HOW TO GUIDE

Electrolysis in energyPRO

Preface

energyPRO is a Windows-based modeling software package for combined techno-economic analysis and optimisation of complex energy projects with a combined supply of electricity and thermal energy from multiple different energy producing units.

The unique programming in energyPRO optimises the operations of the plant including energy storage (heat, fuel, cold and electrical storages) against technical and financial parameters to provide a detailed specification for the provision of the defined energy demands, including heating, cooling and electricity use.
energyPRO also provides the user with a detailed financial plan in a standard format accepted by international banks and funding institutions. The software enables the user to calculate and produce a report for the emissions by the proposed project.
energyPRO is very user-friendly and is the most advanced and flexible software package for making a combined technical and economic analysis of multi-dimensional energy projects.
For further information concerning the applications of energyPRO please visit www.emd.dk.

Terms of application

EMD International A/S, May 23

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1. Introduction

The electrolysis unit allows you to model the production of hydrogen through the usage of electricity and water in energyPRO. Besides electricity consumption and hydrogen production you can model the water consumption and oxygen production of two different electrolysis technologies: alkaline electrolysis (AE) and polymer membrane electrolysis (PEM).

This How To Guide contains two main parts:

Section 2 – How to set up the electrolyser module in energyPRO. A step-by-step guide.
Section 3 – Method of the calculations in energyPRO

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2. How to setup the electrolyser in energyPRO

The energyPRO project case called: “Electrolyser with PVs and wind turbines on the day ahead market” can be accessed from the English Project examples in the start window of energyPRO, please see Figure 1. The project is used in this guide to illustrate the electrolyser in energyPRO.

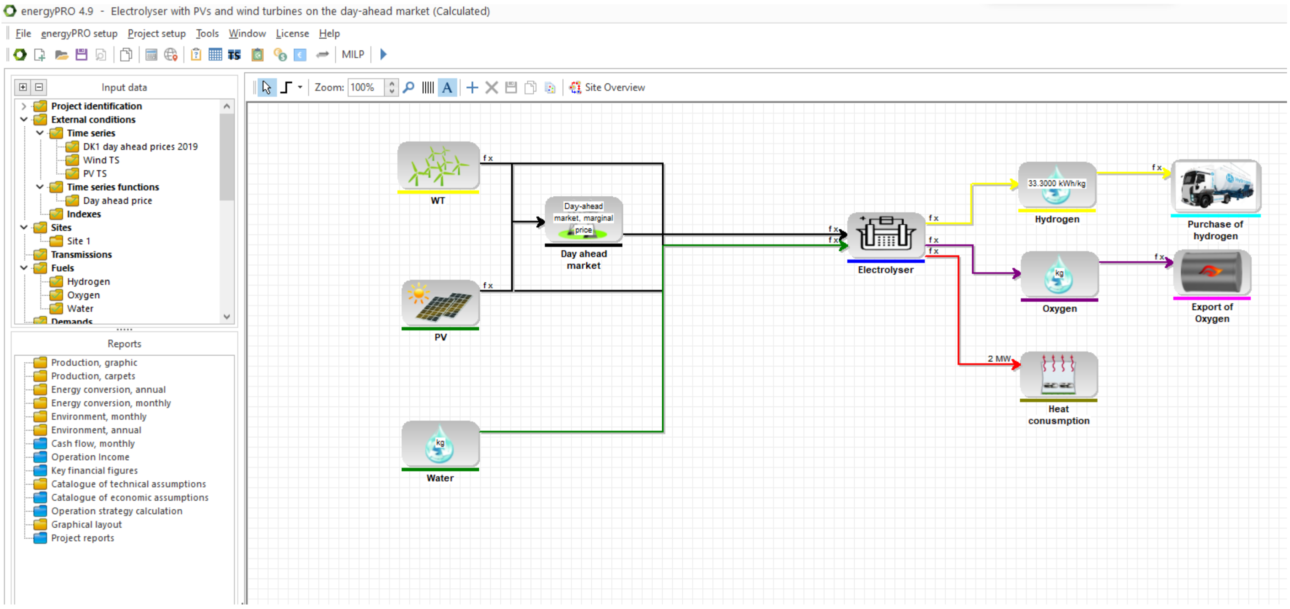

Figure 1. The energyPRO project case, “Electrolyser with PVs and wind turbines on the day-ahead market”, used in this HowToGuide

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2.1 Step 1: Allowing fuel producing units

Go to Project setup and choose Project identification and Advanced settings. Choose "Fuel producing energy units in project". Please see Figure 2.

