Future City Hydrogen: Reality or Utopia?
Michel Tamarzians
A techno-economical feasibility study of an optimal stand-alone Solar-Electrolyzer-Battery-FuelCell system for residential utilization

by

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An electronic version of this thesis is available at http://repository.tudelft.nl/.
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Michel Tamarzians, Delft, May 2019
“The 20th century was the age of the Petroleum Economy while the 21st Century is certainly the age of the Solar-Hydrogen Economy”

-Warren D. Reynolds [1]-
Abstract

The population worldwide is growing rapidly which leads to an increase of the energy demand. Simultaneously, the established energy resources are being depleted and contribute negatively to the climate. The necessity for a sustainable and inexhaustible energy source, to deal with the increasing energy demand in an ecological friendly approach, will play a key role in the 21st century.

One of the most predictable and inexhaustible renewable energy sources is the Sun. Nevertheless, changing weather conditions, like rain and clouds, winter and summer, result in daily and seasonal fluctuations. A reliable stand-alone solar system requires a profound storage method to tackle the daily and seasonal fluctuations that can potentially result in deficit or dumped energy.

Generally, a battery bank is adopted in stand-alone solar systems, but the low energy density makes a battery bank not suitable as a seasonal storage method. A seasonal storage method can be implemented by the production and consumption of the chemical product hydrogen. Hydrogen has a high energy density compared to batteries (142 MJ/kg vs 0.95 MJ/kg [2, 3]), but the low round-trip efficiency prevents implementing hydrogen as a daily storage method. For a highly reliable and optimal sized stand-alone energy system, a combination of both a battery bank and the chemical product hydrogen are used as a profound storage method. The combined storage method can be used in times of excess and deficit energy. This results in a so called stand-alone hybrid PV-Electolyzer-Battery-FC energy system.

In this final thesis project a stand-alone hybrid PV-Electolyzer-Battery-FC energy system is modelled and optimized to determine the current and future feasibility, both technologically and economically, for residential utilization. A simulation model of the hybrid energy system is designed in TRNSYS. The model is optimized by minimizing the loss of load probability (LLP) and levelized cost of energy (LCOE) for the stand-alone hybrid PV-Electolyzer-Battery-FC energy system at residential level in TRNOPT. Several cases are optimized based on the electrical, heat and mobility demand. The used optimization method is a combination of particle swarm optimization (PSO) and Hooke-Jeeves optimization algorithms implemented by GenOpt.

It is established that the proposed stand-alone hybrid PV-Electolyzer-Battery-FC is technically feasible for the fulfillment of the annual electrical demand of a typical Dutch household. The feasible system size consists of 19 PV modules, battery capacity of 25.5 kWh and a tank volume of 1.24 m$^3$ for a LCOE of 1.04 €/kWh. If the future prices of the main components can be reduced to 0.01 €/W for PV, 0.01 €/Wh for battery and 0.01 €/W for electrolyzer and fuel cell the hybrid system can potentially reach a LCOE of 0.28 €/kWh. Reduction of the prices can be realized by large scale production, large scale implementation and technology maturity. In the end, a LCOE of 0.17 €/kWh can be realized by renewable energy systems if these future prices are realized and the following conditions are met: (1) fully covered roof area by PV modules and (1) the production, consumption and storage of hydrogen should be centralized to scatter the infrastructure costs over all the consumers. This can induce a so called hydrogen economy in the future, whereby the hydrogen gas can be the sustainable link between the increasing energy demand and the depleting fossil fuels.
# List of Symbols

**Abbreviations**

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<tr>
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<td>AC</td>
<td>Alternate Current</td>
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<td>AEC</td>
<td>Alkaline Electrolyzer Cell</td>
</tr>
<tr>
<td>AFC</td>
<td>Alkaline Fuel Cell</td>
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<tr>
<td>AGM</td>
<td>Absorbed Glass Mat</td>
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<tr>
<td>AOI</td>
<td>Angle Of Incidence</td>
</tr>
<tr>
<td>BTL</td>
<td>Battery To Load</td>
</tr>
<tr>
<td>CdTe</td>
<td>Cadmium Telluride</td>
</tr>
<tr>
<td>CIGS</td>
<td>Copper Indium Gallium Selenide</td>
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<tr>
<td>DC</td>
<td>Direct Current</td>
</tr>
<tr>
<td>DMFC</td>
<td>Direct Methanol Carbonate Fuel Cell</td>
</tr>
<tr>
<td>DoD</td>
<td>Depth of Discharge</td>
</tr>
<tr>
<td>EC-DMC</td>
<td>Ethylene Carbonate–DiMethyl Carbonate</td>
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<tr>
<td>ETC</td>
<td>Experimental Test Conditions</td>
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<tr>
<td>FCTL</td>
<td>Fuel Cell To Load</td>
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<tr>
<td>FL</td>
<td>Fuzzy Logic</td>
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<tr>
<td>FPSO</td>
<td>Fuzzy Based Particle Swarm Optimization</td>
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<tr>
<td>GenOpt</td>
<td>Generic Optimization Program</td>
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<tr>
<td>HOMER</td>
<td>Hybrid Optimization Model for Electric Renewables</td>
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<tr>
<td>HSS</td>
<td>Hybrid Solar Systems</td>
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<tr>
<td>LCA</td>
<td>Life Cycle Assessment</td>
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<tr>
<td>LCOE</td>
<td>Levelized Cost Of Energy</td>
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<tr>
<td>LLP</td>
<td>Loss of Load Probability</td>
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<tr>
<td>LOE</td>
<td>Loss Of Energy</td>
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<tr>
<td>LSM</td>
<td>Lanthanum Strontium Manganese</td>
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<tr>
<td>MCFC</td>
<td>Molten Carbonate Fuel Cell</td>
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<tr>
<td>MPPT</td>
<td>Maximum Power Point Tracker</td>
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<tr>
<td>Ni-YSZ</td>
<td>Nickle-Yttria-Stabilized Zirconia</td>
</tr>
<tr>
<td>PAFC</td>
<td>Phosphoric Acid Fuel Cell</td>
</tr>
<tr>
<td>PCFC</td>
<td>Protonic Ceramic Fuel Cell</td>
</tr>
</tbody>
</table>
PEBF Photovoltaic-Electrolyzer-Battery-FuelCell
PEMEC Proton Exchange Membrane Electrolyzer Cell
PEMFC Proton Exchange Membrane Fuel Cell
PLR Power to Load Ratio
POA Plane Of Array
PSO Particle Swarm Optimization
PV Photovoltaic
PVMD Photovoltaic Materials and Devices
SDO Simulink Design Optimization
SEI Solid Electrolyte Interface
SoC State of Charge
SOEC Solid Oxide Electrolyzer Cell
SOFC Solid Oxide Fuel Cell
SORFC Solid Oxide Regenerative Fuel Cell
STC Standard Test Conditions
STL Solar To Load
TRNOPT Transient System Simulation Tool Optimization
TRNSYS Transient System Simulation Tool
UV Ultraviolet

