ELECTROLYSIS SYSTEM AND HYDROGEN PROCESSING

STUDENT MANUAL

FINAL DEGREE PROJECT INDUSTRIAL ENGINEERING
STUDENT: JUAN BORRERO MENDOZA
DIRECTOR: FRANCISCA SEGURA MANZANO
ETSI LA RÁBIDA
# CONTENTS

**ABSTRACT** ................................................................................................................................. 3

Main windows.................................................................................................................................. 3

**INSTALLATION AND REQUIREMENTS** ...................................................................................... 5

Installing ......................................................................................................................................... 5

Basic requirement.......................................................................................................................... 5

**THEORETICAL EQUATIONS** ....................................................................................................... 6

Starting conditions: cells installed, production e intensity .......................................................... 6

Heating transmission....................................................................................................................... 6

Water consumption ........................................................................................................................ 8

Hydrogen quantity .......................................................................................................................... 9

Oxygen quantity .............................................................................................................................. 10

PSA: .............................................................................................................................................. 10

**SOFTWARE OPERATION** ........................................................................................................... 12

Settings........................................................................................................................................... 12

**SIMULATION EVENTS** .................................................................................................................. 13

Temperature and tank water level ................................................................................................. 13

Service settings control .................................................................................................................. 14

Purifying process PSA ..................................................................................................................... 16

Pressure control (150%). .................................................................................................................. 17

Over pressure control (175%). ......................................................................................................... 18

**AUTOR RECOMMENDATIONS** ..................................................................................................... 19
ABSTRACT
The aim of this virtual laboratory is to simulate an hydrogen electrolysis system and post-processing cycle in order to ensure its pureness. The tool is split in four main windows, where all the details attached to the simulation are screened and the user can easily control them in order to change the behavior of this chemical process.

Main windows
First of all, we have a short description of the tool.

![Fig 1. Description window](image)

We also have three windows left, where the electrolysis cycle is developed. There is a big one on the right of the screen, which contains elements drawing and control bars. On the left side we have four plot graphics, where the main parameters are shown in their time evolution: produced hydrogen quantity, production rate, temperature of service, tank water level.

We present this guide to expose a further description of the tool and full-explained instructions of how to use the software for a simulation sample.
Fig 2. Main window

Fig 3. Graphics and functions window
INSTALATION AND REQUIREMENTS

Installing
The only requirement to start up the program is double-clicking on .jar file and all the windows will be opened immediately. It is portable and there is no need to install anything, since technical features are quite simple.

Basic requirement
Plug-in Java version 1.5

Windows XP
THEORETICAL EQUATIONS

Math expressions used to approach the electrolysis behavior are explained in this section.

Starting conditions: cells installed, production e intensity

To solve installed cell number, we make equal demanded production with hydrogen produced, so with atomic weight, electron numbers and Faraday theorem, we obtain the result.

\[
\text{Demanded production} \quad \leftrightarrow \quad \text{Hydrogen produced}
\]

\[ P \cdot v_{H_2} = n_{H_2} \cdot R \cdot T \quad (a) \]

\[ V_{H_2} = v_{H_2} \cdot N_{\text{celda}} \quad (b) \]

\[ n_{H_2} = \frac{n_{\text{eq}}}{2} = \frac{I \cdot t}{2N_{\text{Fa}}} \quad (c) \]

\[ N^{\circ} \text{ celdas} = \frac{\text{Prod} \cdot P_{\text{atm}} \cdot 10^3}{I \cdot R \cdot T_{\text{serv}}} \quad (1) \]

Ec. 1 Installed cell number

Prod: Hydrogen produced (Nm³)

P_{atm} : Pressure (aprox 10 kPa)

I: Current supplied to stack (A)

T_{serv} : Stack service temperature (aprox 353 K)

R: Ideal Gas Constant (0.082 l/mol·K)

N_{Fa}: Faraday constant (26.81 Ah/eq)

Intensity, production and cells installed are mathematically related to themselves. Any variation in one of them provokes variation on the other two.

User is able to change production rate and intensity, through slide control at the top of the main window. Therefore, number of cells installed isn’t controlled by the user, so changes in intensity and/or production rate will only change number of cells, keeping the other two according to the user setting. We can take this setting whenever we want before or during the simulation. However, since we cannot modify a real electrolysis stack when is on, we highly recommend setting the values before playing the electrolysis.

Further information about parameters settings will be provided in following sections.