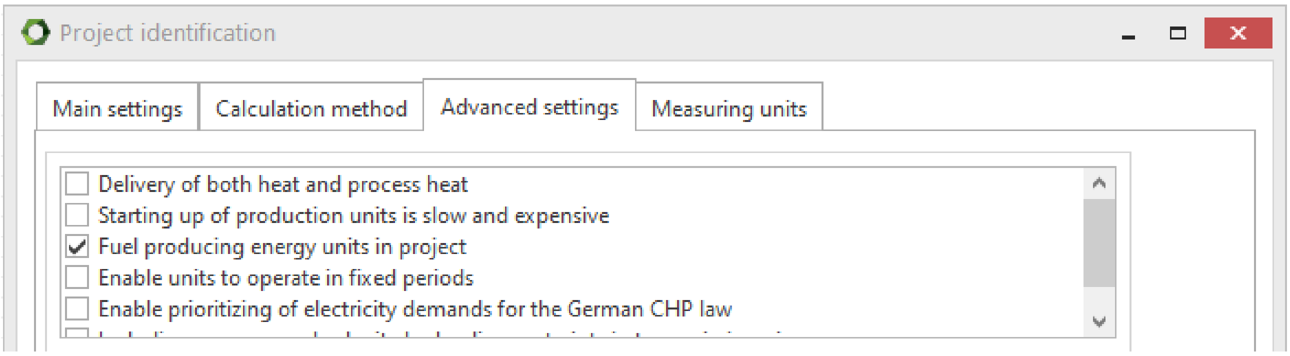

Figure 2. Allow fuel producing units in Project identification and Advanced settings.

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2.2 Step 2: Add an electrolyser unit and fuels to the project

An electrolyser is added just as any other energy conversion unit, as shown in Figure 3.

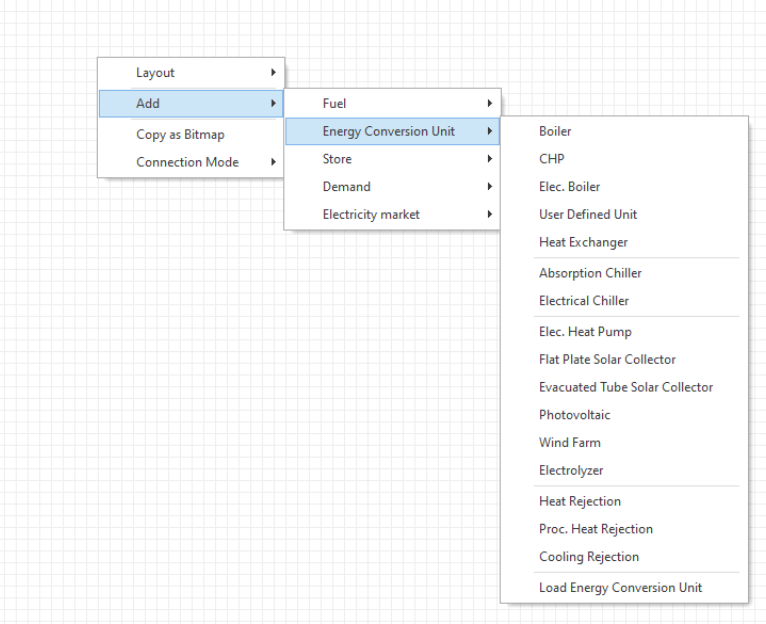

Figure 3. Add a new electrolyser by right click a site and choosing "Add>Energy Conversion Unit>Electrolyser"

Next you need to add all fuels that you want to have modelled in connection to the electrolyser by selecting "Add>Fuel>Load Fuel", as seen in Figure 4.