**Pressure [Pa]**

\[ p_{\text{amb}} \] Ambient pressure
\[ p_{\text{gas}} \] Pressure hydrogen gas in tank
\[ p_{\text{H}_2O} \] Partial pressure water (vapor)
\[ p_{\text{H}_2} \] Partial pressure hydrogen
\[ p_{\text{i}} \] Input pressure gas
\[ p_{\text{O}_2} \] Partial pressure oxygen
\[ p_{\text{out}} \] Output pressure gas
\[ p_{\text{tank}} \] Tank pressure maximum

**Constants**

\[ c \] Speed of light \[ 299\,792\,458 \text{ m s}^{-1} \]
\[ F \] Faraday constant \[ 96485 \text{ A s mol}^{-1} \]
\[ g \] Gravitational acceleration \[ 9.81 \text{ m s}^{-2} \]
\[ h \] Planck's constant \[ 6.626 \cdot 10^{-34} \text{ J s} \]
\[ k_B \] Boltzmann's constant \[ 1.380 \cdot 10^{-23} \text{ J K}^{-1} \]
Abstract

Elementary charge \( q \) [1.602 \( \cdot 10^{-19} \) C] 
ideal gas constant \( R \) [8.314 J mol\(^{-1}\) K\(^{-1}\)]

Cost [€]

- \( F_{Cd} \): Fuel costs in year \( d \)
- \( I_{Cd} \): Investment costs in year \( d \)
- \( M_{Cd} \): Maintenance costs in year \( d \)
- \( R_{Cd} \): Replacement costs in year \( d \)

Energy [kWh]

- \( E_{batt,max} \): Maximum available energy capacity battery
- \( E_{batt,min} \): Minimum available energy capacity battery
- \( E_{batt,rated} \): Rated energy capacity battery
- \( E_{batt}(t) \): Energy capacity battery at time \( t \)
- \( E_{batt}(t-1) \): Energy capacity battery at time \( t-1 \)
- \( E_{EV} \): Consumed energy electrical vehicle
- \( E_{H}^W \): Heat demand winter period
- \( E_{L}^d \): Daily electrical load demand
- \( E_{L}^W \): Electrical load demand winter period
- \( E_{pv} \): Generated energy by PV array
- \( E_{sys} \): Energy provided to system

Chemical Formula

- \( C_6 \): Graphite
- \( CO_2 \): Carbon Dioxide
- \( e^- \): Electrons
- \( H^+ \): Hydrons
- \( H^- \): Hydride Ion
- \( H_2 \): Hydrogen
- \( H_2O \): Water
- \( H_2SO_4 \): Sulfuric Acid
- \( K^+ \): Potassium Ion
- \( KOH \): Potassium Hydroxide
- \( LaNi_5 \): Lanthanum Nickel
- \( Li^+ \): Lithium Ion
- \( Li_4Ti_5O_{12} \): Lithium Titanate Oxide
- \( LiAsF_6 \): Lithium Hexafluoroarsenate Monohydrate
Abstract

LiBF₄  Lithium Tetrafluoroborate  
LiC₆  Lithium Graphite  
LiCF₃SO₃  Lithium Triflate  
LiClO₄  Lithium Perchlorate  
LiCoO₂  Lithium Cobalt Oxide  
LiFePO₄  Lithium Iron Phosphate  
LiMn₂O₄  Lithium Manganese Oxide  
LiNiCoAlO₂  Lithium Nickel Cobalt Aluminium Oxide  
LiNiMnCoO₂  Lithium Nickel Manganese Cobalt Oxide  
LiPF₆  Lithium Hexafluorophosphate  
M⁺  Metal Ion  
Na⁺  Sodium Ion  
NaOH  Sodium Hydroxide  
O₂  Oxygen  
OH⁻  Hydroxide Ion  
Pb  Lead  
Pb²⁺  Lead Ion  
PbO₂  Lead Dioxide  
PbSO₄  Lead Sulfate  
SO₄²⁻  Sulfate Ion  
Y₂O₃  Yttrium Oxide  
ZrO₂  Zirconium Oxide

**Irradiance \([W \, m^{-2}]\)**

\(G_{Beam}\)  Beam Irradiance  
\(G_{Circumsolar}\)  Circumsolar region irradiance  
\(G_{Diffuse}\)  Sky Diffuse Irradiance  
\(G_{Dome}\)  Sky dome irradiance  
\(G_{Ground}\)  Ground reflective Irradiance  
\(G_{Horizon}\)  Sky horizon irradiance  
\(G_{mETC}\)  Irradiance on module at ETC  
\(G_{mSTC}\)  Irradiance on module at STC  
\(G_{NOMT}\)  Irradiance at normal operation module temperature conditions  
\(G_{POASTC}\)  Plane of array irradiance on module at STC  
\(G_{POA}\)  Plane of Array Irradiance
Current [A]