Heating transmission

One important aspect about heating transmission we should consider is that it isn’t constant. The stack is filled with water, which contains an electrolyte in order to power up its electrical conductivity. The influence of this substance on the temperature and conductivity is shown on this graphic, obtained from a commercial electrolyser.
Fig 4. Electric transference-temperature

Red line remarks our working range on the plot (KOH (30%)). Obtaining the math expression is trivial using a linear regression. Finding out conductivity and, as we know the length of the stack, the impedance is easy to figure out using this expression.

\[ R = \frac{1}{C \cdot L} \quad (2) \]

Ec. 2 Resistance calcule

\[ R: \text{Resistance (Ω)} \quad C: \text{Electrical conductivity (siemens)} \quad L: \text{Length (m)} \]

Going back to the linear expression in the plot, we put impedance instead of conductivity and we get the relation between resistance and temperature

\[ R(Ω) = 8 \cdot 10^9 \cdot T^2 - 1,3 \cdot 10^{-4} \cdot T + 0,055 \quad (3) \]

Ec 3: Resistance/temperature relation

Using the formula which explains Joules effect, we can solve the relation between resistance and heat transference.

\[ E(kW) = \frac{I^2 \cdot R}{1000} \rightarrow \text{Effeto Joule} \left( E = \dot{Q} \right) \rightarrow Q = \Delta T \cdot c_p \cdot m \rightarrow \frac{\partial T}{\partial t} = \frac{E}{c_p \cdot m} \]

\[ \frac{\partial T}{\partial t} = \frac{I^2 \cdot (8 \cdot 10^9 \cdot T^2 - 1,3 \cdot 10^{-4} \cdot T + 0,055)}{1000 \cdot c_p \cdot m} \quad (4) \]

Ec 4: Temperature and energy balance

\[ I: \text{Supied current (A)} \quad Q: \text{Produced heat} \]

\[ c_p: \text{Heat constant (kJ/kg·K)} \quad R: \text{Resistance (Ω)} \]

\[ E: \text{Energy (W)} \quad m: \text{Stack mass (kg)} \]

\[ \frac{\partial T}{\partial t}: \text{Temperature diferencial.} \]
Expression (4) will be used in the early beginning of the simulation. If the stack temperature reaches service value, settled in 80ºC by the commercial provider, the expression turns in a constant equation, perturbed by a sinoidal noise.

\[ T_{serv} = 353 + \sin(t) \] (5)

**Ec 5. Sinoidal temperatura noise**

**Water consumption**

Assuming an initial production rate, we develop the resolution using density and atomic weight properties to solve how many grams of water we need to satisfy this demanded rate.

\[
\frac{\text{Prod}}{\text{h}} \left( \frac{\text{Nm}^3}{\text{h}} \right) \cdot \frac{\rho_{H_2}}{\text{kg/m}^3} = \frac{m_{H_2}}{\text{kg/h}} \rightarrow \frac{m_{H_2}}{\text{kg/h}} = \frac{\rho_{H_2}}{2 \cdot 10^{-3} \text{kg/mol}} = \frac{\text{moles}}{\text{h}}
\]

\[
m_{H_2O}(\text{moles/h}) \cdot \frac{18g}{\text{mol}} = \text{Cons}_{H_2O}(\frac{g}{\text{h}}) \cdot \frac{1}{\rho_{H_2O}(\frac{\text{kg}}{\text{m}^3})} \rightarrow \text{Cons}_{H_2O} (\text{l/h})
\]

\[
\frac{\partial V_{H_2O}}{\text{dt}} = \text{Cons}_{H_2O} \left( \frac{\text{h}}{\text{h}} \right) \cdot \frac{1 \text{m}^3}{1000 \text{l}} \cdot \frac{1 \text{ h}}{3600 \text{ s}} \cdot \frac{\text{m}^3}{\text{s}}
\]

\[
\text{Cons}_{H_2O} = \frac{\text{Prod} \cdot \rho_{H_2} \cdot 0,5 \cdot p_{atH_2O}}{10^6}
\]

\[
\frac{\partial V_{H_2O}}{\text{dt}} = \frac{\text{Prod} \cdot \rho_{H_2} \cdot p_{atH_2O}}{7,2 \cdot 10^6} \text{ m} \] (6)

**Ec 6. Water consumption**

- Cons\(_{H_2O} \): Pumped water (l/h)
- Prod: Production rate (Nm\(^3\)/h)
- p\(_{atH_2O} \): Water molar weight (g/mol)
- \( \rho_{H_2} \): Hydrogen density kg/Nm\(^3\)
- \( \partial V_{H_2O}/\text{dt} \): Water consumption (m\(^3\)/s)

