Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Supporting information

Industrial feasibility of anodic hydrogen peroxide production through photoelectrochemical water splitting: a techno-economic analysis

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Maximum solar-to-hydrogen (STH) efficiency modelling

To determine the maximum solar-to-hydrogen (STH) efficiency for a tandem photocatalytic device consisting of dual photoabsorbers, a hydrogen evolution reaction (HER) cathode and a hydrogen peroxide evolution reaction (HPER) anode (see Figure 1), we used the web-based model developed by Seger *et al.*[1] The input parameters used are given in Table S1.

Table S1. Relevant input parameters used to calculate the maximum STH efficiency in our model. Unless stated otherwise, checkboxes are not checked and not mentioned in the table.

Parameter	**Input value**
Reactor temperature	298 K
Water depth	2 cm
Ohmic resistance	0 Ω cm^2
Modified light absorption parameters	Yes
Parasitic light loss (top cell absorber)	10 %
Light absorption (top cell absorber)	100 % when $E_p > E_g$*
Parasitic light loss (bottom cell absorber)	10 %
Light absorption (bottom cell absorber)	100 % when $E_p > E_g$*
Dark saturation current	x 100 of theoretical minimum
Shunt resistance	10 kΩ cm^2
Series resistance	1 Ω cm^2
Thermodynamic reaction potential	1780 mV
Faradaic efficiency	100 %
Reduction overpotential at 1 mA/cm^2	35 mV
Tafel slope for reductive reaction	40 mV/decade
Oxidation overpotential	150 mV
Electrolyte used	1 M H_2SO_4
Average ionic path length	0.5 cm
Precision and plotting options	Yes
Current step size	25 μA/cm^2
Bandgap range (top cell absorber)	2.6 to 1.4 eV
Bandgap interval (top cell absorber)	10 meV
Bandgap range (bottom cell absorber)	1.8 to 0.7 eV
Bandgap interval (bottom cell absorber)	10 meV
Current precision in i-V curve	1 x Current step size (in μA/cm^2)
Voltage precision in i-V curve	0.1 mV

* E_p and E_g are defined as photon energy and bandgap energy respectively

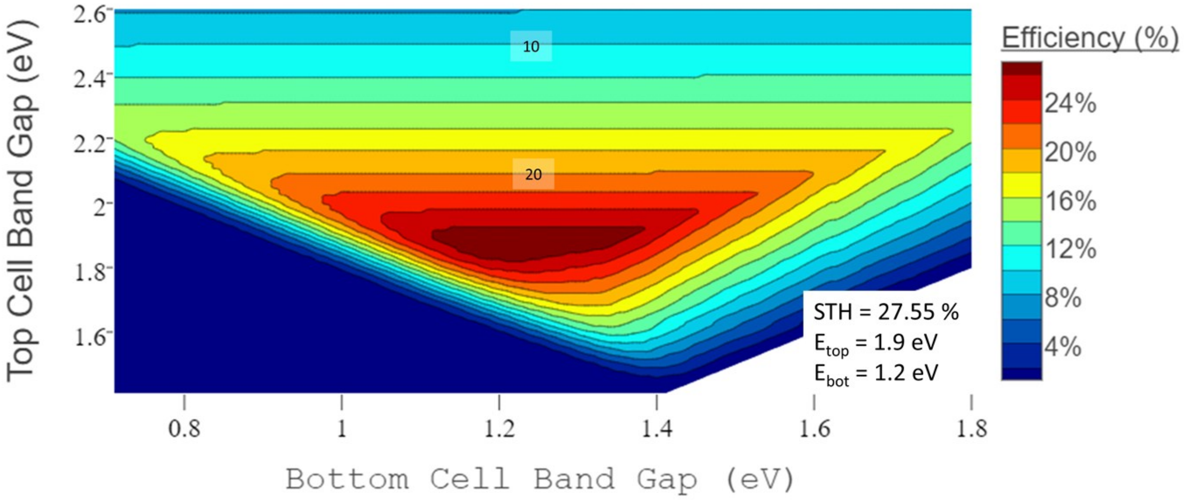

Figure S1. *Contour plot demonstrating the STH efficiency as a function of the bandgaps of the top cell and the bottom cell absorbers in 1.0 M* H_2SO_4 *with 150 mV overpotential. A maximum STH efficiency of 27.55 % is found with top and bottom cell band gaps of 1.9 eV and 1.2 eV respectively.*

Maximum STH efficiency modelling for a bicarbonate solution

As an alternative to sulfuric acid (H_2SO_4), bicarbonate-containing solutions might be used. Several studies have demonstrated that bicarbonate-containing electrolytes significantly improve selectivity towards H_2O_2 production.[2-4] Furthermore, when $BiVO_4$ is used as the HPER anode, the onset potential would be roughly 350 mV.[2] Using the web-based model developed by Seger *et al.*[1] once more, adopting an overpotential of 350 mV for the oxidation potential and using 1.0 M $KHCO_3$, we find the contour plot in Figure S2. The maximum achievable STH efficiency is now calculated to be 23.10 % with top and bottom cell band gaps of 2.0 eV and 1.5 eV respectively.

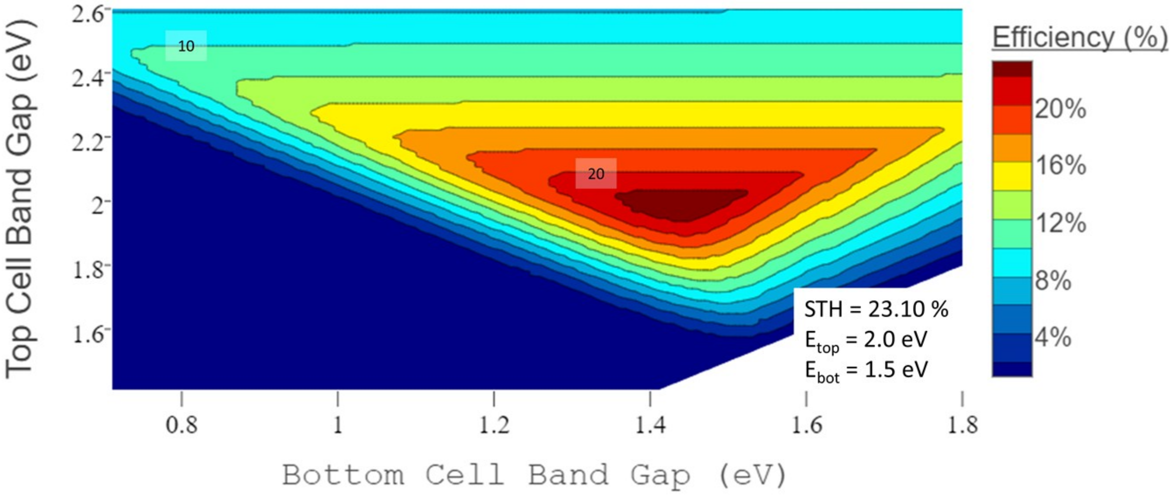

Figure S2. *Contour plot demonstrating the solar-to-hydrogen (STH) efficiency as a function of the bandgaps of the top cell and the bottom cell absorbers in 1.0 M* $KHCO_3$ *with 350 mV overpotential. A maximum STH efficiency of 23.1 % is found with top and bottom cell band gaps of 2.0 eV and 1.5 eV respectively.*