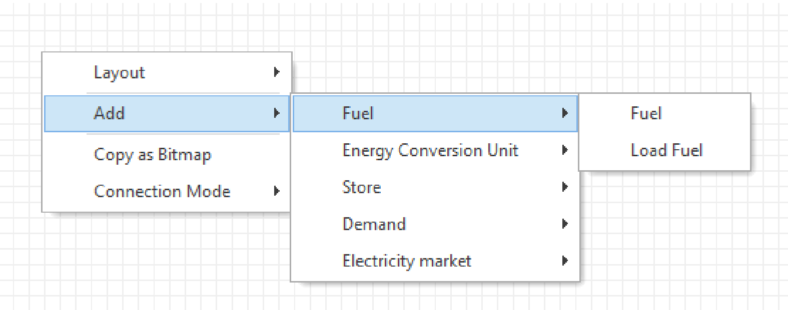

Figure 4. Loading fuels into the project

The fuels Water, Hydrogen and Oxygen can be loaded into the project from your folder energyPRO Data as seen in Figure 5.

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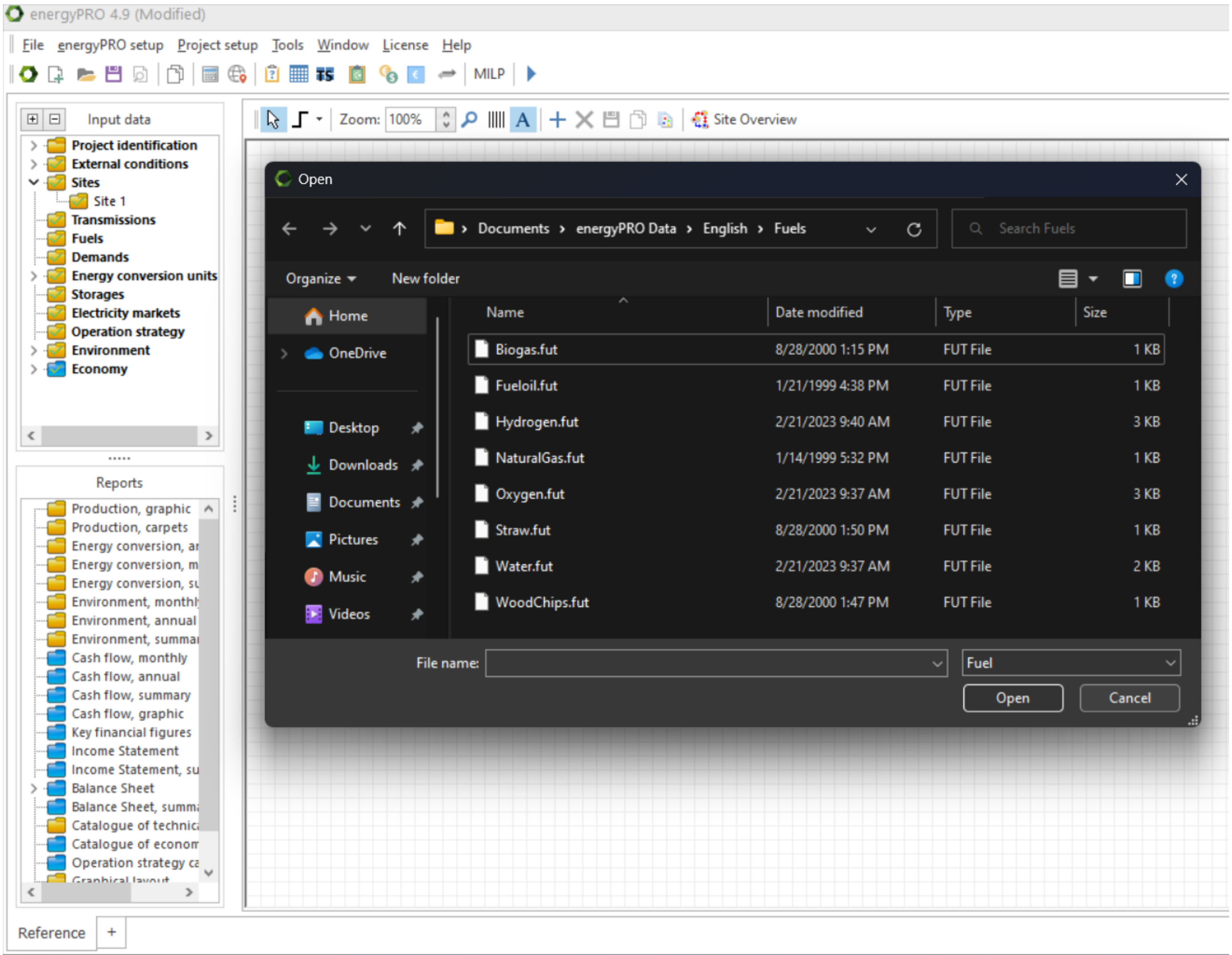