The plot shown by the software means how fast water tank is emptying from an initial level of 20 liters. When a security low level is reached, user is asked to refill the tank or end up the simulation.
Hydrogen quantity

According to production rate required, we have to consider tank measurement (50 l) and pressure factor (Z~1). Pressure will rise to a required value in order to put the hydrogen available to emission.

\[
V_{H2} = \frac{N^0 \text{celdas} \cdot I \cdot t \cdot R \cdot T_{serv}}{P_{atm} \cdot 10^3} \quad (Ec 1)
\]

Demanded production \(\leftarrow\rightarrow\) Produced hydrogen

\[
\frac{\partial C_a}{\partial t} = V_{H2} \left(\frac{Nm^3}{K}\right) = \frac{N^0 \text{celdas} \cdot I \cdot t \cdot R \cdot T_{serv}}{3,6 \cdot 10^3} \quad (7)
\]

\[
\frac{\partial C_a}{\partial t} = \frac{N^0 \text{celdas} \cdot I}{2N_{Fa}} \cdot R \cdot T_{serv} \quad (8)
\]

\[
C_a = \frac{V_{tanque} \cdot P}{Z} \rightarrow P = \frac{C_a}{V_{tanque}} \quad (Ec 7. Hydrogen produced volume)
\]

\[
Ec 8. Pressure level on hydrogen vessel
\]

\[
C_a: \text{Hydrogen produced (Nm}^3/\text{s})
\]
\[
N^0 \text{celdas: Installed cells}
\]
\[
I: \text{Supplied intensity (A)}
\]
\[
T_{serv}: \text{Service temperature (aprox 353 K)}
\]
\[
R: \text{Ideal gas constant (0.082 l/mol·K)}
\]

\[
N_{Fa}: \text{Faraday number (26.81 A·h/eq)}
\]
\[
V_{tanque}: \text{Hydrogen vessel capacity}
\]
\[
Z: \text{Pressure factor}
\]
\[
P: \text{Pressure (bares)}
\]

As far as pressure is getting higher on the tank, there is programmed some warning measurements to avoid failures and explosions in the system. These steps are following explained.
Oxygen quantity
Oxygen production is developed at the same rhythm as hydrogen does, but with a half of its quantity. It is saved in a single tank, so when the top level is reached, the content is fully exhausted to the atmosphere. There is no pressure control over this product, as the empty procedure is always the same.

PSA:
Purifying process PSA is started when the hydrogen comes out from the stack, partly cleaned from humidity. System is compound by two tanks filled with porous elements made from alumina, called drying vessel. The adsorption capacity of the alumina is about 0.8 vol% (molar) of water into hydrogen. Alumina adsorption needs cleaning phases in regular basis, using hydrogen which is refilled back in to the tank. All in all, we have two tanks doing the cleaning in alternative working in order to have a regular purification.

This process is working if the system is turn on and production valve is opened. We can easily check the status looking at the LED panel in the main window.

**Fig 7. PSA timeline and values.**

<table>
<thead>
<tr>
<th>Purifying process PSA</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>T0</strong></td>
<td>1200 s</td>
</tr>
<tr>
<td><strong>T1</strong></td>
<td>600 s</td>
</tr>
<tr>
<td><strong>T2</strong></td>
<td>120 s</td>
</tr>
<tr>
<td><strong>T4</strong></td>
<td>4,8 s</td>
</tr>
<tr>
<td><strong>T5</strong></td>
<td>475,2 s</td>
</tr>
</tbody>
</table>
SOFTWARE OPERATION
To begin with the simulation, we have to double-click on the java file and immediately all the windows will be displayed on the screen. Abstract window is shown backwards, so we can look up information there without interrupting.

Settings
Main window contains all the control system to apply any change over the start conditions. At the bottom, we have time buttons related to the simulation evolution.

![Fig 8. Button panel](image)

At the top we can see to slides to set up parameters (production and intensity) and a scope to see the measurement of cell numbers installed.

![Fig 9. Slide bar panel](image)

As we have seen in the previous section, these three values are related to each other, Intensity and production are input data, so we keep the value set up by the user and cell number installed is fluctuating depending on the setting. The best choice is to set our simulation condition at the beginning and keep it stable during the whole time. If we have to make some changes, you’d better reset the tool and make another simulation. Furthermore, it is the real procedure to develop, because it’s hard and dangerous to make electrical variations and impossible to plug/unplug cells during the operation.