Flow chart for the calculation of the levelized cost of hydrogen

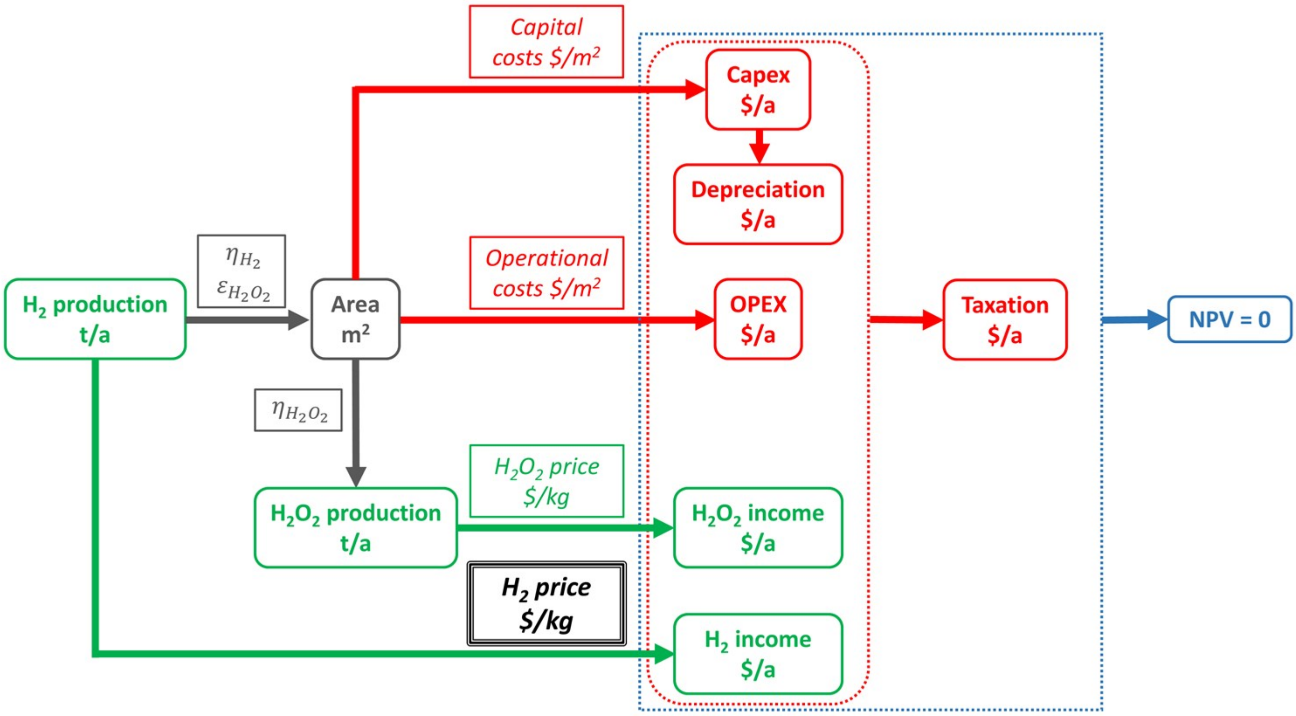

Figure S3. *(Simplified) flow chart depicting the model used to calculate the levelized cost of hydrogen;* i.e. *the H_2 price is calculated to provide a net present value of 0. Please note that for the area and the H_2O_2 production, only the input parameters are given which are fluctuated throughout this study (the STH efficiency η_{H_2}, the Faradaic efficiency towards H_2O_2 at the anode $\varepsilon_{H_2O_2}$ and the STHP efficiency $\eta_{H_2O_2}$). Furthermore, the H_2O_2 price is fluctuated in this study, as well as the material costs (incorporated in the CAPEX).*

Mathematical calculations

Calculation of solar-to-hydrogen (STH) efficiency. The solar-to-hydrogen (STH) efficiency, or H_2 efficiency η_{H_2}, is calculated by:[5]

$$\eta_{H_2} = \frac{P_{H_2}out}{P_{Total}in} = \frac{P_{H_2}out}{P_{Solar}in} = \frac{J_{op}\,[A\,cm^{-2}]\,*\,\Delta E_{H_2}\,[V]\,*\,\varepsilon_{H_2}}{P_{Solar}in\,[W\,cm^{-2}]} \qquad \text{(S1)}$$

where $P_{H_2}out$ is the power output stored in the hydrogen produced (in W cm^{-2}), $P_{Total}in$ is the power put in the system (in W m^{-2}), $P_{Solar}in$ is the power provided by solar illumination (in W cm^{-2}), J_{op} is the operating current density of the PEC device (in A cm^{-2}), ΔE_{H_2} is the potential difference (in V) between the half-reactions corresponding to the hydrogen evolution reaction at the cathode and the oxidation reaction occurring at the anode and ε_{H_2} is the Faradaic efficiency of the hydrogen production.

Now, we should consider the potentials of the half-reactions 1, 2 and 4 in the main manuscript. Because E^0 (H^+/H_2) = 0 V vs RHE and E^0 (O_2/H_2O) = 1.23 V vs RHE, ΔE_{H_2} would be 1.23 V if oxygen is the sole product evolved at the anode. In such case, the Faradaic efficiencies of H_2 and O_2 production would be identical, *i.e.* $\varepsilon_{H_2} = \varepsilon_{O_2}$. Similarly, when H_2O_2 is the sole product formed, ΔE_{H_2} is only +1.78 V (E^0 (H_2O_2/H_2O) = +1.78 V vs RHE)) and $\varepsilon_{H_2} = \varepsilon_{H_2O_2}$. In our model, we assume that only H_2 is produced at the cathode, and only O_2 and H_2O_2 are produced at the anode. Therefore, we can assume that $\varepsilon_{H_2} = 1$ and that $\varepsilon_{H_2O_2} + \varepsilon_{O_2} = 1$. Using this information, we can redefine $\Delta E_{H_2} * \varepsilon_{H_2}$ as follows:

$$\Delta E_{H_2}[V] * \varepsilon_{H_2} = \Delta E_{H_2O_2}[V] * \varepsilon_{H_2O_2} + \Delta E_{O_2}[V] * \varepsilon_{O_2} = \Delta E_{H_2O_2}[V] * \varepsilon_{H_2O_2} + \Delta E_{O_2}[V] * \left(1 - \varepsilon_{H_2O_2}\right) \qquad \text{(S2)}$$

with $\Delta E_{H_2O_2} = 1.78\,V$ and $\Delta E_{O_2} = 1.23\,V$. Implementing equation S2 in equation S1 yields:

$$\eta_{H_2} = \frac{P_{H_2}out}{P_{Solar}in} = \frac{J_{op}\,[A\,cm^{-2}]\,*\,\left(\Delta E_{H_2O_2}\,[V]\,*\,\varepsilon_{H_2O_2} + \Delta E_{O_2}\,[V]\,*\,\left(1 - \varepsilon_{H_2O_2}\right)\right)}{P_{Solar}in\,[W\,cm^{-2}]} \qquad \text{(S3)}$$

Calculation of solar-to-hydrogen peroxide (STHP) efficiency. The solar-to-hydrogen peroxide (STHP) efficiency, or H_2O_2 efficiency $\eta_{H_2O_2}$, can be calculated using:

$$\eta_{H_2O_2} = \frac{P_{H_2O_2}out}{P_{Solar}in} = \frac{J_{op}\,[A\,cm^{-2}]\,*\,\Delta E_{H_2O_2}\,[V]\,*\,\varepsilon_{H_2O_2}}{P_{Solar}in\,[W\,cm^{-2}]} \qquad \text{(S4)}$$

The STHP efficiency can also be defined as a function of the STH efficiency through the following mathematical steps:

$$\frac{\eta_{H_2O_2}}{\eta_{H_2}} = \frac{J_{op}\,[A\,cm^{-2}] \,*\, \Delta E_{H_2O_2}\,[V] \,*\, \varepsilon_{H_2O_2}}{P_{Solar}\,in\,[W\,cm^{-2}]} * \frac{P_{Solar}\,in\,[W\,cm^{-2}]}{J_{op}\,[A\,cm^{-2}] \,*\, \bigl(\Delta E_{H_2O_2}\,[V] \,*\, \varepsilon_{H_2O_2} + \Delta E_{O_2}\,[V] \,*\, (1}$$

(S5)

$$\frac{\eta_{H_2O_2}}{\eta_{H_2}} = \frac{\Delta E_{H_2O_2}\,[V] \,*\, \varepsilon_{H_2O_2}}{\Delta E_{H_2O_2}\,[V] \,*\, \varepsilon_{H_2O_2} + \Delta E_{O_2}\,[V] \,*\, \left(1 - \varepsilon_{H_2O_2}\right)} \tag{S6}$$

$$\eta_{H_2O_2} = \frac{\eta_{H_2}}{1 + \frac{\Delta E_{O_2}\,[V]}{\Delta E_{H_2O_2}\,[V]} \,*\, \left(\frac{1}{\varepsilon_{H_2O_2}} - 1\right)} \tag{S7}$$

Calculation of required panel area. The area of PEC panel required is calculated as follows. First, we define the necessary area:

$$Area = \frac{N_{H_2,\,total}}{N_{H_2}\,per\ area} \tag{S8}$$

where $N_{H_2,\,total}$ is the desired total amount of H_2 produced in the industrial plant and $N_{H_2}\,per\ area$ is the amount of H_2 produced per area. The latter can be calculated as follows:

$$N_{H_2}\,per\ area\,[mol\,m^{-2}] = \frac{E_{H_2}\,[kJ\,m^{-2}]}{\Delta G^0{}_{r,\,H_2}\,[kJ\,mol^{-1}]} \tag{S9}$$

where E_{H_2} is the energy input in the system used to produce H_2 (not to be confused with ΔE_{H_2} in the previous sections!) and $\Delta G^0{}_{r,\,H_2}$ is the Gibbs free energy required to produce one mole of H_2. The energy input for the production of H_2 can be calculated fairly simply from the solar-to-hydrogen efficiency and the solar energy input:

$$E_{H_2}\,[kJ\,m^{-2}] = \eta_{H_2} * E_{solar\ input}\,[kJ\,m^{-2}] \tag{S10}$$

