Thermoptim model of a SOFC burning methane

Let us call α the molar ratio of water and methane flows (α must be greater than 1 so that all methane can be processed).

At the anode, given the high operating temperature of SOFC, we can consider that the whole fuel is converted by the cracking reaction:

$CH_4 + \alpha\, H_2O \rightarrow CO + 3\, H_2 + (\alpha - 1)\, H_2O$ (ΔH_v = 206 140 kJ/kmol)

Then, only a fraction τ (rate of fuel use) is transformed in the cell, the rest coming out of it. The overall reaction giving the output species is written:

For the part used:

$\tau\,(CO + 3\, H_2 + 2\, O_2 + (\alpha - 1)\, H_2O) \rightarrow \tau\,(CO_2 + (\alpha + 2)\, H_2O)$ (ΔH_0 = - 1 008 450 τ kJ/kmol)

Heat of reaction ΔH_0 is calculated here by considering that water remains in the gaseous state due to the temperature (LHV).

For the unused part:

$(1 - \tau)\,(CO + 3\, H_2 + (\alpha - 1)\, H_2O)$

We therefore get at the anode outlet:

$(1 - \tau)\, CO + \tau\, CO_2 + 3\,(1 - \tau)\, H_2 + (3\,\tau + \alpha - 1)\, H_2O$

Of the amount used, a fraction ε is directly converted into electricity, and $(1 - \varepsilon)$ is transformed into heat (some of which is used for steam cracking).

Moreover, λ being a parameter representing the incoming air, oxygen is removed from the oxidizer air at the cathode:

Intake air: $\lambda\,(O_2 + 3{,}76\, N_2)$

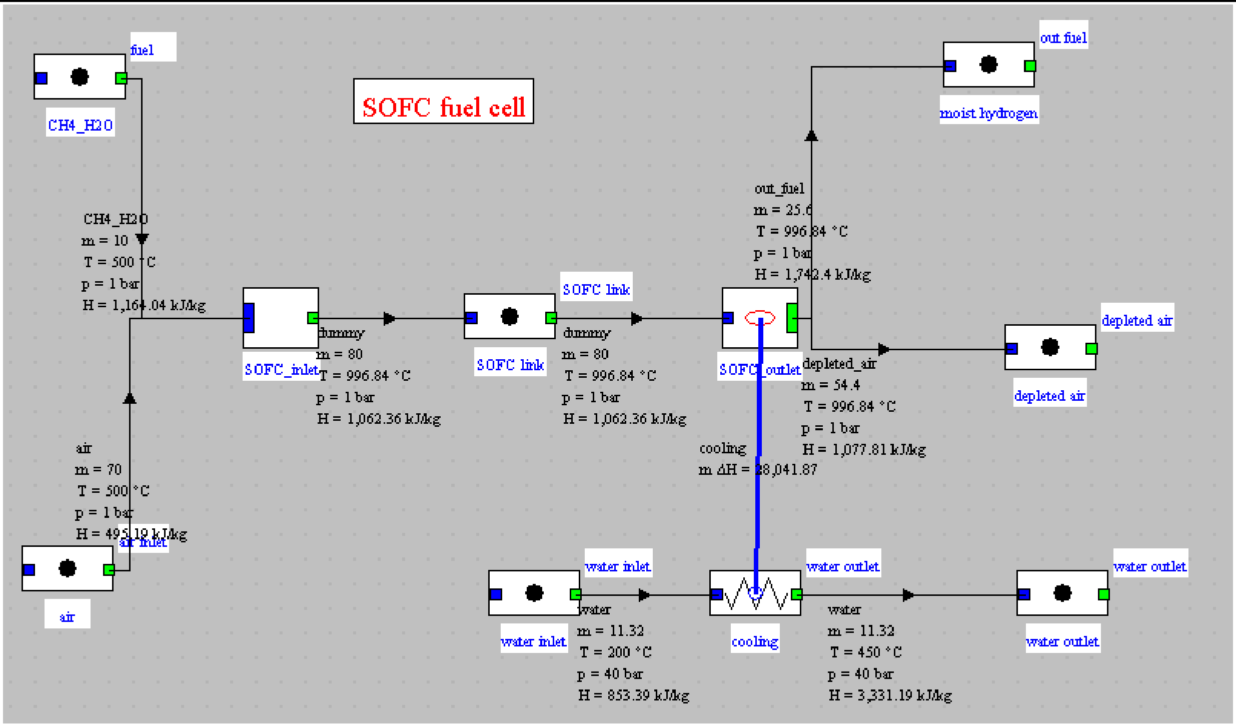
depleted air exiting: $(\lambda - 2\,\tau)\, O_2 + 3{,}76\,\lambda\, N_2$