\( I \)  Operating current PV module
\( I_D \)  Dark diode current
\( I_L \)  Photo current generated
\( I_{ley} \)  Electrolyzer stack current
\( I_{fc} \)  Fuel Cell stack current
\( I_{mpPSTC} \)  Maximum Power Point current at STC
\( I_{mpp} \)  Maximum Power Point Current
\( I_{scSTC} \)  Short circuit current at STC
\( I_{sc} \)  Short Circuit Current

Volumetric flow [m³ s⁻¹]

\( \phi_v \)  Volumetric flow
\( \phi_{vc\text{cooling}} \)  Volumetric flow cooling water
\( \phi_{vdemi} \)  Volumetric flow DEMI water
\( \psi_{H_2\text{practical}} \)  Practical quantity hydrogen
\( \psi_{H_2\text{theoretical}} \)  Theoretical quantity hydrogen

Mass flow [kg s⁻¹]

\( \phi_m \)  Mass flow
\( \phi_{mdump}(t) \)  Mass flow dumped at time \( t \)
\( \phi_{mH_2} \)  Mass flow hydrogen
\( \phi_{m\text{in}}(t) \)  Mass flow in at time \( t \)
\( \phi_{mo_2} \)  Mass flow oxygen
\( \phi_{m\text{out}}(t) \)  Mass flow out at time \( t \)

Lengths [m]

\( \lambda \)  Wavelength light
\( h_{fc} \)  Height cell
\( h_{\text{plate}} \)  Height end plate
\( L_{\text{frame}} \)  Average distance between PEM fuel cell and air
\( t_{fc} \)  Thickness cell
\( t_{\text{memb}} \)  PEM thickness
\( t_{\text{plate}} \)  Thickness end plate
\( w_{fc} \)  Width cell
\( w_{\text{plate}} \)  Width end plate

Molar flow [mol s⁻¹]
\( \phi_{\text{molarH}_2} \) Molar flow hydrogen
\( \phi_{\text{molarO}_2} \) Molar flow oxygen
\( \phi_{\text{molarH}_2O} \) Molar flow demi water

**Molar mass \([\text{kg mol}^{-1}]\)**

- \( M_{\text{H}_2O} \) Molar mass water
- \( M_{\text{H}_2} \) Molar mass hydrogen
- \( M_{\text{O}_2} \) Molar mass oxygen

**Other Symbols**

- \( \beta \) Transport number for water \([-\]
- \( \Delta G^\circ \) Standard internal Energy change \([\text{kJ mol}^{-1}]\)
- \( \Delta H^\circ \) Standard enthalpy change \([\text{kJ mol}^{-1}]\)
- \( \Delta S^\circ \) Standard entropy change \([\text{kJ mol}^{-1}]\)
- \( \eta_{\text{EV}} \) Driving ability electrical vehicle \([\text{km kWh}^{-1}]\)
- \( \eta_{\text{GV}} \) Driving ability gasoline vehicle \([\text{km liter}^{-1}]\)
- \( \eta_{\text{HV}} \) Driving ability hydrogen vehicle \([\text{km liter}^{-1}]\)
- \( \gamma \) Ideality factor diode corresponding to semiconductor material
- \( \mu_{\text{isc}} \) Temperature coefficient short circuit current \([\% \degree\text{C}^{-1}]\)
- \( \mu_{\text{mppt}} \) Temperature coefficient maximum power point \([\% \degree\text{C}^{-1}]\)
- \( \mu_{\text{VocNOC}} \) Temperature coefficient open circuit voltage at NOTC \([\% \degree\text{C}^{-1}]\)
- \( \mu_{\text{Voc}} \) Temperature coefficient open circuit voltage \([\% \degree\text{C}^{-1}]\)
- \( \tau \) Fraction of incident light absorbed by crystalline module
- \( C_{\text{rate}} \) Charge/Discharge energy rate \([\%]\)
- \( C_{\text{teley}} \) Thermal capacitance electrolyzer \([\text{J K}^{-1}]\)
- \( C_{\text{tc}} \) Thermal capacitance fuel cell \([\text{J K}^{-1}]\)
- \( d \) Year
- \( d_a \) Autonomy days
- \( E_{\text{gSTC}} \) Semiconductor bandgap energy crystalline silicon at STC
- \( E_g \) Bandgap energy semiconductor \([\text{eV}]\)
- \( E_{\text{ph}} \) Photon energy \([\text{eV}]\)
- \( h_{\text{air}} \) Heat transfer coefficient air \([\text{W m}^{-2} \text{ K}^{-1}]\)
- \( h_{f\theta H_2O} \) Fraction of demi water vaporized \([\text{W m}^{-1} \text{ K}^{-1}]\)
- \( k_{\text{fc}} \) Thermal conductivity fuel cell material \([\text{W m}^{-1} \text{ K}^{-1}]\)
- \( m_{\text{HV}} \) Consumed mass by hydrogen vehicle \([\text{kg}]\)
- \( N \) Polytropic constant
Abstract

\( n \) Moles
\( n_s \) Number of cells in series
\( r \) Discount rate
\( R_s \) Series resistance module
\( r_1 \) Ohmic resistance coefficient
\( r_2 \) Ohmic resistance coefficient
\( R_{sh} \) Parallel resistance module
\( R_{tey} \) Thermal resistance electrolyzer
\( R_{f_{fc}} \) Thermal resistance fuel cell
\( s_1 \) Overvoltage electrodes
\( t_1 \) Overvoltage electrodes
\( t_2 \) Overvoltage electrodes
\( t_3 \) Overvoltage electrodes
\( v_{wind} \) Wind speed
\( x_{evap} \) Enthalpy of water vaporization
\( y \) Project lifetime
\( z \) Number of electrons
\( k_{isen} \) Isentropic constant

