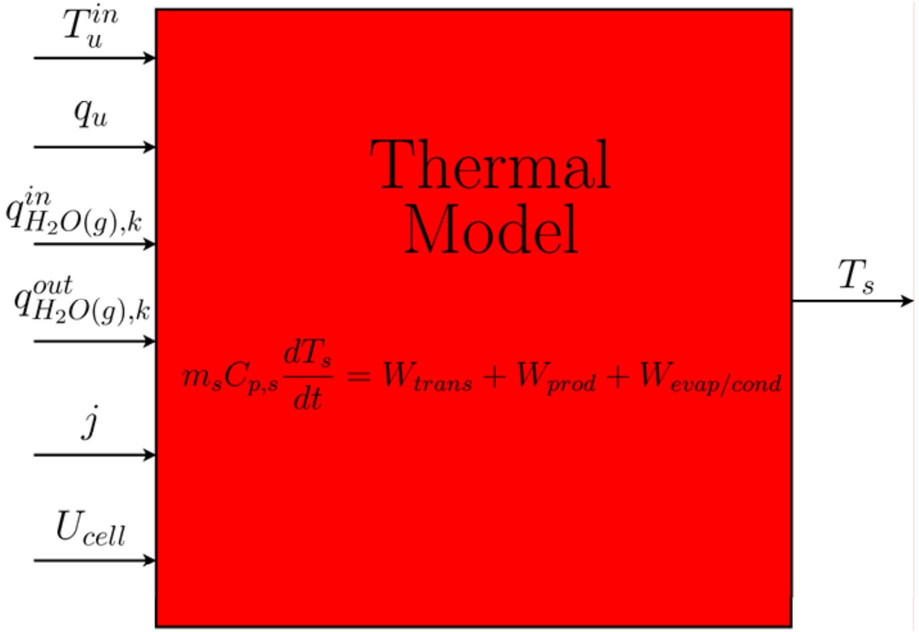
- All the fluids have same outlet temperature taken as the stack temperature:

$$T_u^{out} = T_s, \;\; u \in \{a, c, cool\}$$

- All the cells have the same voltage, stack voltage is then : $U_s = N_{cell} U_{cell}$

- Heat production from reaction:





With:

- T_u^{in}: inlet temperature of the fluid in the channel $u \in \{a, c, cool\}$
- q_u: inlet mass flow of the channel u
- $q^{in}_{H_2O(g),k}, q^{out}_{H_2O(g),k}$: inlet and outlet gas water mass flows in the electrode $k \in \{a, c\}$

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Stack Efficiency

Assumptions:

➢ The heat transfer and the *CO* chemical power received by the stack are not taken into account in this efficiency

$$r_s = \frac{\mathbb{P}_{elec}}{\mathbb{P}^{in}_{chem}} = \frac{U_s A_{act} j}{N_{cell} (LHV)_{H_2} q^{in}_{H_2,a}} \Rightarrow r_s = \frac{U_s}{R_a N_{cell} E^0}$$

Where:

$$q^{in}_{H_2,a} = M_{H_2} \frac{R_a A_{act} j}{2F}$$

$$E^0 = M_{H_2} \frac{(LHV)_{H_2}}{2F}$$

With:

- A_{act}: Active area
- $(LHV)_{H_2}$: Low heat value of hydrogen
- M_{H_2}: Molar mass of hydrogen
- F: Faraday constant
- R_a: Anode stoichiometry
- E^0: Thermo-neutral potential