Figure 5. Predefined fuels in energyPRO

Next, you need to assign the fuels to the electrolyser. In the unit, at minimum, a fuel must be assigned to the hydrogen output, while at maximum three fuels can be assigned (hydrogen, oxygen and water). A fuel is assigned to the hydrogen production by selecting it in the drop-down menu right of "Hydrogen output", as seen in Figure 6.

These pre-created fuels are all quantified in the unit [kg]. The unit kg is required for the fuels representing hydrogen, oxygen and water, even if the fuels are created manually. If a different unit is selected, the results obtained from the calculation will not be correct. Furthermore, if for the fuel representing the hydrogen production of the electrolyser, the energy content is specified to be different from 33,3 kWh/kg, the result of water and oxygen consumption and production is incorrect.

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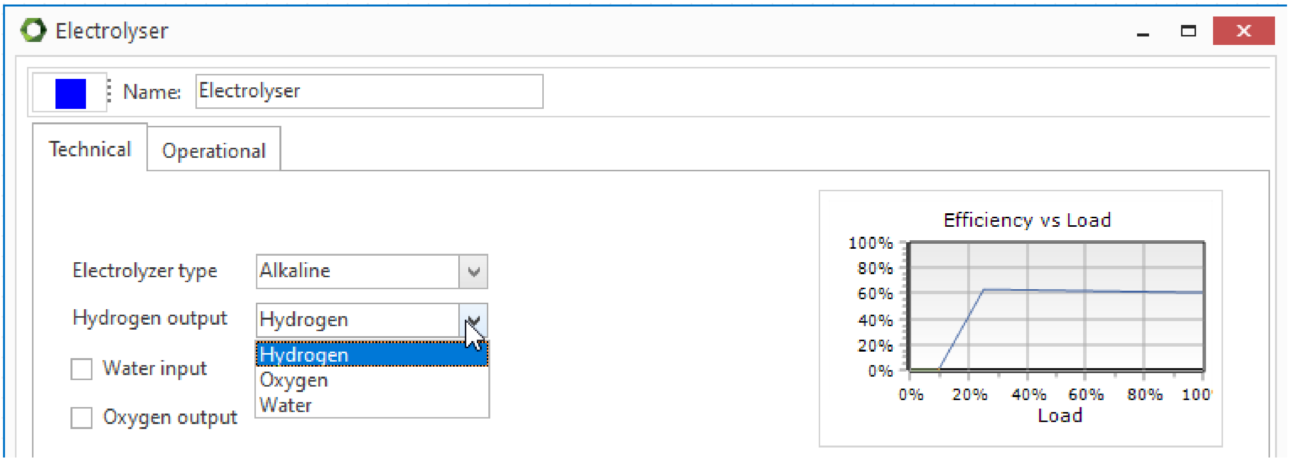

Figure 6. Assigning a fuel to the hydrogen production

The other fuels can be assigned if needed. To assign them, the respective checkbox to the left must be checked. Then the loaded or created fuel can be selected from a drop-down. Figure 7 shows the unit menu if both oxygen and water are activated and the correspondingly named fuels assigned. The fuels can also be named differently than in the example.