The production of H_2 occurs over two pathways, either due to the production of H_2O_2 or O_2. Assuming that H_2 is produced at a Faradaic efficiency of 100 % and that H_2O_2 and O_2 are the only products at the counter-electrode, we can define:

$$\Delta G^0{}_{r,\,H_2}\,[kJ\,mol^{-1}] = \varepsilon_{H_2O_2} * \Delta G^0{}_{r,\,H_2O_2}\,[kJ\,mol^{-1}] + \varepsilon_{O_2} * \Delta G^0{}_{r,O_2}\,[kJ\,mol^{-1}] \tag{S11}$$

or, using $\varepsilon_{H_2O_2} + \varepsilon_{O_2} = 1$:

$$\Delta G^0{}_{r,\,H_2}\,[kJ\,mol^{-1}] = \varepsilon_{H_2O_2} * \Delta G^0{}_{r,\,H_2O_2}\,[kJ\,mol^{-1}] + (1 - \varepsilon_{H_2O_2}) * \Delta G^0{}_{r,O_2}\,[kJ\,mol^{-1}] \tag{S12}$$

Here, $\Delta G^0{}_{r,\,H_2O_2}$ is the Gibbs free energy involved in the electrochemical production of H_2O_2 from water (reaction 5 in main manuscript, $\Delta G^0{}_{r,\,H_2O_2}$ = 354 kJ per mole of H_2 formed)[6, 7], and $\Delta G^0{}_{r,O_2}$ the Gibbs free energy involved in the electrochemical production of O_2 from water (reaction 3 in main manuscript, $\Delta G^0{}_{r,O_2}$ = 237 kJ per mole of H_2 formed)[6, 7]. Implementing equations S10 and S12 into equation S9 yields:

$$N_{H_2}\,per\ area\left[mol\,m^{-2}\right] = \frac{\eta_{H_2} * E_{solar\ input}\left[kJ\,m^{-2}\right]}{\varepsilon_{H_2O_2} * \Delta G^0{}_{r,\,H_2O_2}\left[kJ\,mol^{-1}\right] + \left(1 - \varepsilon_{H_2O_2}\right) * \Delta G^0{}_{r,O_2}\left[kJ\,mol^{-1}\right]} \tag{S13}$$

Implementing equation S13 in equation S8 yields:

$$Area\left[m^2\right] = \frac{N_{H_2,\,total}\left[mol\right] * \left(\varepsilon_{H_2O_2} * \Delta G^0{}_{r,\,H_2O_2}\left[kJ\,mol^{-1}\right] + \left(1 - \varepsilon_{H_2O_2}\right) * \Delta G^0{}_{r,O_2}\left[kJ\,mol^{-1}\right]\right)}{\eta_{H_2} * E_{solar\ input}\left[kJ\,m^{-2}\right]} \tag{S14}$$

Knowing that the desired amount of H_2 is specified in tonnes per day, that we can define the solar energy input in kWh m^{-2} d^{-1} and that a capacity factor still needs to be included, we can adapt equation S14 into equation S15:

$$Area\left[m^2\right] = \frac{TPD_{H_2}\left[t\,d^{-1}\right] * 10^6\left[g\,t^{-1}\right] * \left(\varepsilon_{H_2O_2} * \Delta G^0{}_{r,\,H_2O_2}\left[kJ\,mol^{-1}\right] + \left(1 - \varepsilon_{H_2O_2}\right) * \Delta G^0{}_{r,O_2}[k\right.}{\eta_{H_2} * E_{solar\ input}\left[kWh\,m^{-2}\,d^{-1}\right] * 3600\left[s\,h^{-1}\right] * C_f * M_{H_2}\left[g\,mol^{-1}\right]} \tag{S15}$$

where TPD_{H_2} is the desired amount of H_2 produced in tonnes per day, C_f is the capacity factor and M_{H_2} the molar mass of hydrogen (2.02 g mol^{-1}).

Calculation of H_2O_2 amount produced. With the required area known, the amount of H_2O_2 produced ($N_{H_2O_2,\,total}$) can be calculated using:

$$N_{H_2O_2,\,total} = Area * N_{H_2O_2}\,per\ area \tag{S16}$$

where $N_{H_2O_2,\,total}$ is the total amount of H_2O_2 produced and $N_{H_2O_2}\,per\ area$ is the amount of H_2O_2 produced per area. Similarly to the previous section, we can define:

$$N_{H_2O_2}\,per\ area\left[mol\,m^{-2}\right] = \frac{E_{H_2O_2}\left[kJ\,m^{-2}\right]}{\Delta G^0{}_{r,\,H_2O_2}\left[kJ\,mol^{-1}\right]} \tag{S17}$$

$$E_{H_2O_2}\left[kJ\,m^{-2}\right] = \eta_{H_2O_2} * E_{solar\ input}\left[kJ\,m^{-2}\right] \tag{S18}$$

with $E_{H_2O_2}$ being the energy input in the system used to produce H_2O_2 and $\Delta G^0{}_{r,\ H_2O_2}\ [kJ\ mol^{-1}]$ the Gibbs free energy required to produce one mole of H_2O_2, which is 354 kJ per mole of H_2O_2 formed (see reaction 5 in main manuscript).[6, 7] Implementing equations S17 and S18 in equation S16 yields:

$$N_{H_2O_2,\ total}\ [mol] = \frac{Area\ [m^2]\ *\ \eta_{H_2O_2}\ *\ E_{solar\ input}\ [kJ\ m^{-2}]}{\Delta G^0{}_{r,\ H_2O_2}\ [kJ\ mol^{-1}]} \tag{S19}$$

Defining the solar energy input once more in kWh m^{-2} d^{-1}, converting the amount of moles H_2O_2 produced to tonnes of H_2O_2 produced per day, *i.e.* $TPD_{H_2O_2}$, and also introducing a capacity factor C_f here, we adapt equation S19 to equation S20:

$$TPD_{H_2O_2}\ [t\ d^{-1}] = \frac{Area\ [m^2]\ *\ \eta_{H_2O_2} *\ E_{solar\ input}\ [kWh\ m^{-2}\ d^{-1}]\ *\ 3600\ [s\ h^{-1}]\ *\ C_f\ *\ M_{H_2O_2}\ [g\ mol^{-1}]}{\Delta G^0{}_{r,\ H_2O_2}\ [kJ\ mol^{-1}]\ *\ 10^6\ [g\ t^{-1}]} \tag{S20}$$

where $M_{H_2O_2}\ [g\ mol^{-1}]$ is the molar mass of hydrogen peroxide (34.02 g mol^{-1}).