**Power [W]**

\( P_{batt_{load}} \) Power from battery to load
\( P_{batt} \) Power to or from battery
\( P_{batt(t)} \) Instantaneous power to or from battery at time \( t \)
\( P_{comp} \) Compressor power
\( P_{conv_{in}} \) DC input power
\( P_{conv_{out}} \) DC output power
\( P_{def} \) Power deficit
\( P_{demand} \) Power demand
\( P_{dump} \) Power dumped
\( P_{ely} \) Electrolyzer power
\( P_{exc} \) Excess power
\( P_{f_{c_{load}}} \) Power from fuel cell to load
\( P_{fc} \) Fuel Cell power
\( P_{hv} \) Power consumed by hydrogen vehicle
\( P_{load} \) Power delivered to load
Abstract

\( P_{\text{mpp}} \)  Power Maximum Power Point
\( P_{\text{net}} \)  Net power
\( P_{\text{pvtoLoad}} \)  Power from solar to load
\( P_{\text{pv}} \)  Power generated by PV array
\( P_{\text{rated}} \)  Rated power inverter
\( P_{\text{short}} \)  Shortage power
\( P_{\text{tank}} \)  Total required power for consumption or production of hydrogen
\( P_{\text{inDC}} \)  DC input power inverter
\( P_{\text{inmppt}} \)  MPPT charge controller input power
\( P_{\text{outAC}} \)  AC output power inverter
\( P_{\text{outmppt}} \)  MPPT charge controller output power
\( P_{\text{outratedmppt}} \)  Rated power mppt charge controller

**Density [kg m\(^{-3}\)]**

\( \rho_{\text{DEMI}} \)  Density DEMI-water
\( \rho_{\text{fc}} \)  Density fuel cell material
\( \rho_{\text{H}_2\text{O}} \)  Density water
\( \rho_{\text{H}_2} \)  Hydrogen density
\( \rho_{\text{plate}} \)  Density end plate material

**Efficiency [%]**

\( \eta_{\text{battcoul}} \)  Coulombic efficiency battery
\( \eta_{\text{battvolt}} \)  Voltaic efficiency battery
\( \eta_{\text{batt}} \)  Round-trip efficiency battery
\( \eta_{\text{cell}} \)  Solar cell efficiency
\( \eta_{\text{conv}} \)  Efficiency converter
\( \eta_{\text{ely}} \)  Electrolyzer efficiency
\( \eta_{\text{faraday}} \)  Faraday efficiency
\( \eta_{\text{inv}} \)  Efficiency inverter
\( \eta_{\text{mppt}} \)  Efficiency MPPT charge controller
\( \eta_{\text{m}} \)  Module’s efficiency
\( \eta_{\text{poly}} \)  Polytropic efficiency
\( \eta_{\text{pump}} \)  Overall efficiency pump
\( \eta_{\text{stochH}_2} \)  Stochiometric efficiency hydrogen
\( \eta_{\text{stochO}_2} \)  Stochiometric efficiency oxygen
\( \eta_{\text{sys}} \)  Hybrid system efficiency
\[ \eta_{voltage_{el}} \] Voltage efficiency electrolyzer
\[ \eta_{voltage_{fc}} \] Voltaic efficiency fuel cell

**Surface [m^2]**
\[ A_{cell_{pp}} \] Solar cell surface
\[ A_{cell} \] Electrolyzer cell area
\[ A_{module} \] Module's surface
\[ A_{pem} \] PEM membrane electrode area

**Temperature [°C]**
\[ T_m \] Module's temperature
\[ T_{amb} \] Ambient temperature
\[ T_{ely} \] Electrolyzer temperature
\[ T_{gas} \] Temperature Gas
\[ T_{in} \] Input temperature hydrogen gas
\[ T_{m_{ETC}} \] Module’s temperature at ETC
\[ T_{m_{STC}} \] Module’s temperature at STC
\[ T_{NOMT} \] Temperature at normal operation module temperature conditions
\[ T_{out} \] Output temperature hydrogen gas
\[ T_{w_{in}} \] Temperature cooling water in
\[ T_{w_{out}} \] Temperature cooling water out

**State of Charge [%]**
\[ DoD_{bat_{max}} \] Maximum Depth of Discharge battery
\[ SoC_{bat_{ini}} \] Initial State of Charge battery
\[ SoC_{bat_{max}} \] Maximum State of Charge battery
\[ SoC_{bat}(t) \] State of Charge battery at time \( t \)
\[ SoC_{fin} \] Final State of Charge
\[ SoC_{ini} \] Initial State of Charge
\[ SoC_{tank_{ini}} \] Initial State of Charge tank
\[ SoC_{tank}(t) \] State of Charge hydrogen tank at time \( t \)

**Voltage [V]**
\[ V \] Operating voltage PV module
\[ V^o_{rev} \] Reversible voltage standard condition
\[ V^o_{tn} \] Thermoneutral voltage standard condition
\[ V_{act} \] Activation overpotential
\[ V_{cel_{ely}} \] Cell voltage electrolyzer
Abstract

\[ V_{cell} \]: Cell voltage  
\[ V_{comp} \]: Operating voltage compressor  
\[ V_{con} \]: Concentration overpotential  
\[ V_{irrev} \]: Irreversible overpotential  
\[ V_{mpp, STC} \]: Maximum Power Point voltage at STC  
\[ V_{mpp} \]: Maximum Power Point Voltage  
\[ V_{oc, STC} \]: Open circuit voltage at STC  
\[ V_{oc} \]: Open Circuit Voltage  
\[ V_{ohm} \]: Ohmic overpotential  
\[ V_{rev} \]: Reversible voltage  
\[ V_{tn} \]: Thermoneutral voltage  

**Volume [m^3]**

\[ V_{gas}(t) \]: Volume stored hydrogen gas at time t  
\[ V_{gas}(t - 1) \]: Volume stored hydrogen gas at time t-1  
\[ V_{tank} \]: Volume storage tank  

**Heat capacity [J kg^{-1} K^{-1}]**

\[ C_p \]: Specific heat ideal gas at constant pressure  
\[ C_v \]: Specific heat ideal gas at constant volume  
\[ c_{pf, c} \]: Heat capacity fuel cell material  
\[ c_{p, H_2O} \]: Heat capacity water  
\[ c_{p, plate} \]: Heat capacity plate material  