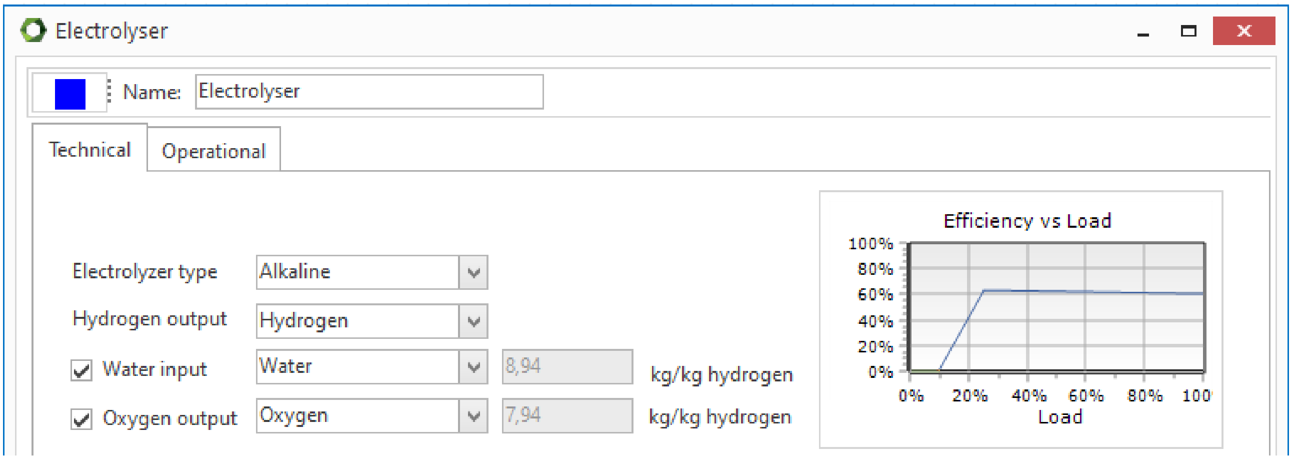

Figure 7. Water and oxygen assigned as fuels

Left of the respective drop-down menu to select the assigned fuel, a value of kg/kg hydrogen shows up. For the water consumption the unit relates to consumed kg of water per produced kg of hydrogen, while for the oxygen production this value expresses the produced kg of oxygen per produced kg of hydrogen.

2.3 Step 3: Entering energy consumption and production

To determine the energetic efficiency and thereby the relation between energy consumption and production, the type of electrolyser is established. In a drop-down menu either “Alkaline” or “Polymer Electrolyte Membrane” can be chosen (see Chapter 3.3 for more details). Furthermore, the electric capacity and the Electricity to Hydrogen

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efficiency need to be entered as seen in Figure 8. As an example, the efficiency is set to 60 % and the electric capacity to 10 MW.