Matlab files (m-files) used in this work

m-file used for contour plot scenario (i)

```
%-------------------Model for near-optimal scenario------------------------
close all
clear,clc
set(0,'DefaultFigureVisible','on')
Mymap                   %m-file used for color definition (not shown here)

%--------------------------Input parameters -------------------------------
PX_H2O2_B=0.85;         %Basecase H2O2 price ($ kg-1)
PX_H2O2_H=1.2;          %Maximum H2O2 price ($ kg-1)
PX_H2O2_L=0.5;          %Minimum H2O2 price ($ kg-1)
C_Materials=60;         %Combined costs of photoabsorbers, cathode and
                        anode ($ m-2)
Replacement=7;          %Replacement time of the PEC cell module (in years)
STH_Max=27.55;          %Maximum solar to hydrogen efficiency (%)
FE_H2O2=100;            %Faradaic efficiency towards H2O2 production (%)

Bias_No='no';           %Additional PV bias is not allowed

PX_H2_SR=1.4;           %H2 price through steam reforming ($ kg-1)
PX_H2_ClassicPEC=10;    %H2 price through 'classic' water splitting with O2
                        at the anode ($ kg-1)

%--------Calculations of the LCH based on the maximum STH efficiency-------
f=@(PX_H2)
H2_NPV(STH_Max,FE_H2O2,PX_H2O2_B,PX_H2,Bias_No,C_Materials,Replacement);
                        %Calculation of H2 price at the basecase H2O2 price
[PX_H2_B]=fsolve(f,3);

f=@(PX_H2)
H2_NPV(STH_Max,FE_H2O2,PX_H2O2_H,PX_H2,Bias_No,C_Materials,Replacement);
                        %Calculation of H2 price at the maximum H2O2 price
[PX_H2_H]=fsolve(f,3);

f=@(PX_H2)
H2_NPV(STH_Max,FE_H2O2,PX_H2O2_L,PX_H2,Bias_No,C_Materials,Replacement);
                        %Calculation of H2 price at the minimum H2O2 price
[PX_H2_L]=fsolve(f,3);

PX_H2=[PX_H2_L,PX_H2_B,PX_H2_H];
                        %H2 price at the minimum, basecase and maximum H2O2
                        price

%----Calculation of the LCH as function of STH efficiency and H2O2 price---
 [PX_H2O2,Eff_H2]=meshgrid(0.5:0.014:1.2,5:0.5:30);
                        %Definition of the H2O2 price (PX_H2O2) and the
                        solar-to-hydrogen efficiency (Eff_H2)
H2price=zeros(51,51);
for x=1:length(PX_H2O2);
   for y=1:length(Eff_H2);
       f=@(PX_H2)
H2_NPV(Eff_H2(x,y),FE_H2O2,PX_H2O2(x,y),PX_H2,Bias_No,C_Materials,Replaceme
nt);
       [H2price(x,y)]=fsolve(f,3);
   end
end
```

```
%---Contour plot of H2 price as function of STH efficiency and H2O2 price--
Contour_PX_H2=figure('Name','H2 Price (Optimal
conditions)','NumberTitle','off','Position',[0 0 1600 1000]);
hold on
contourf(PX_H2O2,Eff_H2,H2price)
[C,h]=contour(PX_H2O2,Eff_H2,H2price);
c=colorbar('Direction','reverse','TickLabelInterpreter','latex','FontSize',
35,'Ticks',[-15,-10,-5,0,5,10,15,20,25]);
c.Label.String='H_2 price ($ kg^{-1})';
c.Label.FontSize=35;
colormap(MyMap7)
caxis([-15,25])
axis([0.5 1.2 5 30])
ax=gca;
ax.FontSize=35;
ax.XTick=([0.5,0.7,0.85,1,1.2]);
ax.YTick=([5,10,15,20,25,30]);
ax.TickLabelInterpreter='latex';
ax.XGrid='on';
ax.GridLineStyle='--';
grid on
ax.GridLineStyle='-';
ax.GridAlpha=0.4;
ax.XAxis.MinorTick='on';
ax.XAxis.MinorTickValues= 0.5:0.05:1.2;
ax.YAxis.MinorTick='on';
ax.YAxis.MinorTickValues= 5:1:30;
ax.XLabel.String='H_2O_2 price ($ kg^{-1})';
ax.XLabel.FontSize=40;
ax.YLabel.String='STH efficiency (%)';
ax.YLabel.FontSize=40;
ax.Title.String='H_2/H_2O_2 PEC configuration, optimal conditions';
ax.Title.FontSize=35;
ax.Layer='top';
h.LevelListMode='manual';
h.LevelList=[-20,-17.5,-15,-14.5,-12.5,-10,-7.5,-5,-2.5,-
1,0,1,2,3,5,7.5,10,15,20,30,40,50];
h.TextList=[-20,-17.5,-15,-14.5,-12.5,-10,-7.5,-5,-2.5,-
1,0,1,2,3,5,7.5,10,15,20,30,40,50];
clabel(C,h,'FontSize',35,'FontWeight','bold','LabelSpacing',1000,'Interpret
er','latex')

%----Plot of the maximum STH efficiency (27.55 %) (in the contour plot)----
plotSTH=plot([0.5 0.85 1.2],[STH_Max STH_Max
STH_Max],'Marker','o','MarkerEdgeColor','k','MarkerFaceColor','k','MarkerSi
ze',8,'LineStyle','-','LineWidth',3.5,'Color','k');

%---------Plot of the STH efficiency at 10 % (in the contour plot)---------
plotSTH10=plot([0.5 0.85 1.2],[10 10 10],'LineStyle','--
','LineWidth',2.5,'Color','k');

%-----Calculation and plot of the H2 price through steam reforming (in the
contour plot)------
Price_H2O2=[0.5:0.014:1.2];
H2price_SR=zeros(1,51);
for y=1:length(Price_H2O2);
    f=@(Eff_H2)
H2_NPV(Eff_H2,FE_H2O2,Price_H2O2(y),PX_H2_SR,Bias_No,C_Materials,Replacemen
t);
       [H2price_SR(y)]=fsolve(f,3);
```

```
end
plotPX_H2_SR=plot(Price_H2O2,H2price_SR,'Marker','none','Color','r','LineSt
yle','--','LineWidth',3.5);

%---Calculation and plot of H2 price through 'classic' PEC water splitting
(in the contour plot)---
H2price_ClassicPEC=zeros(1,51);
for y=1:length(Price_H2O2);
    f=@(Eff_H2)
H2_NPV(Eff_H2,FE_H2O2,Price_H2O2(y),PX_H2_ClassicPEC,Bias_No,C_Materials,Re
placement);
       [H2price_ClassicPEC(y)]=fsolve(f,3);
end
plotPX_H2_ClassicPEC=plot(Price_H2O2,H2price_ClassicPEC,'Marker','none','Co
lor','b','LineStyle','--','LineWidth',3.5);

hold off

print(Contour_PX_H2,'-dpng','D:\UT_2018\Papers\HP Techno-economics
paper\Resubmission\Updated M-files\_Adjusted m-files_optimal
scenario\Contour_PX_H2_Optimal.PNG')

%--------------------------------------Output of values---------------------
---------------------
PX_H2             %Levelized cost of hydrogen at the minimum, basecase and
                  maximum H2O2 price (at maximum STH efficiency)

[NPV,TOTAL_CAPEX,TOTAL_OPEX,TOTAL_CAPEX_PEC_Cell,TOTAL_CAPEX_HardBoS,TOTAL_
CAPEX_SoftBoS,Area]=H2_NPV(STH_Max,FE_H2O2,PX_H2O2_B,PX_H2_B,Bias_No,C_Mate
rials,Replacement)
%The following parameters are returned:
%NPV - Net present value (should approach 0)
%TOTAL_CAPEX - Total CAPEX costs
%TOTAL_OPEX - Total OPEX costs
%TOTAL_CAPEX_PEC_Cell - Total CAPEX costs of the PEC cell (including PV
module costs)
%TOTAL_CAPEX_HardBoS - Total CAPEX costs of the hard balance of systems
%TOTAL_CAPEX_SoftBoS - Total CAPEX costs of the soft balance of systems
%Area - Total required area of cathodic (or anodic) material
```