If we make changes during the operation, we must consider that Electric power value shown below stack drawing is related to the relation explained before. Changes in intensity mean change in cell number, so electric power keep constant if we want to keep the same value of cell number; we have to set it manually through modifying production rate. Therefore, production rate variation means changes in electric power. Due to the complex relation among these factors, we should make the settings while the operation is paused.
SIMULATION EVENTS

Temperature and tank water level
The first message to appear on the screen will happen when the stack reaches its service temperature. It depends on the intensity applied, but heating period lasts a few seconds. This is the window we will see.

![Service temperature graph](image1)

**Fig 10. Service temperature window and its graphic.**

Water level is also a value which can control in different ways, tank drawing, display below this picture or graphic plot. Empty rate is simulated by equation (6), but disconnection during pressure warning. The minimum level is 1 liter, and in this point user will be asked for a decision:

![Water tank diagram](image2)
If we click on YES button, the tank will be refilled to his initial level (20 l). Otherwise, NO button will stop the operation and system goes back to his reset status, holding on for a new simulation.

**Service settings control.**
Pressure measures starts when tank hydrogen level reaches 100% of its capacity, that is to say, 20 bar.

So, we will be noticed of production conditions are available and will be able to decide the next step:
If we choose Open Valve, tank level will stand in a value of 105% (21 bares). This is over dimensioned to compensate losses in piping.

If we take the other choice, hydrogen will keep filling the tank until we reach the next pressure check point.

Cancel button doesn’t stand for nothing; we have to take one of the previous choices.

After this checkpoint, a new option will appear on button panel, controlling valve operation.

This button allows us to open the valve to interrupt filling operation. From this moment, hydrogen input and output are equal, so tank level is established in a constant value and PSA stage is getting.

On the other hand, if valve is already opened, we have the choice of closing output and continue filling the tank from the level we had at this moment. Notice that it is necessary to double click the button, because the default option for valve is to open.
We have control over the valve and tank level until it reaches 150%, where it is the next check point.

**Purifying process PSA**
From the moment we decide to open the valve and emitting hydrogen, Pressure Swing Adsorption (PSA) process will be started. The stages which happen during the drying period were explained in previous paragraphs. Here you are a chronogram explanation from the spanish version of the tool.

![Fig 14. PSA chronogram](image-url)
Pressure control (150%).
Whatever had happened before about tank level, if the pressure on it gets a 150% of capacity, an alert window shows up on the screen, asking for a decision:

![Alert Window](image)

Despite being 100% the accurate conditions for hydrogen production, hydrogen tank is capable to support a 30 bar pressure forces. Upper to this value, we are not in a safe environment.

If we open the valve, hydrogen is sent to consumption and PSA starts working. Besides, electric power in the stack is reduced to a 50% in order to decrease over pressure level. So, this problem is getting fixed as well as we save some electric resource (we can see on the scope below the stack how kW number is lower than before. Therefore, this period will last until level becomes a 100% again. If we interrupt this operation closing the valve, the tank will be refilled as it was doing before, as we can see on status diagram. Opening and closing in this moment will make these previous results.

So that, if we avoid this measurement, level keeps going up without any control. If we decide later to open the valve, electric measurements won’t take place, because we avoided them before, so hydrogen tank will keep a constant level without empty.
Over pressure control (175%)

Last check point takes place when level gets to a level of 175%, meaning 35 bar. Graphic correspondence is visible when the drawing is fully colored. Message shown is as it follows.

User is not allowed to make a decision anymore. Therefore, electric source is immediately unplugged and an exhaust valve is opened. So, the system doesn't have any input and two ways of output. This measurement means that we need to reduce hydrogen level as soon as possible, so we have this extra valve, which we can see on this screen capture below:
Now, empty rate is twice of the filling rate. Closing the tank is forbidden in this stage, so if user closes the valve, all hydrogen escapes through exhaust valve, and PSA stop working. No way of refill hydrogen tank. This stage lasts until hydrogen level reaches again a 100%. To sum up, a behavior plot is displayed below in a schematic way:

![Graph](image)

**Fig 18. Tank level evolution**

**AUTOR RECOMMENDATIONS**

- Read carefully section “Software operation/Settings” to have a full knowledge about relation between parameters.
- If we choose OPEN VALVE on the first pressure control and we decide to close again later, we have to click TWICE because default valve option is to open it, which is currently selected. Look for further information in Theoretic Equations section.
- Making single simulations for each condition is highly recommended. It will avoid failures and mistakes about data interpretation and results. If you decide anyway do it in the same session, you should pause the program and take in consideration all the given instructions about parameters.