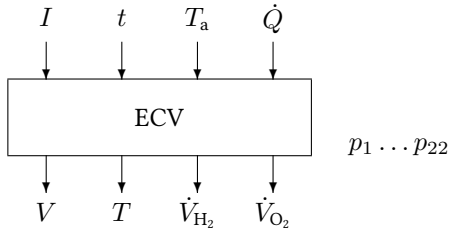
Block ECV

The ECV block simulates an electrolysis cell.



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Function	se0011
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Inputs

1 Current I / A
2 Time t / s
3 Ambient temperature T_a / °C
4 Heating / cooling power $\dot{Q}$ / W

Outputs

1 Voltage V / V
2 Cell temperature T / °C
3 Volume flow hydrogen $\dot{V}_{H_2}$ / $m_n^3\ s^{-1}$
4 Volume flow oxygen $\dot{V}_{O_2}$ / $m_n^3\ s^{-1}$

Parameters

1 Mode
  0 The cell temperature depends on the thermal parameters of the electrolysis cell and the inputs of the block; the initial value of the cell temperature is given by parameter number 22.
  1 The cell temperature is given by input 3
2 Area of a single cell A_c / m^2
3 Number of cells in series N_s

4	Number of cells in parallel N_p
5	Molar enthalpy for the reaction ΔH / J mol^{-1}
6	Equilibrium voltage U_{00} / V at reference temperature $T_0 = 298.15$ K
7	Temperature coefficient s / V K^{-1} of the equilibrium voltage
8	Number z of exchanged electrons
9	Stoichiometric factor of the negative elektrode ν_- (H_2 for water electrolysis)
10	Stoichiometric factor of the positive elektrode ν_+ (O_2 for water electrolysis)
11	Current yield factor $\epsilon_- \leq 1$ of the negative elektrode (H_2 for water electrolysis)
12	Current yield factor $\epsilon_+ \leq 1$ of the positive elektrode (O_2 for water electrolysis)
13	Exchange current densitiy coefficient C_0 / kA m^{-2}
14	Activation energy coefficient of the charge transfer C_1 / K
15	Limiting current density at reference temperature D_0 / kA m^{-2}
16	Temperature coefficient D_1 / kA m^{-2} K^{-1}
17	Conductivity coefficient at reference temperature K_0 / kΩ^{-1} m^{-2}
18	Temperature coefficient K_1 / kΩ^{-1} m^{-2} K^{-1}
19	Heat transfer coefficient K_V / W
20	Temperature exponent m
21	Heat capacity C_eff / J K^{-1}
22	Initial value of cell temperature / °C

Strings

None

Description

The model of an electrolysis cell has two parts: an electrical model and a thermal model based on an energy balance.

Electrical model

The relationship between voltage V_c of a single electrolysis cell and current density j is given by

$$V_\mathrm{c} = V_0 + \frac{4RT}{zF} \ln\left(\frac{j}{2j_\mathrm{A}} + \sqrt{\left(\frac{j}{2j_\mathrm{A}}\right)^2 + 1}\right) + \frac{RT}{zF} \ln\left(\frac{j_\mathrm{G}}{j_\mathrm{G} - j}\right) + j r_\mathrm{c}$$

where

V_0	Equilibrium voltage / V
R	Universal gas Constant 8.314 J mol^{-1} K^{-1}
z	Number of exchanged electrons
F	Faraday Constant 96 494 A s/mol
T	Cell temperature / °C

j_A	Exchange current density / A m^{-2}
j_G	Limiting current density / A m^{-2}
r_c	Ohmic resistance coefficient / Ω m^2

This equation is valid for current densities in the range $j_\mathrm{A} \leq j < j_\mathrm{G}$.

The operating point of the electrolysis block is given by

$$\begin{aligned} V &= V_\mathrm{c} N_\mathrm{s} \\ I &= j A_\mathrm{c} N_\mathrm{p} \end{aligned}$$

where

N_s	Total number of cells in series
N_p	Total number of cells in parallel
A_c	Active area of a single cell / m^2

The variables $V_0, j_\mathrm{A}, j_\mathrm{G}$ and r_c depend on the cell temperature

$$\begin{aligned} V_0 &= V_{00} + s(T - T_0) \\ j_\mathrm{A} &= C_0 \exp\left(-C_1/T\right) \\ j_\mathrm{G} &= D_0 \exp\left(-D_1/T\right) \\ r_\mathrm{c} &= \left(K_0 + K_1(T - T_0)\right)^{-1} \end{aligned}$$

where

V_{00}	Equilibrium voltage / V at reference temperature
s	Temperature coefficient of equilibrium voltage / $\mathrm{V\,K}^{-1}$
T_0	Reference temperature 298.15 K
T	Cell temperature / K
C_0	Exchange current densitiy coefficient / $\mathrm{kA\,m}^{-2}$
C_1	Activation energy coefficient of the charge transfer / K
D_0	Limiting current density at reference temperature / $\mathrm{kA\,m}^{-2}$
D_1	Temperature coefficient / $\mathrm{kA\,m}^{-2}\,\mathrm{K}^{-1}$
K_0	Conductivity coefficient at reference temperature / $\mathrm{k\Omega\,m}^{-2}$
K_1	Temperature coefficient / $\mathrm{k\Omega\,m}^{-2}\,\mathrm{K}^{-1}$