The model retained is the following (classes SOFCCH4inlet.java and SOFCCH4outlet.java):

- species composition is given by solving the equations above: we determine the molar flow rates of fuel and humidified air at the inlet, which provides values for α and λ, we deduce the molar flow at the output, the values of τ and ε being read on the screen;
- heat released by fraction $\tau\,(1 - \varepsilon)$ of the fuel is used to provide the energy needed to heat gas and by steam cracking.

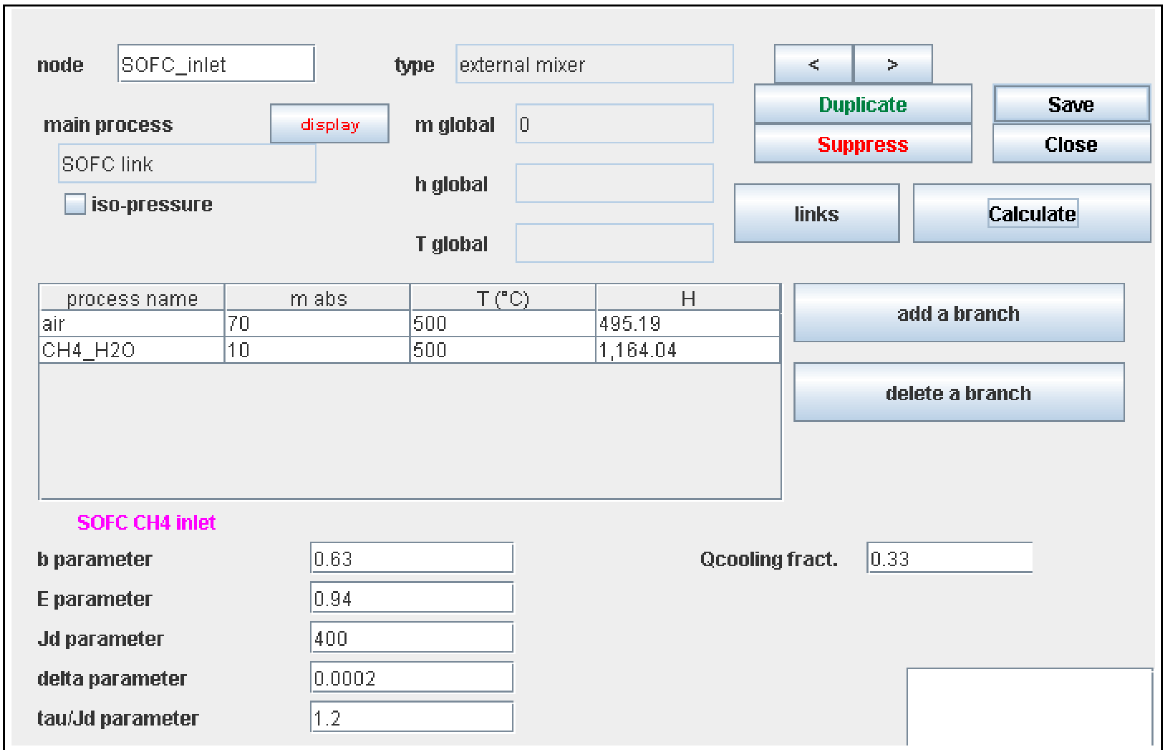
The enthalpy released is equal to τ ΔH0. It is divided into electricity ($\varepsilon\,\tau\,\Delta H_0$), and heat required for steam cracking (ΔH_v) and heating of gas ($\tau\,(1 - \varepsilon)\,\Delta H_0 - \Delta H_v$).