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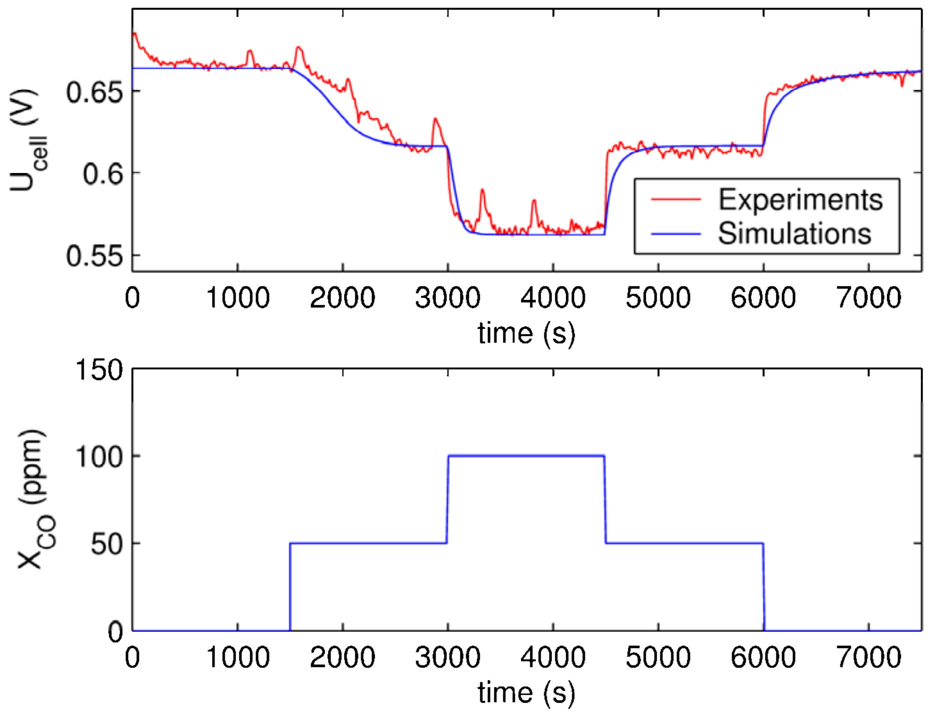
Experimental Results & Model Validation

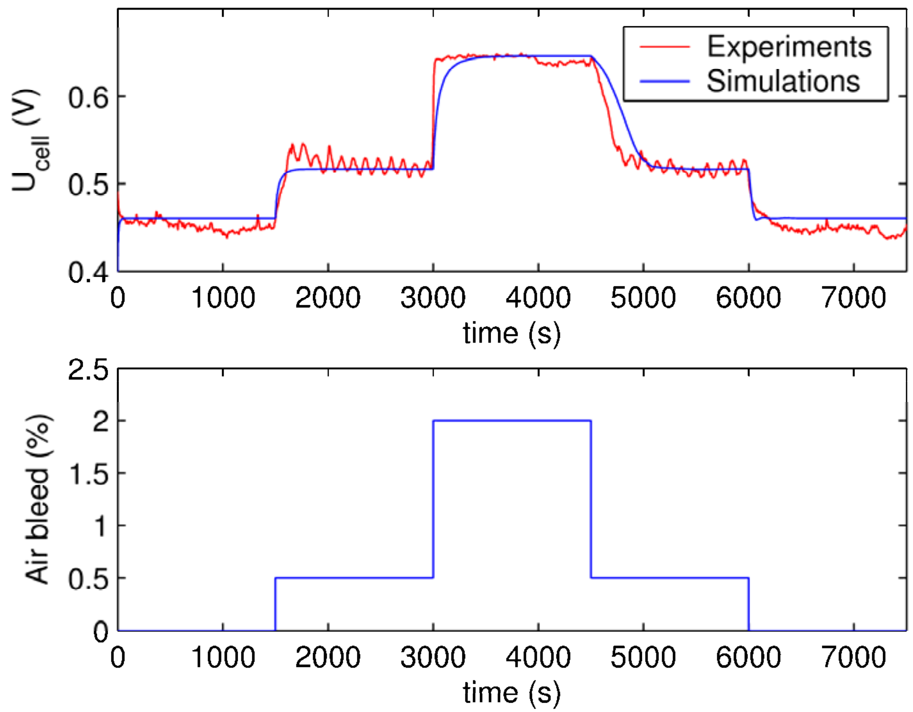
(a) 70°C and 50ppm *CO*
(b) 80°C and 100ppm *CO*
(c) 90°C and 200ppm *CO*

All the tests were performed by 3M

(d)