m-file used for the contour plot in scenario (ii)

```
%-----------Model for literature-based state-of-the-art scenario-----------
close all
clear,clc
set(0,'DefaultFigureVisible','on')
Mymap                       %m-file used for color definition (not shown here)

%---------------------------Input parameters ------------------------------
PX_H2O2_B=0.85;            %Basecase H2O2 price ($ kg-1)
PX_H2O2_H=1.2;             %Maximum H2O2 price ($ kg-1)
PX_H2O2_L=0.5;             %Minimum H2O2 price ($ kg-1)
C_Photoanode=50;           %Costs of photoanode ($ m-2)
C_PV=70;                   %Costs of photovoltaic module ($ m-2)
Replacement=7;             %Replacement time of the PEC cell module (in years)

STH_PV=10.1;                %Solar-to-hydrogen efficiency based on literature
                           (%)
FE_H2O2=98;                 %Faradaic efficiency towards H2O2 production based
                           on literature (%)
STH_Max = 13.4;             %Maximum solar-to-hydrogen efficiency obtainable
                           when BiVO4 is used as a photoanode for H2O2
                           production (%)

Bias_In='In';              %Additional PV bias is allowed

PX_H2_SR=1.4;              %H2 price through steam reforming ($ kg-1)
PX_H2_ClassicPEC=10;       %H2 price through 'classic' water splitting with O2
                           at the anode ($ kg-1)

%-Calculations of the LCH based on the STH efficiency adopted from
literature-
f=@(PX_H2)
H2_NPV(STH_PV,FE_H2O2,PX_H2O2_B,PX_H2,Bias_In,C_Photoanode,C_PV,Replacement
);                         %Calculation of H2 price at the basecase H2O2 price
[PX_H2_In_B]=fsolve(f,3);

f=@(PX_H2)
H2_NPV(STH_PV,FE_H2O2,PX_H2O2_H,PX_H2,Bias_In,C_Photoanode,C_PV,Replacement
);                         %Calculation of H2 price at the maximum H2O2 price
[PX_H2_In_H]=fsolve(f,3);

f=@(PX_H2)
H2_NPV(STH_PV,FE_H2O2,PX_H2O2_L,PX_H2,Bias_In,C_Photoanode,C_PV,Replacement
);                         %Calculation of H2 price at the minimum H2O2 price
[PX_H2_In_L]=fsolve(f,3);

PX_H2_In=[PX_H2_In_L,PX_H2_In_B,PX_H2_In_H];
                           %H2 price at the minimum, basecase and maximum H2O2
                           price

%---Calculations of the LCH based on the maximum STH efficiency for BiVO4--
f=@(PX_H2)
H2_NPV(STH_Max,FE_H2O2,PX_H2O2_B,PX_H2,Bias_In,C_Photoanode,C_PV,Replacemen
t);                        %Calculation of H2 price at the basecase H2O2 price
[PX_H2_Max_B]=fsolve(f,3);
```

```
f=@(PX_H2)
H2_NPV(STH_Max,FE_H2O2,PX_H2O2_H,PX_H2,Bias_In,C_Photoanode,C_PV,Replacemen
t);                     %Calculation of H2 price at the maximum H2O2 price
[PX_H2_Max_H]=fsolve(f,3);

f=@(PX_H2)
H2_NPV(STH_Max,FE_H2O2,PX_H2O2_L,PX_H2,Bias_In,C_Photoanode,C_PV,Replacemen
t);                     %Calculation of H2 price at the minimum H2O2 price
[PX_H2_Max_L]=fsolve(f,3);

PX_H2_Max=[PX_H2_Max_L,PX_H2_Max_B,PX_H2_Max_H];
                        %H2 price at the minimum, basecase and maximum H2O2
                        price

%----Calculation of the LCH as function of STH efficiency and H2O2 price---
[PX_H2O2,Eff_H2]=meshgrid(0.5:0.014:1.2,5:0.5:30);
                        %Definition of the H2O2 price (PX_H2O2) and the
                        solar-to-hydrogen efficiency (Eff_H2)
H2price=zeros(51,51);
for x=1:length(PX_H2O2)
   for y=1:length(Eff_H2)
       f=@(PX_H2)
H2_NPV(Eff_H2(x,y),FE_H2O2,PX_H2O2(x,y),PX_H2,Bias_In,C_Photoanode,C_PV,Rep
lacement);
       [H2price(x,y)]=fsolve(f,3);
   end
end

%--Contour plot of H2 price as function of STH efficiency and H2O2 price---
Contour_PX_H2=figure('Name','U_PV = 1.9 V; FE = 98
%','NumberTitle','off','Position',[0 0 1600 1000]);
hold on
contourf(PX_H2O2,Eff_H2,H2price)
[C,h]=contourf(PX_H2O2,Eff_H2,H2price);
c=colorbar('Direction','reverse','TickLabelInterpreter','latex','FontSize',
35,'Ticks',[-15,-10,-5,0,5,10,15,20,25]);
c.Label.String='H_2 price ($ kg^{-1})';
c.Label.FontSize=35;
colormap(MyMap7)
caxis([-15,25])
axis([0.5 1.2 5 30])
ax=gca;
ax.FontSize=35;
ax.XTick=([0.5,0.7,0.85,1,1.2]);
ax.YTick=([5,10,15,20,25,30]);
ax.TickLabelInterpreter='latex';
ax.XGrid='on';
ax.GridLineStyle='--';
grid on
ax.GridLineStyle='-';
ax.GridAlpha=0.4;
ax.XAxis.MinorTick='on';
ax.XAxis.MinorTickValues= 0.5:0.05:1.2;
ax.YAxis.MinorTick='on';
ax.YAxis.MinorTickValues= 5:1:30;
ax.XLabel.String='H_2O_2 price ($ kg^{-1})';
ax.XLabel.FontSize=40;
ax.YLabel.String='STH efficiency (%)';
ax.YLabel.FontSize=40;
ax.Title.String='U_{PV} = 1.9 V; FE = 98 %, literature based';
ax.Title.FontSize=35;
```

```
ax.Layer='top';
h.LevelListMode='manual';
h.LevelList=[-20,-17.5,-15,-14.5,-12.5,-10,-7.5,-5,-2.5,-
1,0,1,2,3,5,7.5,10,15,20,30,40,50];
h.TextList=[-20,-17.5,-15,-14.5,-12.5,-10,-7.5,-5,-2.5,-
1,0,1,2,3,5,7.5,10,15,20,30,40,50];
clabel(C,h,'FontSize',35,'FontWeight','bold','LabelSpacing',1000,'Interpret
er','latex')

%------Plot of the STH efficiency derived from literature (in the contour
plot)------
plotSTH=plot([0.5 0.85 1.2],[STH_PV STH_PV
STH_PV],'Marker','o','MarkerEdgeColor','k','MarkerFaceColor','k','MarkerSiz
e',8,'LineStyle','-','LineWidth',3.5,'Color','k');

%------Plot of the calculated maximum STH efficiency for BiVO4 (in the
contour plot)------
plotSTH=plot([0.5 0.85 1.2],[STH_Max STH_Max STH_Max],'LineStyle','--
','LineWidth',2.5,'Color','k');

%------Calculation and plot of the H2 price through steam reforming (in the
contour plot)------
Price_H2O2=[0.5:0.014:1.2];
H2price_SR=zeros(1,51);
for y=1:length(Price_H2O2)
    f=@(Eff_H2)
H2_NPV(Eff_H2,FE_H2O2,Price_H2O2(y),PX_H2_SR,Bias_In,C_Photoanode,C_PV,Repl
acement);
       [H2price_SR(y)]=fsolve(f,3);
end
plotPX_H2_SR=plot(Price_H2O2,H2price_SR,'Marker','none','Color','r','LineSt
yle','--','LineWidth',3.5);

%-Calculation and plot of H2 price through 'classic' PEC water splitting
(in the contour plot)-
H2price_ClassicPEC=zeros(1,51);
for y=1:length(Price_H2O2)
    f=@(Eff_H2)
H2_NPV(Eff_H2,FE_H2O2,Price_H2O2(y),PX_H2_ClassicPEC,Bias_In,C_Photoanode,C
_PV,Replacement);
       [H2price_ClassicPEC(y)]=fsolve(f,3);
end
plotPX_H2_ClassicPEC=plot(Price_H2O2,H2price_ClassicPEC,'Marker','none','Co
lor','b','LineStyle','--','LineWidth',3.5);

hold off

print(Contour_PX_H2,'-dpng','D:\UT_2018\Papers\HP Techno-economics
paper\Resubmission\Updated M-files\_Adjusted m-
files_literature_based\H2price_Literature.png')

%---------------------------Output of values------------------------------
PX_H2_In           %Levelized cost of hydrogen at the minimum, basecase and
                   maximum H2O2 price (at STH efficiency based on
                   literature)
PX_H2_Max          %Levelized cost of hydrogen at the minimum, basecase and
                   maximum H2O2 price (at maximum STH efficiency possible
                   for BiVO4)
```

```
[NPV,TOTAL_CAPEX,TOTAL_OPEX,TOTAL_CAPEX_PEC_Cell,TOTAL_CAPEX_HardBoS,TOTAL_
CAPEX_SoftBoS,Area]=H2_NPV(STH_PV,FE_H2O2,PX_H2O2_B,PX_H2_In_B,Bias_In,C_Ph
otoanode,C_PV,Replacement)
%The following parameters are returned:
%NPV - Net present value (should approach 0)
%TOTAL_CAPEX - Total CAPEX costs
%TOTAL_OPEX - Total OPEX costs
%TOTAL_CAPEX_PEC_Cell - Total CAPEX costs of the PEC cell (including PV
module costs)
%TOTAL_CAPEX_HardBoS - Total CAPEX costs of the hard balance of systems
%TOTAL_CAPEX_SoftBoS - Total CAPEX costs of the soft balance of systems
%Area - Total required area of cathodic (or anodic) material
```

m-file ‘H2_NPV’ used for scenario (ii)