**Optimization parameters**

\[ a \]: Multiplier for pilot point Hooke-Jeeves algorithm  
\[ c \]: Multiplier for interior penalty function  
\[ c_1 \rho_1 \]: Cognitive acceleration of the particle in PSO algorithm  
\[ c_2 \rho_2 \]: Social acceleration of the swarm in PSO algorithm  
\[ f'(x) \]: Augmented objective function  
\[ f(x) \]: Objective function  
\[ i \]: \( i^{th} \) particle PSO algorithm  
\[ k \]: \( k^{th} \) generation PSO algorithm  
\[ n_g \]: Number of generations PSO algorithm  
\[ n_p \]: Number of particles PSO algorithm  
\[ p_b \]: Personal best location particle PSO algorithm  
\[ p_g \]: Global best location particle PSO algorithm
$v_i$ Velocity of the $i^{th}$ particle of PSO algorithm

$x_i$ Location of the $i^{th}$ particle of PSO algorithm

$x_0$ Base point Hooke-Jeeves algorithm

$x_1$ Best next point Hooke-Jeeves algorithm

$x_2$ Pilot point Hooke-Jeeves algorithm

$x_3$ New pilot Hooke-Jeeves algorithm

**Heat transfer [J s$^{-1}$]**

$\dot{Q}_{cool}$ Heat loss cooling water

$\dot{Q}_{evap}$ Evaporative heat loss cathode

$\dot{Q}_{gen}$ Generated heat

$\dot{Q}_{loss}$ Ambient heat loss

$\dot{Q}_{net}$ Net heat difference

$\dot{Q}_{rest}$ Rest heat difference

$\dot{Q}_{comp}$ Heat compressor
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1. Introduction

1.1. Motivation
According to the United Nations the population size worldwide is growing rapidly. A growing population requires more cultivation preventing starvation, more fresh and clean water preventing health issues and inexhaustible energy sources so that even in the darkest and coldest corners of the world there may be light. In a nutshell, population growth will result in an increase of energy consumption. Figure 1.1 gives an insight on the growth of both the population and energy demand in the future.

![Figure 1.1: World population and Energy demand growth](image)

Although the population growth of industrialized countries is negligible compared to the total growth of the world population -as can be seen in figure 1.1- the energy consumption is higher than the rest of the world in 2015, see figure 1.2, and tends to increase because of economic prosperity in the industrialized countries.
To manage the population growth and prevent water, food or energy scarcity it is essential to look into the prospects of available energy sources. Currently, fossil fuels are used because of the low cost and the detailed technological knowledge available in the energy sector. The artificial production of carbon dioxide by burning fossil fuels and releasing into the atmosphere has an impact on the climate change. One of the critical effects of the climate change is on the stratospheric ozone layer. A damaged ozone layer not only results in temperature rise due to greenhouse gasses but also in a diminished absorption of UV-light resulting in possible health issues such as cancer. Besides burning fossil fuels, also the extraction of natural gasses negatively impacts the climate. Due to gas extractions, soils are sagged resulting in earth quakes. The current consumption of fossil fuels is not only harmful for the climate due to the emitted carbon dioxide but also exhaust the resources at a higher rate than the earth can replenish. This year for the third year in row the number one on the list of world problems to be dealt with is the climate change and destruction of natural resources. To put it more concrete, on the 8th of December 2015, the Belfer Center for Science and International Affairs of the Harvard Kennedy School wrote an article stating that “Climate Change is the issue of the millennial generation” [7]. In plain English: the energy industry requires a radical change towards more sustainable and inexhaustible energy sources.

1.2. Solar & Storage

1.2.1. Solar Energy

The largest, most predictable, inexhaustible and the main source which powers other renewable energy sources is the Sun (except for geothermal and tidal) [8]. Although the energy retrieved from the Sun is inexhaustible and predictable, the drawback is that the intensity and visible hours received by the earths surface varies due to weather conditions -such as clouds and rain- and because of the location. Resulting in both daily and seasonal fluctuations as shown in figures 1.3a and 1.3b. The daily fluctuations can be dealt with by short term storage methods and the seasonal can be dealt with by long term storage methods so that a stand-alone solar energy system becomes more viable. Stand-alone energy systems are systems that are often used in remote areas where no utility grid is present of viable to develop. Like power generation in rural areas of developing countries [9, 10], backup energy for telecommunication networks [11], water pumping in agriculture [12] and many more. Although each stand-alone solar energy system has its own purpose, the general components are photovoltaic
(PV) modules, power/charge controller and storage.

![Graph](image)

**Figure 1.3:** (a) Daily fluctuation solar energy [13]. (b) Seasonal fluctuation solar energy [14].

### 1.2.2. Electrochemical energy

A well researched and one of the oldest way of storage, is electrochemical energy storage where electricity is stored under a chemical form. In the late 18\textsuperscript{th} century scientists began to conduct more experiments till 1766 when Henry Cavendish recognized hydrogen as a discrete substance and in 1800 the first battery was created by Volta. This principle is achieved by an electrolysis process that will be explained more in detail in chapter 2. In this storage technique both the electrical and chemical energy share the same carrier, namely the electron. Two familiar electrochemical storage methods are battery storage and storage in chemical bonds.

In today’s modernity a lead-acid battery is commonly used in stand-alone energy systems due to their straightforward charge/discharge cycle, high round-trip efficiency of 80% [9], and low cost. However, the disadvantage is that lead-acid batteries not only have a low energy density, but also negatively impact the environment after the disposal of the lead plates and the sulphuric acid. And due to the relative short life cycle it has to be replaced more frequently during the lifetime of the entire system. Another disadvantage is the self-discharge of a lead acid battery which varies at different ambient temperatures. At an environmental temperature of 20°C, the self-discharge is roughly 3-5% per month and needs definite recharging after 12 month of storage while a temperature of 30°C requires a recharge after 6 months. Self-discharge decreases the shelf life of batteries and the State of Charge (SoC). Consequently, the battery with a low SoC during long term periods causes sulfation. Another main battery technology, that is not commonly used in stand-alone systems, is lithium-ion and is comprehensively discussed in 2.3.