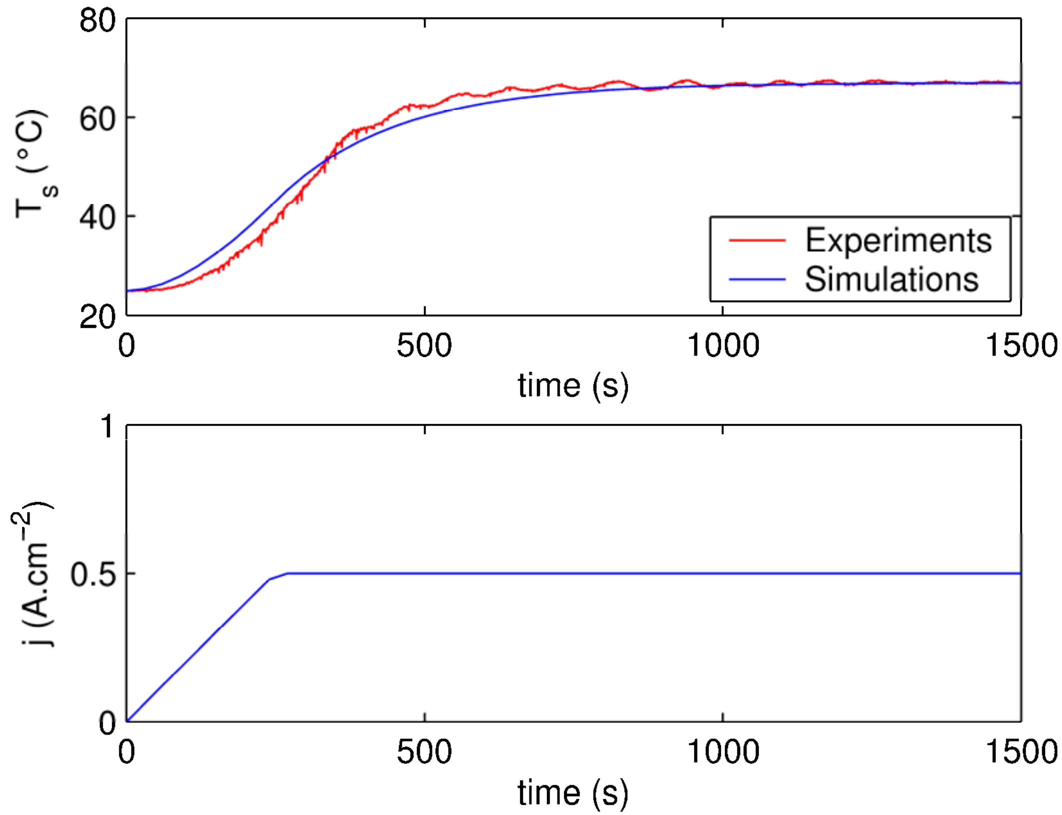
(e)



(d) Variation of inlet *CO* with no air bleed

(e) Variation of air bleed with a fixed inlet *CO*

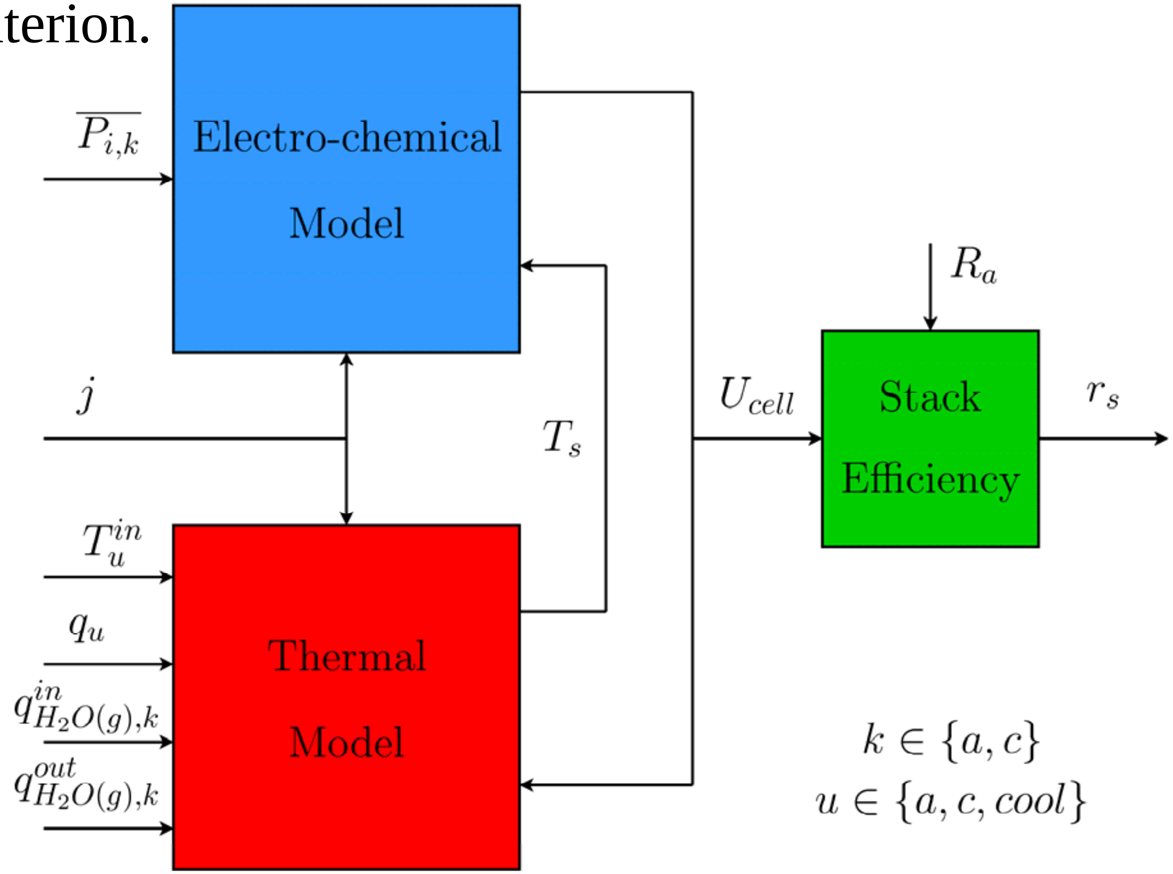
(f)