Gas yield

Only part of the current goes into the main cell reaction. Losses are described by a *current yield factor*

$$\epsilon = 1 - \frac{\sum I_{\text{side}} + I_{\text{shunt}} + I_{\text{reco}} + I_{\text{leak}}}{I}$$

where

I_{side}	Current losses due to different side reactions / A
I_{shunt}	Current losses due to ohmic shunt resistances / A
I_{reco}	Current losses due to recombinations / A
I_{leak}	Current losses due to leaks / A

Following Faradays Law $\int I \,\mathrm{d}t = nzF$, where n is the mol number, F the Faraday Constant $96\,494\,\mathrm{As/mol}$ and z is the number of exchanged charges, for the current I we have

$$V_x = \nu_x \epsilon \frac{\int I \,\mathrm{d}t}{zF} \frac{N_{\text{L}}}{N_{\text{A}}} N_{\text{s}}$$

norm cubic meter of gas x from the electrolysis block, where

ν_x	Stoichiometric coefficient of gas x ($\nu_{\text{H}_2} = 1,\ \nu_{\text{O}_2} = 1/2$),
ϵ	Current yield factor
N_{L}	Loschmidt number $6.022 \times 10^{23}\,\mathrm{mol}^{-1}$
N_{A}	Avogadro constant $2.687 \times 10^{25}\,\mathrm{m}^{-3}$
N_{s}	Number of cells in series

Thermal model

The thermal model is based on an energy balance

$$P_{\text{el}} + \dot{Q} - \dot{Q}_{\text{V}} - \Delta H \frac{I N_{\text{s}}}{zF} - C_{\text{eff}} \frac{\mathrm{d}T}{\mathrm{d}t} = 0$$

where

P_{el}	Electrical input power $U \times I$ / W
$\dot{Q}$	Heating ($\dot{Q} > 0$) or cooling ($\dot{Q} < 0$) power / W
$\dot{Q}_{\text{V}}$	Radiation and konvection losses / W
ΔH	Molar enthalpy for the reaction / $\mathrm{J\,mol}^{-1}$
C_{eff}	Heat capacity / $\mathrm{J\,K}^{-1}$]

The losses $\dot{Q}_\mathrm{V}$ are given by

$$\dot{Q}_\mathrm{V} = K_\mathrm{V} \left(\frac{T - T_\mathrm{a}}{\Delta T_0} \right)^{1+m}$$

with the heat transfer coefficient K_V / W and $\Delta T_0 = 1\,\mathrm{K}$. [1]

[1] The coefficients K_V, m and C_eff can be determined by a simple experiment: Given a constant electrolysis current I, after some time a steady state temperature T_∞ will be reached. From eq. **??** we have

$$\begin{aligned} \ln \dot{Q}_\mathrm{V} &= \ln \left(UI + \dot{Q} - \Delta H \frac{I N_\mathrm{s}}{zF} \right) \\ &= \ln K_\mathrm{V} + (1+m) \ln \left(\frac{T_\infty - T_\mathrm{a}}{\Delta T_0} \right) \end{aligned}$$

If the measurement is done with different current values I, the coefficients K_V and m can be determined by a linear regression (using block FITLIN, for example).

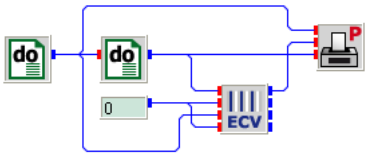
If T_∞ is reached and the current is switched off at t_off the temperature of the electrolysis block decreases till $t_\mathrm{ref} > t_\mathrm{off}$ to T_ref. Since in this case $P_\mathrm{el} = 0$ it follows for all $t > t_\mathrm{off}$ that

$$\frac{\mathrm{d}T}{\mathrm{d}t} = \frac{1}{C_\mathrm{eff}} \left(\dot{Q} - K_\mathrm{V} \left(\frac{T - T_\mathrm{a}}{\Delta T_0} \right)^{1+m} \right)$$

By integration from T_∞ to T_ref and the assumptions $T_\mathrm{a} = \mathrm{const}$ and $\dot{Q} = 0$ it follows

$$C_\mathrm{eff} = \frac{m K_\mathrm{V} (t_\mathrm{ref} - t_\mathrm{off})}{((T_\mathrm{ref} - T_\mathrm{a})/\Delta T_0)^{-m} - ((T_\infty - T_\mathrm{a})/\Delta T_0)^{-m}}$$

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Two nested DO blocks vary temperature (outer block) and current (inner block) from 50 to 120 °C in steps of 10 °C and from 0 to 40 A in steps of 0.01 A, respectively. The time input is set to zero by a CONST block because the ECV block is operated in “Cell temperature given by input 3” mode.

A parametric PLOTP block displays the electrolyser’s voltage-current characteristics.