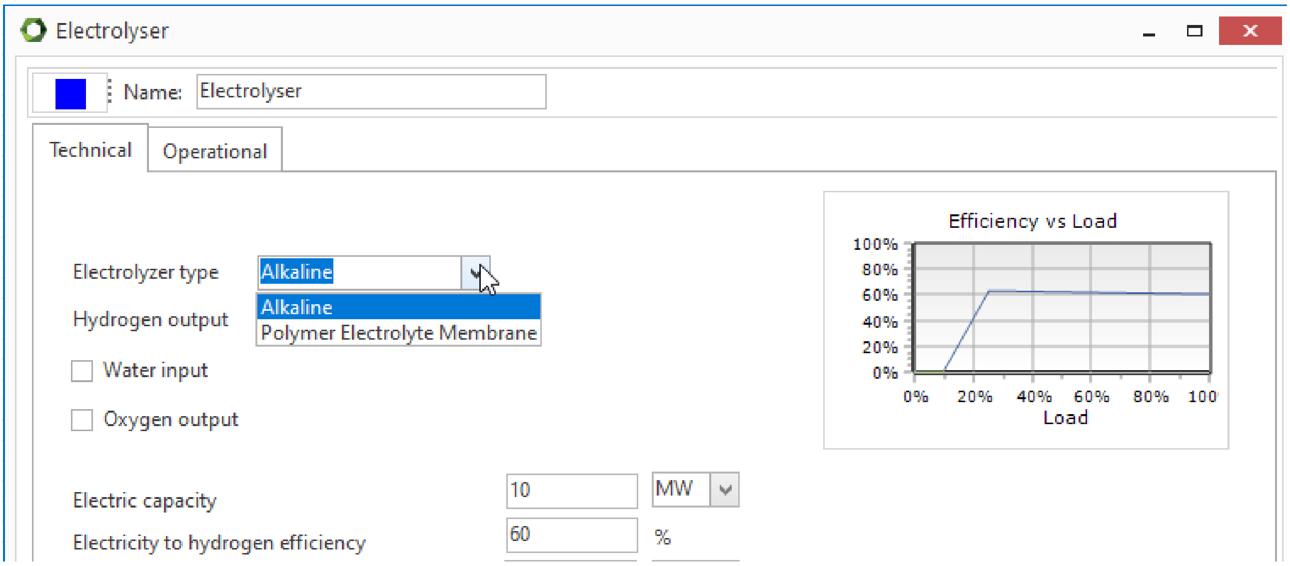

Figure 8. Setting the energetic parameters Capacity, Efficiency and Type of Eletcrolyzer

Additionally, a heat production and a minimal load can be added by checking the respective checkboxes. The heat production is entered as an absolute value, while the minimal load as entered as a percentage of electric capacity, as seen in Figure 9. The minimal load is referring to the lowest part load that the electrolyser can run at.