Figure below shows the synoptic view of the fuel cell. The settings used are similar to that of the hydrogen-powered cell model: inlet gas temperature 500 °C, flow rate 10 g/s for fuel, and 80 g/s for air.



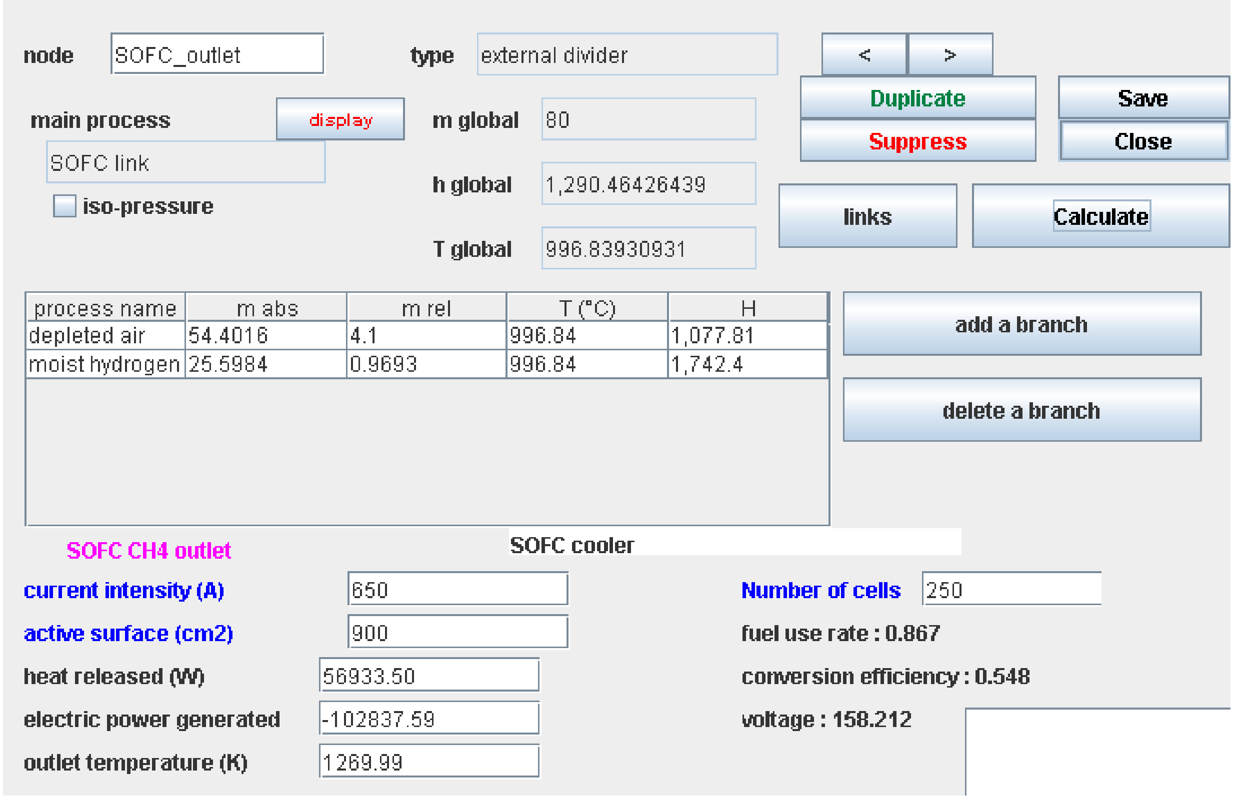
Synoptic view of the SOFC cell

The figure below shows the upstream mixer screen where appear the settings of the electric model, the fuel utilization rate and the fraction of the thermal power extracted by the thermocoupler.



Screen of the mixer upstream of the SOFC

The SOFC component screen is shown in Figure below. We have taken a fuel utilization rate of almost 85%, corresponding to the figure announced by Siemens and Westinghouse for this type of cell operating with natural gas.