(*Note: the m-file* `H2_NPV` *is almost identical for scenario (i), with a few alterations: the inputs for* `C_Photoanode` *and* `C_PV`*, along with the constant* `C_Cathode`*, have been replaced with an input for the combined costs of photoabsorbers, cathode and anode. Furthermore, no photovoltaic module is involved for scenario (i), so* `C_In=0`)

```
function[NPV,TOTAL_CAPEX,TOTAL_OPEX,TOTAL_CAPEX_PEC_Cell,TOTAL_CAPEX_HardBoS,TOTAL_CAPEX_SoftBoS,Area]=H2_NPV(Eff_H2,FE,PX_H2O2,PX_H2,Bias,C_Photoanode,C_PV,Replacement)

%PX_H2 = H2 price (output) ($ kg-1)
%Eff_H2 = Solar-to-hydrogen (STH) efficiency (%)
%FE = Faradaic efficieny towards hydrogen peroxide (%)
%PX_H2O2 = H2O2 price ($ kg-1)
%Bias = Definition whether additional PV bias is allowed ('In' means it is)
%C_Photoanode = Costs of the photoanode material ($ m-2)
%C_PV = Costs of photovoltaic module when used ($ m-2)
%Replacement = Replacement time (a)

%---------------------------Technical constants----------------------------
Cf=0.95;                %Capacity factor
Ps=6.19;                %Solar energy input (KWh m-2 d-1)
TPD=10;                 %H2 production scale (t d-1)
Er_H2O2=354;            %Gibbs free energy required for H2O2 formation (kJ mol-1 H2)
Er_O2=237;              %Gibbs free energy required for O2 formation (kJ mol-1 H2)
M_H2=2.02;              %Molar mass H2 (g mol-1)
M_H2O2=34.02;           %Molar mass H2O2 (g mol-1)
Rep=Replacement;        %Replacement time (years). Only 3, 7 and 12 years can be entered.

%------------------------------CAPEX constants-----------------------------
C_Glass=10;             %Costs glass ($ m-2)
C_Housing=21;           %Costs housing ($ m-2)
C_Cathode=5;            %Costs cathode ($ m-2)
C_Membrane=50;          %Costs membrane ($ m-2)
C_Assembly=20;          %Costs assembly of the PEC cell module ($ m-2)
C_In=C_PV;              %Costs photovoltaic module ($ m-2)
C_No=0;                 %Costs when no photovoltaic module is used ($ m-2)

Inst=0.2;               %Installement costs: 20% of initial investment + replacement costs
Cont=0.3;               %Contingency costs: 30% of initial investment
Engi=0.05;              %Engineering and design costs: 5% of initial investment

Sys_H2=11.5*1000000;    %H2 gas system ($)
Sys_H2O=2.6*1000000;    %H2O piping system ($)
Sys_H2O2=2.6*1000000;   %H2O2 piping system ($)
Sys_Sep=5*1000000;      %H2O2 and H2O seperator ($)
Sys_Cont=6*1000000;     %Process control system ($)

Rep_7=0.75;             %Replacement costs after 7 years: 75% of initial CAPEX costs
Rep_14=0.6;             %Replacement costs after 14 years: 60% of initial CAPEX costs

%--------------------OPEX and other economic constants---------------------
```

```
Ins=0.02;                %Insurence costs: 2% of initial CAPEX of PEC module
                         and hard BoS per year
C_Labor=4.5*1000000;     %Labor costs ($ a-1)
n=20;                    %Project lifetime in years
Inf=0.019;               %Inflation rate
r=0.1;                   %Discount rate
tax=0.389;               %Tax rate (over profit only)

%---------------------Calculation area and H2O2 income-----------------------

Area=(TPD*1e6*((Er_H2O2*(FE/100))+(Er_O2*(1-
(FE/100)))))/((Eff_H2/100)*Ps*3600*Cf*M_H2);
                         %Calculation of area (m2)
Prod_H2O2=(Area*((Eff_H2/100)/(1+((Er_O2/Er_H2O2)*((1/(FE/100))-
1))))*Ps*3600*Cf*M_H2O2)/(Er_H2O2*1e6);
                         %Calculation of H2O2 production (t d-1)
In_H2O2=(Prod_H2O2*365)*PX_H2O2*1000;
                         %Yearly income of H2O2 ($ a-1)

%-----------------Calculation CAPEX costs and depreciation------------------

Ifin1={'In'};            %Definition whether a photovoltaic module is
                         applied or not. 'In' means that a photovoltaic
                         module is used.
If1=strcmpi(Bias,Ifin1);
if If1==1
    C_Bias=C_In;
else
    C_Bias=C_No;
end

C_Cell=C_Glass+C_Housing+C_Cathode+C_Membrane+C_Assembly+C_Photoanode+C_Bia
s;
%PEC cell module cost (including potential photovoltaic module) ($ m-2)
CAPEX_Cell=C_Cell*Area;
%CAPEX - PEC cell module costs ($)

CAPEX_HardBoS=Sys_H2+Sys_H2O2+Sys_H2O+Sys_Cont+Sys_Sep;
%CAPEX - Hard BoS costs ($)

CAPEX_Cell_Inst=CAPEX_Cell*Inst;
%Installation costs of PEC cell ($)
CAPEX_C_Inst=CAPEX_HardBoS*Inst;
%Installation costs of hard BoS ($)
CAPEX_Cont=(CAPEX_Cell+CAPEX_HardBoS)*Cont;
%Contingency costs of PEC cell and hard BoS ($)
CAPEX_Engi=(CAPEX_Cell+CAPEX_HardBoS)*Engi;
%Engineering & design costs of PEC cell and hard BoS ($)
CAPEX_SoftBoS=CAPEX_Cell_Inst+CAPEX_C_Inst+CAPEX_Cont+CAPEX_Engi;
%CAPEX - Soft BoS costs ($)

CAPEX_TOT=CAPEX_Cell+CAPEX_SoftBoS+CAPEX_HardBoS;
%Total CAPEX costs ($)

DEP_C=(CAPEX_HardBoS+CAPEX_C_Inst+CAPEX_Cont+CAPEX_Engi)/(n);
%Depriciation of the BoS (excluding the PEC cell installation) ($)

%--------------------------Calculation OPEX costs--------------------------
```

```
OPEX_Ins=(CAPEX_Cell+CAPEX_HardBoS)*Ins;
%OPEX - Insurance costs ($)
OPEX_Labor=C_Labor;
%OPEX - Labor costs ($)
OPEX_TOT=OPEX_Ins+OPEX_Labor;
%Total OPEX costs ($)

%-------------------------Calculation of H2 Income-------------------------
In_H2=TPD*365*PX_H2*1000;
%Income of H2 ($ a-1)

%-------------------------Initial matrix creation--------------------------
%A Matrix containing the value of different debits and credits is defined.