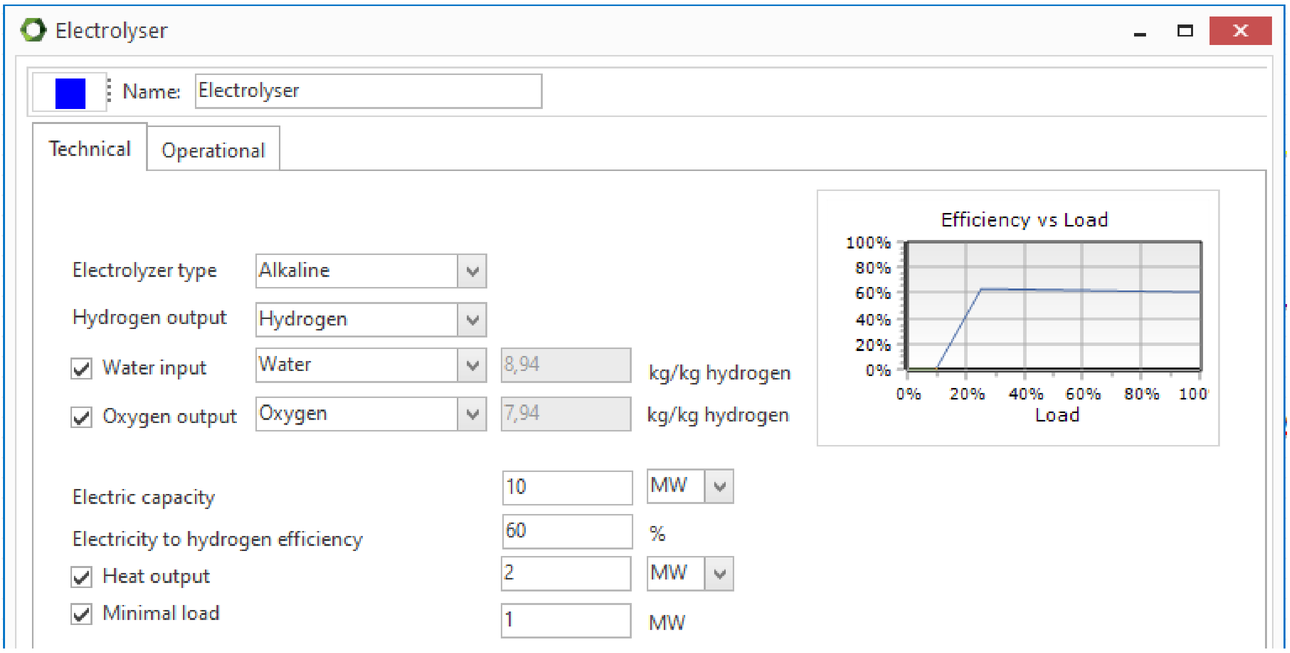

Figure 9. Entering a heat production and a minimal load

The entered minimal load is not allowed to be higher than 25 % for Alkaline and 27 % for Polymer Membrane Electrolysis, to be entered as electric capacity in MW. In this case it is set to 10 MW electric capacity.

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The entered heat output, as heat production capacity during nominal load, should not exceed

$$(1 - \eta_{H2,out,peak}) \cdot E_{cap}$$

Where:

$\eta_{H2,out,peak}$ is the highest possible efficiency of electric input to hydrogen production and not the nominal efficiency entered in Figure 8

E_{cap} is the nominal electric capacity of the electrolyser.

This is due to the way the electrolyser is modelled (see Chapters 3.3 and 3.5).

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3. The electrolyser modelling method used in energyPRO

3.1 Input for the Model

- Nominal efficiency of the Electrolyser [%] (relating hydrogen production to electricity consumption)
- Electric Capacity of the Electrolyser [MW]

Further optional inputs:

- Heat output [MW]
- Minimal load [MW]

3.2 General constants:

- Molar weight of hydrogen: 1,00784 g/mol
- Molar weight of oxygen: 15,999 g/mol
- Lower heating value of hydrogen: 33,3 kWh/kg

3.3 Creating a load curve for an electrolyser

Since an electrolyser is very flexible to change its load, it is important to be able to know how the efficiency varies with the applied load. The efficiency in this document is related to, as suggested by *Buttler et al. (2018)* for energy applications, the lower heat value of hydrogen [1]. The relative change in efficiency is however assumed to be similar. For the two mentioned technologies different load curves are assumed:

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Table 1. Part load behaviour of different electrolyser types

[%] of nominal load	Alkaline Electrolysis (AE) [%] of nominal efficiency	Polymer Electrolyte Membrane Electrolysis (PEM) [%] of nominal efficiency
25 (AE)/ 27 (PEM)	105	115
100	100	100

The data point in the middle refers to the peak efficiency of the electrolyser system, also referred to as $\eta_{H2,out,peak}$. It is seen in Figure 10 as the points where both curves show the highest efficiency, close after 20 % of their nominal load.