The second form of electrochemical storage mentioned is storing electricity in chemical bonds such as ammonia, hydrogen and hydrocarbons. In these mentioned chemical bonds a hydrogen bond can be found. A hydrogen bond is the attractive force between the hydrogen attached to an electronegative atom of one molecule and an electronegative atom of a different molecule [15]. In the case of ammonia, a hydrogen atom creates a hydrogen bond with nitrogen atom. The hydrocarbon consist of a hydrogen bond between carbons and hydrogen and the hydrogen itself is a hydrogen bond between two hydrogen atoms. Hydrogen as the most abundant chemical element can be found in water and is produced in an electrolytic process where water is split into hydrogen and oxygen molecules in an endothermic process. As stated by Rashidi [16], “the storage of electrical energy in the form of hydrogen compound is favored due to the fact that hydrogen is a clean emission free product for production, storage and consumption.” Hydrogen has a higher energy density, either stored as liquid, gas or in metal hydrids, compared to batteries (142 MJ/kg vs 0.95 MJ/kg) [2, 3]. In turn, hydrogen and oxygen molecules produce electricity in an exothermic process with water as byproduct. Although hydrogen seems promising as a long term storage method, the requirement of additional auxiliary components for production, storage and consumption of hydrogen thwarts the direction towards a complete energy storage in the way of only chemical bonds. All the additional auxiliary components required for the implementation of hydrogen storage in stand-alone solar energy systems results in a low well-to-wheel efficiency of 4-6% [17–19].
In addition, potential self-discharge of hydrogen and the wide flammability range of 4-74% [20] in air can lead to flammable situations or even explosions. Therefore, great cares have to be taken to embrace hydrogen storage.

1.3. Hybrid Solar Systems

Hybrid Solar Systems (HSS) are typical stand-alone solar energy systems with a battery bank, that are expanded by the addition of a storage method in the form of hydrogen and the essential components. Hydrogen implementation into stand-alone energy systems in contrast to batteries is the new kid on the block. Even though hydrogen is a well known chemical element and is used profoundly in other chemical process as fixation of nitrogen from the air in the Haber ammonia process, hydrogenation of fats and oils, methanol production, hydro-cracking, rocket fuel, welding, filling balloons, as liquid in superconductivity studies and many others [21], it is still not comprehensively explored as a promising storage method in energy systems.

In 2009 Chun-Hua Li et al. [22] performed a study on optimizing, analyzing and comparing three stand-alone renewable energy systems, (1) PV+Battery, (2) PV+Electrolyzer+FC and (3) PV+Battery+Electrolyzer+FC, to meet the load requirement. Each configuration is single optimized for the minimum cost or maximum efficiency. The study concludes that the high efficiency of the battery and low cost of hydrogen tank helps the PV+Battery+Electrolyzer+FC system to meet the load with a lower system cost, higher system efficiency and less solar modules as compared to the other two studied systems. Jérémy Lagorse et al. [23] modelled and intuitively sized the system configurations shown in figure 1.3, (a) PV/Battery/FC, (b) PV/Electrolyzer/FC and (c) PV/Battery/Electrolyzer/FC to meet the load demand and evaluated the energy cost of each system configuration being 0.519 €/kWh, 4.9439 €/kWh and 0.6459 €/kWh respectively. While configuration “a” is the cheapest but not completely autonomous, the best option is configuration “c” which is completely autonomous at an acceptable energy cost.

![Diagram](image)

Figure 1.4: Illustrative configurations of the studied system by Lagorse. (a) Load provided by PV, Battery and FC with an external hydrogen tank. (b) Load provided by PV, Electrolyzer, FC and storage tank. (c) Load provided by PV, Battery, Electrolyzer, FC and storage tank. [23].

Especially in some cases, such as telecommunication networks in remote area [11], a higher energy cost for a PV/Battery/Electrolyzer/FC is accepted if that comes with a 100% reliability. A more recent study in 2016 by Belmonte et al. [24] compared a PV/Battery system and a PV/Electrolyzer/FC system for a case study in Turin Italy. The systems were intuitively sized to provide a maximum power consumption of 3kW and compared from a technical and economical point of view and a life cycle assessment (LCA) was performed. The results showed that technically and economically a PV/Battery system based on battery is more mature than a hydrogen energy system while the hydrogen technology is preferred from an environmental perspective (LCA) due to the lower burden. The outgrow of electrolyzers and fuel cells from a niche market can positively influence the hydrogen technology both technically and economically. In the paper by Halimi Rashidi et al. [16], a system optimization is performed for a stand-alone hybrid solar-hydrogen with the focus on the optimal design of a stand-alone hybrid solar-hydrogen energy system to provide reliable supply with minimum cost during the 20-years system life using Fuzzy based Particle Swarm Optimization (FPSO). Two proposed configurations are optimized and analyzed. One is PV-Electrolyzer-Battery-FC and the other is PV-Electrolyzer-FC. Results show that a hybrid system combining battery and hydrogen has higher global efficiency, 50%, at a lower total
system cost of $2,589,580.

The prosperous results of stand-alone hybrid PV-Electrolyzer-Battery-FC (PEBF) energy systems [22–24] boosted the academic world to enhance more research and perhaps even a complete transition of the energy economy. In 2004 the U.S. National Research Council [25] and the American Physical Society [26] published the technical opportunities and further improvements towards a hydrogen economy. A hydrogen economy is a future ideology for a clean energy economy. In a hydrogen economy the focus will be on producing hydrogen, storing hydrogen, transportation of hydrogen and conversion of hydrogen to electrical energy to meet the energy demand as a low-carbon energy source when combined with renewable sources. The first step towards a so-called hydrogen economy is in depth feasibility study of such a system for residential implementation.