M_In_H2=zeros(1,21);          %Definition of income of H2 in year y
M_In_H2O2=zeros(1,21);        %Definition of income of H2O2 in year y
M_OPEX=zeros(1,21);           %OPEX Costs in year y
M_DEP_C=zeros(1,21);          %Depriciation of the BoS in year y
M_DEP_Cell=zeros(1,21);       %Depriciation of the PEC cell in year y
M_CAPEX=zeros(1,21);          %CAPEX Costs in year y
M_Af_TAX=zeros(1,21);         %Additional yearly tax paid in year y
M_DCF=zeros(1,21);            %Discounted cash flow in year y
M_Cum_DCF=zeros(1,21);        %Cumulative discounted cash flow in year y

%----------------------------------Further creation of matrix--------------
--------------------


for y=1:21
    M_In_H2(y)=In_H2;
%Each year, the income of hydrogen is identical
    M_In_H2O2(y)=In_H2O2;
%Each year, the income of hydrogen peroxide is identical
    M_OPEX(y)=OPEX_TOT*(1+Inf)^y;
%Each year, the OPEX costs increase due to inflation with (1+inf)^year
    M_DEP_C(y)=DEP_C;
%Each year, the deprecitation of the BoS (excluding the PEC cell
installation) is identical
end

M_In_H2(1)=0;
%Before operation, there is no H2 income
M_In_H2O2(1)=0;
%Before operation, there is no H2O2 income
M_OPEX(1)=0;
%Before operation, there are no OPEX costs
M_DEP_C(1)=0;
%Before operation, there are no depreciation costs of the system

%In the next session, the total CAPEX costs (in $) over the whole project
%lifetime is calculated when the replacement time is 3, 7 or 12 years.
%First, the total CAPEX costs are defined in year 1. Then, after the cell
%is replaced every n years (with n = 3, 7 or 12), replacement costs for
%both the PEC cell and the installation are charged. The replacement costs
%for n = 3 and n = 12 are estimated on the basis of intra- and
%extrapolation using the replacement costs for n = 7. The depreciation of
%the PEC cell (including the PEC cell installation) is calculated
%afterwards.

if Rep==3
        M_CAPEX(1)=CAPEX_TOT;
```

```
        M_CAPEX(4)=(CAPEX_Cell*(1-(1-Rep_7)*(3/7)))*(1+Inst);
        M_CAPEX(7)=(CAPEX_Cell*(1-(1-Rep_7)*(6/7)))*(1+Inst);
        M_CAPEX(10)=(CAPEX_Cell*(Rep_7-(Rep_7-Rep_14)*(2/7)))*(1+Inst);
        M_CAPEX(13)=(CAPEX_Cell*(Rep_7-(Rep_7-Rep_14)*(5/7)))*(1+Inst);
        M_CAPEX(16)=(CAPEX_Cell*(Rep_7-(Rep_7-Rep_14)*(8/7)))*(1+Inst);
        M_CAPEX(19)=(CAPEX_Cell*(Rep_7-(Rep_7-Rep_14)*(11/7)))*(1+Inst);
    for y=2:4
        M_DEP_Cell(y)=(CAPEX_Cell*(1+Inst))/Rep;
    end
    for y=5:7
        M_DEP_Cell(y)=(M_CAPEX(4))/Rep;
    end
    for y=8:10
        M_DEP_Cell(y)=(M_CAPEX(7))/Rep;
    end
    for y=11:13
        M_DEP_Cell(y)=(M_CAPEX(10))/Rep;
    end
    for y=14:16
        M_DEP_Cell(y)=(M_CAPEX(13))/Rep;
    end
    for y=17:19
        M_DEP_Cell(y)=(M_CAPEX(16))/Rep;
    end
    for y=20:21
        M_DEP_Cell(y)=(M_CAPEX(19))/Rep;
    end
elseif Rep==7
        M_CAPEX(1)=CAPEX_TOT;
        M_CAPEX(8)=(CAPEX_Cell*Rep_7)*(1+Inst);
        M_CAPEX(15)=(CAPEX_Cell*Rep_14)*(1+Inst);
    for y=2:8
        M_DEP_Cell(y)=(CAPEX_Cell*(1+Inst))/Rep;
    end
    for y=9:15
        M_DEP_Cell(y)=(M_CAPEX(8))/Rep;
    end
    for y=16:21
        M_DEP_Cell(y)=(M_CAPEX(15))/Rep;
    end
elseif Rep==12
        M_CAPEX(1)=CAPEX_TOT;
        M_CAPEX(13)=(CAPEX_Cell*(Rep_7-(Rep_7-Rep_14)*(5/7)))*(1+Inst);
    for y=2:13
        M_DEP_Cell(y)=(CAPEX_Cell*(1+Inst))/Rep;
    end
    for y=14:21
        M_DEP_Cell(y)=(M_CAPEX(13))/Rep;
    end

else
    error('Only a replacement years of 3, 7 and 12 accepted')
end

M_DEP=M_DEP_C+M_DEP_Cell;
%Calculation of the total depreciation ($)

M_REV=M_In_H2+M_In_H2O2-M_OPEX-M_CAPEX-M_DEP;
%Calculation of the revenue ($)
```

```
for y=1:21
    if M_REV(y)>0
        M_Af_TAX(y)=M_REV(y)*(1-tax);
%Calculation of the revenue after tax subtraction ($). Tax is only applied
when a profit is made.
    else M_Af_TAX(y)=M_REV(y);
    end
end

M_CF=M_Af_TAX+M_DEP;
%Calculation of the cash flow ($)

for y=1:21
    M_DCF(y)=M_CF(y)/((1+r)^(y-1));
%Calculation of the discounted cash flow in the year y ($)
end

for y=1:21
M_Cum_DCF(y)=sum(M_DCF(1:y));
%Calculation of the cumulative discounted cash flow ($)
end

%-------------------------------------Final matrix creation----------------
--------------------
M_all=[M_In_H2;M_In_H2O2;M_CAPEX;M_OPEX;M_DEP_C;M_DEP_Cell;zeros(1,21);M_RE
V;M_Af_TAX;zeros(1,21);M_CF;M_DCF;M_Cum_DCF]/1000000;

% The matrix consists of (1) Income H2 (2) Income H2O2 (3) CAPEX costs (4)
OPEX costs (5) Depriciation of the BoS (excluding the PEC cell
installation) (6) Cell depriciation (including the PEC cell installation)
(7) Line of zeroes (8) Revenue (9) Revenue after tax subtraction (10) Line
of zeroes (11) Cash flow (12) Discounted cash flow (13) Cumulative
discounted cash flow. All prices are in M$.

NPV=sum(M_DCF)/1000000;             %Calculation of the NPV (M$)

TOTAL_CAPEX=sum(M_CAPEX)/1000000;  %Total CAPEX costs in M$
TOTAL_OPEX=sum(M_OPEX)/1000000;    %Total OPEX costs in M$

TOTAL_CAPEX_PEC_Cell =
(CAPEX_Cell+CAPEX_Cell*Rep_7+CAPEX_Cell*Rep_14)/1000000;
%Total CAPEX cell costs (for replacement every 7 years) (M$)
TOTAL_CAPEX_HardBoS = CAPEX_HardBoS/1000000;
%Total CAPEX Hard BoS costs (for replacement every 7 years) (M$)
TOTAL_CAPEX_SoftBoS =
(CAPEX_SoftBoS+CAPEX_Cell*Rep_7*Inst+CAPEX_Cell*Rep_14*Inst)/1000000;
%Total CAPEX Soft BoS costs (for replacement every 7 years) (M$)

end
```