SOFC component screen

The gas compositions that are obtained are given in Figures below.

component name	molar fraction	mass fraction
H2O	0.52	0.5488451
CH4 ` methane	0.48	0.4511549

Fuel, flow-rate 10 g/s, LHV: 22,562 kJ/kg

component name	molar fraction	mass fraction
N2	0.781	0.7555302
Ar	0.009	0.01241636
O2	0.21	0.2320534

Air, flow-rate 80 g/s

component name	molar fraction	mass fraction
CO	0.03265306	0.0410301
CO2	0.2122449	0.4190309
H2	0.09795918	0.008858684
H2O	0.6571429	0.5310803

Fuel at the outlet, flow-rate 25.6 g/s, LHV: 1,477 kJ/kg

component name	molar fraction	mass fraction
N2	0.9782662	0.9721497
Ar	0.01127323	0.01597628
O2	0.01046053	0.01187401

O_2-depleted air, flow-rate 64.4 g/s

Model implementation

The main changes to the fuel cell model are displayed on the screen: it is essentially the calculation of the composition of gases leaving the anode and that of the thermal power generated, which is reduced by the heat of reaction required for steam cracking

```
//nombre de moles du fuel en sortie / number of moles of fuel at the outlet
double xCO2=tau*(beta+1)+gamma;
double xH2O=(delta+3.)*tau + alpha -1;
double xCO=(1-tau)*(beta+1);
double xH2=(delta+3.)*(1-tau);
double sigma=xCO2+xH2O+xCO+xH2;

Util.updateMolarComp(fuelComp,gasComp[0], xCO/sigma);
Util.updateMolarComp(fuelComp,gasComp[1], xCO2/sigma);
Util.updateMolarComp(fuelComp,gasComp[2], xH2/sigma);
Util.updateMolarComp(fuelComp,gasComp[3], xH2O/sigma);


double current = -Vtot*intens;
double Qlib= (-DH0*tau-DHvapo)*molFlowCH4+current;

double fractQthermo=Util.lit_d(inletSOFC.Qex_value.getText());//

double Qcool=Qlib*fractQthermo;
Qlib=Qlib-Qcool;
double mcool=inletSOFC.fuelFlow+inletSOFC.airFlow;

epsi = -current/(-DH0*tau-DHvapo)/molFlowCH4;
JLabel11.setText("conversion efficiency : "+Util.aff_d(epsi,3));
```

Model of the cell with recycling

At the anode inlet, we get:

$CH_4 + \alpha\ H_2O + \beta\ CO + \gamma\ CO_2 + \delta\ H_2$

Steam cracking being supposed complete (with the condition $\alpha \geq 1$), the composition after cracking is:

$(\alpha -1)\ H_2O + (\beta +1)\ CO + \gamma\ CO_2 + (\delta +3)\ H_2$

For the part used:

$\tau\ [(\beta +1)\ CO + (\delta +3)\ H_2 + ((\beta +\delta)/2 +2)\ O_2] \rightarrow \tau\ [(\beta +1)\ CO_2 + (\delta +3)\ H_2O]$

For the unused part:

$(\alpha -1)\ H_2O + \gamma\ CO_2 + (1 - \tau)[(\beta +1)\ CO + (\delta +3)\ H_2]$

We therefore get at the anode outlet:

$[\alpha -1 + \tau\ (\delta +3)]\ H_2O + [\gamma + \tau\ (\beta +1)]\ CO_2 + (1 - \tau)\ (\beta +1)\ CO + (1 - \tau)\ (\delta +3)\ H_2$

At the cathode outlet, we get:

$[\lambda - \tau\ ((\beta +\delta)/2 +2)]\ O_2 + 3{,}76\ \lambda\ N_2$

Influence of pressure on the cell performance

Tests made on Siemens Westinghouse cells have shown that the pressure mainly influences the open circuit voltage E.

We choose a model exponential in relation to pressure:

$E = E_0 + E_1\ e^{E_2 P}$

The settings of this equation are defined in the inlet mixer.