One of the first operational stand-alone solar-hydrogen systems is the solar house in Freiburg, discussed by Voss et al. [27], that was operated for a period of 3 years. Three years of experience demonstrated that it is possible to overcome the seasonal mismatch between solar radiation and building energy demand, for heating, domestic hot water, electricity and cooking by long term storage based on hydrogen and short term storage based on lead-acid batteries. In 1998 Oystein Ulleberg [28] published perhaps one of the most comprehensive researches on a hybrid solar-hydrogen renewable energy system. In this PhD dissertation a stand-alone solar-hydrogen system is simulated with the help of the TRNSYS (Transient System Simulation Tool) and with the results from the PV-Electrolyzer-Battery-FC demonstration plant called PHOEBUS in Jülich, Germany, it was concluded that all the developed models were more than accurate enough to perform long-term simulations. Ulleberg also successfully found optimal operation and control strategies for the PHOEBUS system. The PHOEBUS system is an operational fixed system design to meet the load demand of Central Library of Forschungszentrum [29, 30]. In the paper of Singh, Baredar and Gupta [31], a stand-alone solar-hydrogen system, see figure 1.5, is numerically optimally sized and examined for an academic research building located in India at 23°12’N latitude and 77°24’E longitude. The optimization process is divided into two objectives. Primarily, the optimum value of capital and replacement cost for each component is computed with the fuzzy logic (FL) program. Secondly, HOMER (Hybrid Optimization Model for Electric Renewables) software is used to optimize system sized according by minimizing the total system cost while maintaining system reliability. The optimum system design has a capacity shortage of 0% for the minimum total system cost of roughly $47,437, electricity cost of 0.20 $/kWh and an operating cost of 2088 $/year.

In Khemariya et al. [32], for an unelectrified village in India, Jhiriya Kheda, a stand-alone solar-hydrogen system sizing is designed through a numerical optimization process by HOMER software [33] to minimize the per unit cost for a project lifetime of 20 years. To consider the seasonal mismatch,
1.4. Problem Statement

The estimated load is divided into three seasons (winter season, summer season and rainy season). The optimal stand-alone system for the lowest per unit cost of 0.1959 $/kWh is unable to meet load demand 1.7% of the time in a year. Castaneda et al. [34] use a sizing method based on Simulink Design Optimization (SDO) to perform technical optimization for three system configuration, (1) PV+Battery, (2) PV+Electrolyzer+Battery+FC and (3) PV+Electrolyzer+FC. Configuration (2), see figure 1.6, is then analyzed by simulating for three control strategies based on operating modes and combining technoeconomical aspects are considered for the energy management. The criteria for the hybrid system to be met is satisfying the load demand and maintaining certain levels for the battery capacity and hydrogen tank. Simulation results demonstrated reliable electricity supply, while maintaining a certain energy reserve in the storage sources for all three control strategies.

Figure 1.6: Studied configuration of Hybrid Renewable Energy System for three different control strategies [34].

The aforementioned literature shows several stand-alone hybrid solar-hydrogen systems which are either optimized by an intuitive [22–24, 27, 28] or numerical approach [16, 31, 32, 34]. The optimizations are done from a technical perspective [23, 24], an economical perspective [16, 31] and a technoeconomical perspective [34]. All the studies, except for Singh et al. [32], only considers seasonal fluctuations at the energy generation side instead of both energy generation and energy demand side (i.e. cold winters and hot summers). The studies confirm a promising high reliable and low cost effective stand-alone hybrid solar-hydrogen system, but the studied locations are all, except for Castaneda [34], in rural and sunny areas. This raises the question if such systems will also be viable for less sunny and higher energy demand locations like the Netherlands. Lastly, none of the papers discuss the future perspective of stand-alone hybrid solar energy systems for the case that electrolyzers, batteries and fuel cells experience the same learning curve as with solar modules in the last 15 years.

1.4. Problem Statement

This thesis project attempts to extend the already discussed work on stand-alone hybrid solar-hydrogen systems in the literature by the implementation of a optimal sized hybrid stand-alone energy system based on a single primary energy source, the Sun, and a combination of battery and hydrogen for storage and a fuel cell for the back conversion of hydrogen into electricity. Such a system can tackle the short-comings of batteries and hydrogen as single storage methods and smooth out both daily and seasonal fluctuations. The proposed system, shown in figure 1.7, comprises a PV array, a battery, an electrolyzer, a fuel cell, a hydrogen storage system, power conditioning unit(s) and a controller and is abbreviated as PV-Electrolyzer-Battery-FC (PEBF). The system is optimal sized for a Loss of Load Probability of 1% or lower for the lowest possible Levelized Cost of Energy over a lifetime of 25 years.
Figure 1.7: Schematic overview of the proposed stand-alone hybrid PV-Electrolyzer-Battery-FC system.
The detailed literature study in the previous section and the motivation extending the knowledge on this topic helps to form the following research objective:

Assess the feasibility of current and future stand-alone hybrid PV-Electrolyzer-Battery-FC energy systems from a techno-economical point of view, based on a numerical optimal system sizing for a typical household.

The main research objective can be divided into the following sub-objectives:

- Develop a computer simulation model of a stand-alone hybrid PV-Electrolyzer-Battery-FC energy system.
- Obtain an applicable optimization function and algorithm for the proposed simulation model.
- Develop case studies for residential application of the proposed stand-alone hybrid energy system for fulfillment of electrical, heat and mobility demand.
- Assess the techno-economical feasibility of the proposed stand-alone system now and in the future based on optimization.