m-file used for sensitivity analysis

(*Note: functions* `H2_NPV_CAPEX_F` *and* `H2_NPV_OPEX_F` *are not shown here. They are identical to* `H2_NPV`*, with the difference that respectively the CAPEX and OPEX costs can be changed through a multiplication with an input factor. Furthermore, functions* `H2_NPV_`*`X`*, *with* *`X`* *corresponding to an input parameter, are not shown here either. They are identical to* `H2_NPV`*, with the difference that input parameter* *`X`* *can be changed.*)

```
%---Sensitivity analysis for literature-based state-of-the-art scenario----
close all
clear,clc

%----------------------------Input parameters -----------------------------
STH_PV=10.1;            %Solar-to-hydrogen efficiency (%)
FE_H2O2=98;             %Faradaic efficiency towards H2O2 production (%)
C_Photoanode=50;        %Costs of photoanode ($ m-2)
PX_H2O2=0.85;           %Basecase H2O2 price ($ kg-1)
C_PV=70;                %Costs of photovoltaic module ($ m-2)
Replacement=7;          %Replacement time (in years)
Bias_In='In';           %Additional PV bias is allowed
Ps=6.19;                 %Solar energy input (KWh m-2 d-1)
tax=0.389;               %Tax rate (over profit only)
Inf=0.019;               %Inflation rate
C_Labor=4.5*1000000;     %Labor costs ($ a-1)

%-----------------------Initial LCH calculation----------------------------
funct=@(PX_H2)
H2_NPV(STH_PV,FE_H2O2,PX_H2O2,PX_H2,Bias_In,C_Photoanode,C_PV,Replacement);
%Calculation of the H2 price at the basecase H2O2 price
[PX_H2_In]=fsolve(funct,3)

[NPV,TOTAL_CAPEX,TOTAL_OPEX,TOTAL_CAPEX_PEC_Cell,TOTAL_CAPEX_HardBoS,TOTAL_
CAPEX_SoftBoS]=H2_NPV(STH_PV,FE_H2O2,PX_H2O2,PX_H2_In,Bias_In,C_Photoanode,
C_PV,Replacement);

%----------------Sensitivity analysis total CAPEX costs--------------------
CAPEXF_L=0.5;
%Reduction factor for the total CAPEX costs in a positive scenario
CAPEXF_H=2;
%Increase factor for the total CAPEX costs in a negative scenario

f=@(PX_H2)
H2_NPV_CAPEX_F(STH_PV,FE_H2O2,PX_H2O2,PX_H2,Bias_In,C_Photoanode,C_PV,Repla
cement,CAPEXF_L);
[PX_H2_CAPEX_L]=fsolve(f,3);

f=@(PX_H2)
H2_NPV_CAPEX_F(STH_PV,FE_H2O2,PX_H2O2,PX_H2,Bias_In,C_Photoanode,C_PV,Repla
cement,CAPEXF_H);
[PX_H2_CAPEX_H]=fsolve(f,3);

PX_H2_CAPEXF=[PX_H2_CAPEX_L PX_H2_CAPEX_H];
%Hydrogen price using the positive and the negative scenario for the CAPEX
costs

%-----------------Sensitivity analysis total OPEX costs--------------------
OPEXF_L=0.5;
%Reduction factor for the total OPEX costs in a positive scenario
OPEXF_H=2;
%Increase factor for the total OPEX costs in a negative scenario
```

```
f=@(PX_H2)
H2_NPV_OPEX_F(STH_PV,FE_H2O2,PX_H2O2,PX_H2,Bias_In,C_Photoanode,C_PV,Replac
ement,OPEXF_L);
[PX_H2_OPEX_L]=fsolve(f,3);

f=@(PX_H2)
H2_NPV_OPEX_F(STH_PV,FE_H2O2,PX_H2O2,PX_H2,Bias_In,C_Photoanode,C_PV,Replac
ement,OPEXF_H);
[PX_H2_OPEX_H]=fsolve(f,3);

PX_H2_OPEXF=[PX_H2_OPEX_L PX_H2_OPEX_H];
%Hydrogen price using the positive and the negative scenario for the OPEX
costs

%--------------Sensitivity analysis photovoltaic module--------------------
C_PV_L=0.5*C_PV;        %Photovoltaic module costs in a positive scenario
C_PV_H=2*C_PV;          %Photovoltaic module costs in a negative scenario

f=@(PX_H2)
H2_NPV(STH_PV,FE_H2O2,PX_H2O2,PX_H2,Bias_In,C_Photoanode,C_PV_L,Replacement
);
[PX_H2_C_PV_L]=fsolve(f,3);

f=@(PX_H2)
H2_NPV(STH_PV,FE_H2O2,PX_H2O2,PX_H2,Bias_In,C_Photoanode,C_PV_H,Replacement
);
[PX_H2_C_PV_H]=fsolve(f,3);

PX_H2_C_PV=[PX_H2_C_PV_L PX_H2_C_PV_H];
%Hydrogen price using the positive and the negative scenario for the
photovoltaic module costs

%------------------Sensitivity analysis photoanode-------------------------
C_Photoanode_L=C_Photoanode*0.5;
%Photoanode costs in a positive scenario
C_Photoanode_H=C_Photoanode*2;
%Photoanode costs in a negative scenario

f=@(PX_H2)
H2_NPV(STH_PV,FE_H2O2,PX_H2O2,PX_H2,Bias_In,C_Photoanode_L,C_PV,Replacement
);
[PX_H2_C_Photoanode_L]=fsolve(f,3);

f=@(PX_H2)
H2_NPV(STH_PV,FE_H2O2,PX_H2O2,PX_H2,Bias_In,C_Photoanode_H,C_PV,Replacement
);
[PX_H2_C_Photoanode_H]=fsolve(f,3);

PX_H2_C_Photoanode=[PX_H2_C_Photoanode_L PX_H2_C_Photoanode_H];
%Hydrogen price using the positive and the negative scenario for the
photoanode costs

%---------------Sensitivity analysis replacement time----------------------
Rep_L=12;
%Replacement time of the PEC cell module in years in a positive scenario
(in years)
Rep_H=3;
```

```
%Replacement time of the PEC cell module in years in a negative scenario
(in years)

f=@(PX_H2)
H2_NPV(STH_PV,FE_H2O2,PX_H2O2,PX_H2,Bias_In,C_Photoanode,C_PV,Rep_L);
[PX_H2_Rep_L]=fsolve(f,3);

f=@(PX_H2)
H2_NPV(STH_PV,FE_H2O2,PX_H2O2,PX_H2,Bias_In,C_Photoanode,C_PV,Rep_H);
[PX_H2_Rep_H]=fsolve(f,3);

PX_H2_Rep=[PX_H2_Rep_L PX_H2_Rep_H
%Hydrogen price using the positive and the negative scenario for the
replacement time of the PEC cell module

%-----Sensitivity analysis Faradaic efficiency towards H2O2 production-----
FE_H2O2_L=100;
%Faradaic efficiency towards H2O2 production in a positive scenario (%)
FE_H2O2_H=50;
%Faradaic efficiency towards H2O2 production in a negative scenario (%)

f=@(PX_H2)
H2_NPV(STH_PV,FE_H2O2_L,PX_H2O2,PX_H2,Bias_In,C_Photoanode,C_PV,Replacement
);
[PX_H2_FE_H2O2_L]=fsolve(f,3);

f=@(PX_H2)
H2_NPV(STH_PV,FE_H2O2_H,PX_H2O2,PX_H2,Bias_In,C_Photoanode,C_PV,Replacement
);
[PX_H2_FE_H2O2_H]=fsolve(f,3);

PX_H2_FE_H2O2=[PX_H2_FE_H2O2_L PX_H2_FE_H2O2_H];
%Hydrogen price using the positive and the negative scenario for the
Faradaic efficiency towards H2O2 production

%---------Sensitivity analysis solar-to-hydrogen efficiency----------------
STH_PV_L=12.5;
%Solar-to-hydrogen efficiency in a positive scenario (%)
STH_PV_H=7.5;
%Solar-to-hydrogen efficiency in a negative scenario (%)

f=@(PX_H2)
H2_NPV(STH_PV_L,FE_H2O2,PX_H2O2,PX_H2,Bias_In,C_Photoanode,C_PV,Replacement
);
[PX_H2_STH_PV_L]=fsolve(f,3);

f=@(PX_H2)
H2_NPV(STH_PV_H,FE_H2O2,PX_H2O2,PX_H2,Bias_In,C_Photoanode,C_PV,Replacement
);
[PX_H2_STH_PV_H]=fsolve(f,3);

PX_H2_STH_PV=[PX_H2_STH_PV_L PX_H2_STH_PV_H];
%Hydrogen price using the positive and the negative scenario for the solar-
to-hydrogen efficiency

%------------------Sensitivity analysis solar energy input-----------------
Ps_L=8.0;
%Solar energy input in a positive scenario (KWh m-2 d-1)
Ps_H=3.3;
```

```
%Solar energy input in a negative scenario (KWh m-2 d-1)

f=@(PX_H2)
H2_NPV_Ps(STH_PV,FE_H2O2,PX_H2O2,PX_H2,Bias_In,C_Photoanode,C_PV,Replacemen
t,Ps_L);
[PX_H2_Ps_L]=fsolve(f,3);

f=@(PX_H2)
H2_NPV_Ps(STH_PV,FE_H2O2,PX_H2O2,PX_H2,Bias_In,C_Photoanode,C_PV,Replacemen
t,Ps_H);
[PX_H2_Ps_H]=fsolve(f,3);

PX_H2_Ps=[PX_H2_Ps_L PX_H2_Ps_H];
%Hydrogen price using the positive and the negative scenario for the solar
energy input

%------------------------Sensitivity analysis tax rate-----------------------
tax_L=0.10;
%Tax rate in a positive scenario
tax_H=0.55;
%Tax rate in a negative scenario

f=@(PX_H2)
H2_NPV_tax(STH_PV,FE_H2O2,PX_H2O2,PX_H2,Bias_In,C_Photoanode,C_PV,Replaceme
nt,tax_L);
[PX_H2_tax_L]=fsolve(f,3);

f=@(PX_H2)
H2_NPV_tax(STH_PV,FE_H2O2,PX_H2O2,PX_H2,Bias_In,C_Photoanode,C_PV,Replaceme
nt,tax_H);
[PX_H2_tax_H]=fsolve(f,3);

PX_H2_tax=[PX_H2_tax_L PX_H2_tax_H];
%Hydrogen price using the positive and the negative scenario for the tax
rate

%---------------------Sensitivity analysis inflation rate--------------------
Inf_L=0;
%Inflation rate in a positive scenario
Inf_H=0.10;
%Inflation rate in a negative scenario

f=@(PX_H2)
H2_NPV_Inf(STH_PV,FE_H2O2,PX_H2O2,PX_H2,Bias_In,C_Photoanode,C_PV,Replaceme
nt,Inf_L);
[PX_H2_Inf_L]=fsolve(f,3);

f=@(PX_H2)
H2_NPV_Inf(STH_PV,FE_H2O2,PX_H2O2,PX_H2,Bias_In,C_Photoanode,C_PV,Replaceme
nt,Inf_H);
[PX_H2_Inf_H]=fsolve(f,3);

PX_H2_Inf=[PX_H2_Inf_L PX_H2_Inf_H];
%Hydrogen price using the positive and the negative scenario for the
inflation rate

%----------------------Sensitivity analysis labor costs----------------------
C_Labor_L=0.091*1000000;
%Labor costs in a positive scenario ($ a-1)
```

```
C_Labor_H=9.1*1000000;
%Labor costs in a negative scenario ($ a-1)

f=@(PX_H2)
H2_NPV_Labor(STH_PV,FE_H2O2,PX_H2O2,PX_H2,Bias_In,C_Photoanode,C_PV,Replace
ment,C_Labor_L);
[PX_H2_C_Labor_L]=fsolve(f,3);

f=@(PX_H2)
H2_NPV_Labor(STH_PV,FE_H2O2,PX_H2O2,PX_H2,Bias_In,C_Photoanode,C_PV,Replace
ment,C_Labor_H);
[PX_H2_C_Labor_H]=fsolve(f,3);

PX_H2_C_Labor=[PX_H2_C_Labor_L PX_H2_C_Labor_H];
%Hydrogen price using the positive and the negative scenario for labor
costs

%-----------------------------Output of values----------------------------
%All the relevant parameters are returned in the Matlab Command Window and
%exported for further data processing.

PX_H2_In
PX_H2_CAPEXF
PX_H2_OPEXF
PX_H2_C_PV
PX_H2_C_Photoanode
PX_H2_Rep
PX_H2_FE_H2O2
PX_H2_STH_PV
PX_H2_Ps
PX_H2_tax
PX_H2_Inf
PX_H2_C_Labor
```

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