(f) Small stack transient temperature

6 Conclusion

- We have designed a reduced mathematical model of fuel cell stack, which is validated with experimental data.
- It is composed of two coupled sub models and compute the stack efficiency, which can be used as a fault criterion.



- Due to its simplicity in the form of ordinary differential equations of small order, it is well suited for controllers and fault diagnosis algorithms.

Rates of change of anode catalyst coverage fractions:

$$\rho\frac{d\theta_{H,a}}{dt} = k_{fh}\overline{P_{H_2,a}}\left(1-\theta_{H,a}-\theta_{CO,a}-\theta_{O,a}\right) - b_{fh}k_{fh}\theta_{O,a} - j_H - 2k_{oh}\theta_{H,a}\theta_{O,a} \quad (1)$$

$$\rho\frac{d\theta_{CO,a}}{dt} = k_{fc}\overline{P_{CO,a}}\left(1-\theta_{H,a}-\theta_{CO,a}-\theta_{O,a}\right) - b_{fc}k_{fc}\theta_{CO,a} - j_{CO} - k_{oc}\theta_{CO,a}\theta_{O,a} \quad (2)$$

$$\rho\frac{d\theta_{O,a}}{dt} = k_{foa}\overline{P_{O_2,a}}\left(1-\theta_{H,a}-\theta_{CO,a}-\theta_{O,a}\right) - b_{foa}k_{foa}\theta_{O,a} - k_{oh}\theta_{H,a}\theta_{O,a} - k_{oc}\theta_{CO,a}\theta_{O,a} \quad (3)$$

$$\rho\frac{d\theta_{O,c}}{dt} = k_{foc}\overline{P_{O_2,c}}\left(1-\theta_{O,c}\right) - b_{foc}k_{foc}\theta_{O,c} - j \quad (4)$$

Butler-Volmer equation:

$$j_H = 2k_{eh}\theta_{H,a}\sinh\left(\frac{\eta_a}{B_T}\right) \quad (5)$$

$$j_{CO} = 2k_{ec}\theta_{CO,a}\sinh\left(\frac{\eta_a}{B_T}\right) \quad (6)$$

$$j = 2k_{eo}\theta_{O,c}\sinh\left(\frac{\eta_c}{B_T}\right) \quad (7)$$

$$j = j_H + j_{CO} \quad (8)$$

Temperature dependence: $k_i = k_i^0\exp\left(-\frac{E_{k_i}}{RT_s}\right)$, $b_i = b_i^0\exp\left(-\frac{E_{b_i}}{RT_s}\right)$, $B_T = \frac{2RT_s}{F}$

$$M_s C_p^s \frac{dT_s}{dt} = W_{trans} + W_{prod} + W_{evap/cond} \quad (9)$$

Heat transfer: $$W_{trans} = \sum_{u \in \{a,c,cool\}} q_u C_p^u \left(T_u^{in} - T_s \right) \quad (10)$$

Heat generation: $$\begin{aligned} W_{prod} &= (E^0 - U_{cell}) N_{cell} A_{act} j \\ &= (N_{cell} E^0 - U_s) A_{act} j \end{aligned} \quad (11)$$

Water evaporation/ condensation: $$W_{evap/cond} = L_v \sum_{k \in \{a,c\}} \left(q_{H_2O(g),k}^{in} - q_{H_2O(g),k}^{out} \right) \quad (12)$$