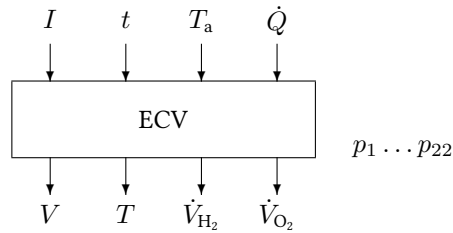


Block ECV

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 $\Delta H / \text{J mol}^{-1}$
6	Equilibrium voltage U_{00} / V at reference temperature $T_0 = 298.15 \text{ K}$
7	Temperature coefficient $s / \text{V K}^{-1}$ of the equilibrium voltage
8	Number z of exchanged electrons
9	Stoichiometric factor of the negative electrode ν_- (H_2 for water electrolysis)
10	Stoichiometric factor of the positive electrode ν_+ (O_2 for water electrolysis)
11	Current yield factor $\epsilon_- \leq 1$ of the negative electrode (H_2 for water electrolysis)
12	Current yield factor $\epsilon_+ \leq 1$ of the positive electrode (O_2 for water electrolysis)
13	Exchange current density coefficient $C_0 / \text{kA m}^{-2}$
14	Activation energy coefficient of the charge transfer C_1 / K
15	Limiting current density at reference temperature $D_0 / \text{kA m}^{-2}$
16	Temperature coefficient $D_1 / \text{kA m}^{-2} \text{K}^{-1}$
17	Conductivity coefficient at reference temperature $K_0 / \text{k}\Omega^{-1} \text{m}^{-2}$
18	Temperature coefficient $K_1 / \text{k}\Omega^{-1} \text{m}^{-2} \text{K}^{-1}$
19	Heat transfer coefficient K_V / W
20	Temperature exponent m
21	Heat capacity $C_{\text{eff}} / \text{J K}^{-1}$
22	Initial value of cell temperature / $^{\circ}\text{C}$

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

$$V_c = V_0 + \frac{4RT}{zF} \ln \left(\frac{j}{2j_A} + \sqrt{\left(\frac{j}{2j_A} \right)^2 + 1} \right) + \frac{RT}{zF} \ln \left(\frac{j_G}{j_G - j} \right) + jr_c$$

where

V_0	Equilibrium voltage / V
R	Universal gas Constant $8.314 \text{ J mol}^{-1} \text{K}^{-1}$
z	Number of exchanged electrons
F	Faraday Constant 96494 A s/mol
T	Cell temperature / $^{\circ}\text{C}$

j_A	Exchange current density / A m^{-2}
j_G	Limiting current density / A m^{-2}
r_c	Ohmic resistance coefficient / $\Omega \text{ m}^2$

This equation is valid for current densities in the range $j_A \leq j < j_G$.

The operating point of the electrolysis block is given by

$$\begin{aligned} V &= V_c N_s \\ I &= j A_c N_p \end{aligned}$$

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_A , j_G and r_c depend on the cell temperature

$$\begin{aligned} V_0 &= V_{00} + s(T - T_0) \\ j_A &= C_0 \exp(-C_1/T) \\ j_G &= D_0 \exp(-D_1/T) \\ r_c &= (K_0 + K_1(T - T_0))^{-1} \end{aligned}$$

where

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

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 $\int I dt = n z F$, where n is the mol number, F the Faraday Constant 96 494 As/mol and z is the number of exchanged charges, for the current I we have

$$V_x = \nu_x \epsilon \frac{\int I dt}{z F} \frac{N_L}{N_A} N_s$$

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 $6.022 \times 10^{23} \text{ mol}^{-1}$

N_A Avogadro constant $2.687 \times 10^{25} \text{ m}^{-3}$

N_s Number of cells in series

Thermal model

The thermal model is based on an energy balance

$$P_{\text{el}} + \dot{Q} - \dot{Q}_v - \Delta H \frac{I N_s}{z F} - C_{\text{eff}} \frac{dT}{dt} = 0$$

where

P_{el} Electrical input power $U \times I$ / W

$\dot{Q}$ Heating ($\dot{Q} > 0$) or cooling ($\dot{Q} < 0$) power / W

$\dot{Q}_v$ Radiation and konvection losses / W

ΔH Molar enthalpy for the reaction / J mol⁻¹

C_{eff} Heat capacity / J K⁻¹]

The losses $\dot{Q}_V$ are given by

$$\dot{Q}_V = K_V \left(\frac{T - T_a}{\Delta T_0} \right)^{1+m}$$

with the heat transfer coefficient K_V / W and $\Delta T_0 = 1$ 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

$$\begin{aligned} \ln \dot{Q}_V &= \ln \left(UI + \dot{Q} - \Delta H \frac{IN_s}{zF} \right) \\ &= \ln K_V + (1+m) \ln \left(\frac{T_\infty - T_a}{\Delta T_0} \right) \end{aligned}$$

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).

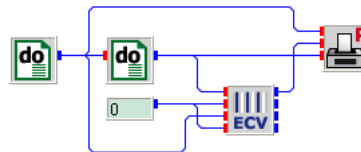
If T_∞ is reached and the current is switched off at t_{off} the temperature of the electrolysis block decreases till $t_{\text{ref}} > t_{\text{off}}$ to T_{ref} . Since in this case $P_{\text{el}} = 0$ it follows for all $t > t_{\text{off}}$ that

$$\frac{dT}{dt} = \frac{1}{C_{\text{eff}}} \left(\dot{Q} - K_V \left(\frac{T - T_a}{\Delta T_0} \right)^{1+m} \right)$$

By integration from T_∞ to T_{ref} and the assumptions $T_a = \text{const}$ and $\dot{Q} = 0$ it follows

$$C_{\text{eff}} = \frac{m K_V (t_{\text{ref}} - t_{\text{off}})}{((T_{\text{ref}} - T_a)/\Delta T_0)^{-m} - ((T_\infty - T_a)/\Delta T_0)^{-m}}$$

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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.