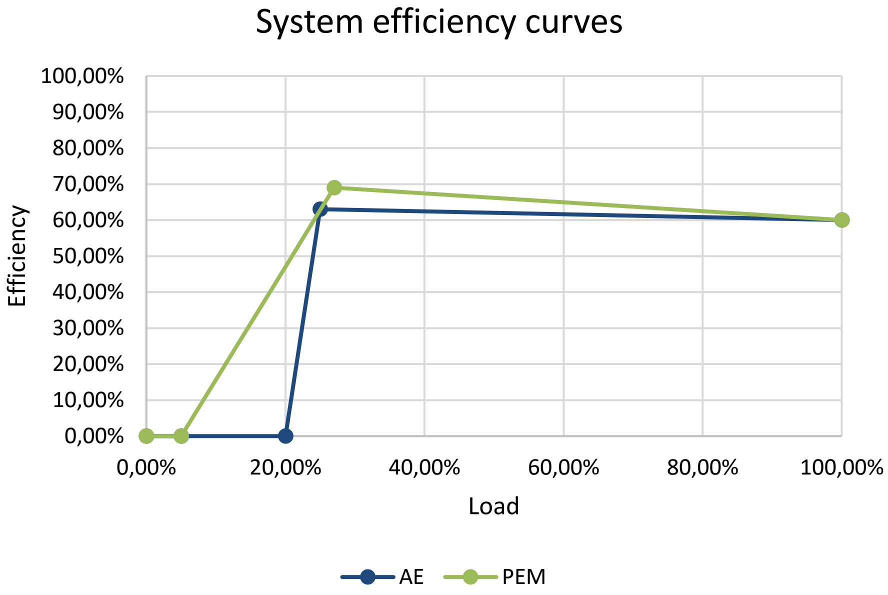

Figure 10: System efficiency of AE and PEM

The shown efficiency curves relate both to AE and PEM with 60 % nominal efficiency, which is entered by the user, as shown in Figure 8. As seen the highest efficiency is reached in part load reaching 63 % and 69 % of efficiency respectively as a result of multiplying the nominal efficiency with the second row of Table 1. This happens because an electrolysers cells are declining in efficiency with higher loads, while an electrolyser's auxiliaries are increasing in efficiency with increasing load [1], [2]. The minimal loads are specified by the user (see Figure 9)to be 5 % of nominal load for the PEM and 20 % for the AE in Figure 10.

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3.4 Hydrogen and Oxygen Production and Water Consumption

The hydrogen production is modelled by multiplying on the electricity consumption with a factor of how much electricity is converted into hydrogen directly. This factor is referred to as efficiency.

The oxygen output is calculated based on the hydrogen output. Therefore, the mass balance to the chemical reaction of splitting water ($2\ H_2O \rightarrow 2\ H_2 + O_2$) is used to calculate the amount of oxygen produced per kg of produced hydrogen. The oxygen output is calculated according to following equation:

Equation 1: Stoichiometry oxygen

$$O_{2,out} = \frac{2 \cdot 15{,}999 \left[\frac{kg}{kmol}\right]}{4 \cdot 1{,}00784 \left[\frac{kg}{kmol}\right]} = 7{,}94\ \frac{kg}{kg\ H_2}$$

The amount of water consumption is also determined based on the hydrogen production, by using the mass balance to the chemical reaction of splitting water.

Equation 2: Stoichiometry water

$$H_2O_{in} = \frac{(2 \cdot 15{,}999 + 4 \cdot 1{,}00784)\left[\frac{kg}{kmol}\right]}{4 \cdot 1{,}00784 \left[\frac{kg}{kmol}\right]} = 8{,}94\ \frac{kg}{kg\ H_2}$$

3.5 Heat output

The heat production is modelled as absolute value. To prevent that the overall system efficiency will increase above 100 %, the heat output at nominal load should not exceed:

$$Maximum\ heat\ output = (1 - \eta_{H2,out,peak}) \cdot E_{cap}$$

Where:

$\eta_{H2,out,peak}$ is the highest possible efficiency of electric input to hydrogen production (LHV) and not the nominal efficiency entered in Figure 8

E_{cap} is the nominal electric capacity of the electrolyser

This is because the model assumes the heat output to be constant from the point of maximum efficiency to nominal efficiency. Thereby, this heat output together with the hydrogen efficiency should not exceed the input of electricity.

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4. Reference list

[1] A. Buttler and H. Spliethoff, “Current status of water electrolysis for energy storage, grid balancing and sector coupling via power-to-gas and power-to-liquids: A review,” *Renewable and Sustainable Energy Reviews*, vol. 82. Elsevier Ltd, pp. 2440–2454, Feb. 01, 2018. doi: 10.1016/j.rser.2017.09.003.

[2] P. Lettenmeier, “Efficiency-Electrolysis White paper,” 2021.

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