1.5. Thesis Approach

The structure of this final thesis project report is similar to the order of the aforementioned sub-objectives for gaining a fundamental understanding about solar-hydrogen energy systems. Up till now the motivation for the topic of this thesis is discussed and a brief literature review is done on the progress of the solar-hydrogen energy systems. In chapter 2 the fundamentals and technologies of PV modules, batteries, electrolyzers, fuel cells and hydrogen storage methods are elaborately described and explained. Thereupon, well-thought decisions are made for adopting the appropriate technologies for the proposed stand-alone hybrid PV-Electrolyzer-Battery-FC energy system. Chapter 3 explains the empirically developed system simulation model in the simulation environment of TRNSYS (Transient System Simulation Tool) on the basis of the physical, chemical and math principles. In chapter 4, the urge of optimization necessary for a potential complex hybrid renewable energy system is discussed. Followed with an elaborate explanation about the adopted optimization algorithms particle swarm optimization (PSO) and Hooke-Jeeves in the optimization environment of Generic Optimization Program (GenOpt) and TRNSYS Optimization (TRNOPT). Chapter 5 describes the different scenario’s of energy demand of a typical household in the Netherlands that will be studied in collaboration with the proposed hybrid system. The adopted simulation model and optimization algorithms are used to find the optimal system sizing corresponding to the lowest levelized cost of energy (LCOE) and a loss of load probability (LLP) of 0-1% for the different scenario’s of energy demand. This is done according to the current and future prices of the components and the results are displayed in chapter 6 followed by a quantitative analysis on the potential of a so called hydrogen economy in the future. Lastly, in chapter 7 the conclusions and recommendations for future work can be found.
Background information

The primary energy source for the proposed stand-alone PV-Electrolyzer-Battery-FC energy system in this thesis is the Sun. The energy of the Sun is collected by the PV array in combination with a Maximum Power Point Tracker (MPPT) while the battery bank and the combination of Electrolyzer-FC-Storage are respectively used for short and long term storage. For a well thought selection process regarding these components, an elaborated explanation is given concerning the principles and the available technologies. Firstly, the fundamentals and technologies of the solar energy are explained in 2.1. Then, the conversion of electrical energy to electrochemical energy (by an electrolyzer) and vice versa (by a fuel cell) and the related technologies are discussed in 2.2. Thirdly, the principles of electrochemical energy in the form of batteries and hydrogen storage are described in 2.3. The reader who is already familiar with these fundamentals and is only interested in the concluding remarks, regarding the selection process of the main components, is kindly invited fast forwarding to section 2.4 for the concluding remarks.

2.1. Solar Energy

Fundamental

The Sun, the energy source for all the living organism on the planet, emits electromagnetic radiation which is partly received by the earths surface. To convert the free and clean energy of the Sun directly into electricity, a PV module is used. A PV module is an essential component of any solar powered energy system and each PV module consists of multiple solar cells. The different types of solar cell can be categorized in crystalline silicon cells, thin-film cells and multi-junction cells, shown in figure 2.1. The names of the different solar cell types are based on the semiconductor material implemented in the solar cell. Creation of voltage and electric current upon exposure to light is a physical and chemical phenomenon, dependent of the semiconductor materials, also known as the photovoltaic effect.
The emitted incident irradiation by the Sun has a broad spectrum, see figure 2.2. According to quantum mechanics, electromagnetic radiation can behave as a wave but also as discrete packages of energy. This is also known as the wave-particle duality. In terms of classical mechanics it is assumed that radiation comes in packages of energy and thus shows the behaviour of particles [36]. But the propagation of light through space or at reflection and refraction at a flat interface shows wave character [37]. For the principle of photovoltaic effect, the incoming light has both wave and particle characteristics. Energy quanta in light are also known as photons where the photons present in the short wavelength of the light have a larger energy than the photons present in the longer wavelength of the light. Energy of such a photon is defined by the Planck–Einstein relation:

\[ E = \frac{h \cdot c}{\lambda} \]  

(2.1)

where \( h \) is the constant of Planck, \( c \) is speed of light and \( \lambda \) is the wavelength of the light.

Figure 2.2: The spectrum of the Sun [38].
Upon impact of the material to the incident light, the photons consisting of a larger energy \( E_{ph} \), dependent of frequency and defined by eq. 2.1, than the bandgap \( E_g \) of the semiconducting material will be absorbed \([37]\), see figure 2.3a. After absorption of the photon, the energy is employed to excite an electron to the conduction band. This results in the generation of electron-hole pairs. Next, the electron-hole pairs are separated through a semipermeable membrane layer inside the solar cells to prevent recombination. The electrons travel to the n-type layer, whereas the “holes” travel through the membrane to the p-type layer. Electrons travel via the external circuit and generate electric current before being collected and recombined with the “holes”. For a typical silicon solar cell, the holes gather at the p-type layer at the back of the solar cell and are recombined there with the externally arrived electrons. An illustrated overview of this principle is given in figure 2.3b.

Illuminated solar cells have a characteristic current-voltage curve dependent on the environmental conditions, such as received irradiation, ambient temperature and the solar cell’s temperature, and will be discussed in detail in 3.2.3. Figure 2.4 represents the characteristic current-voltage and power-voltage curve of a typical silicon solar cell under a certain irradiation level with its characteristic external parameters. The current-voltage curve is a plot of the operating output voltage versus the generated current. Subsequently, the power-voltage curve is determined by plotting the product of current and voltage, for all possible combinations of current and voltage in the range of open circuit and short circuit conditions. The open circuit voltage \( V_{OC} \) of a solar cell is measured when no load is connected upon illumination and the short circuit current \( I_{SC} \) is the generated current upon illumination. The short circuit current is measured by when the solar cell output connectors are shorted together. Maximum power point \( P_{mpp} \) is found where the derivative of the power-voltage curve, \( \frac{dP}{dV} = 0 \). The correlative voltage and current of the maximum power point are called maximum power point voltage \( V_{mpp} \) and maximum power point current \( I_{mpp} \). The ratio between the maximum power point \( P_{mpp} \) and the received plane of incident irradiance \( G_{POA} \) and surface of the cell \( A_{cell,po} \) defines the solar cell’s efficiency. The efficiency of a solar cell is expressed by:

\[
\eta_{cell} = \frac{P_{mpp}}{G_{POA} \cdot A_{pv,cell}} \cdot 100\%
\]
Under any operational circumstances, solar cells have a single operating point where the values of the current and voltage of the cell result in a maximum power output [40]. The highest power yield of a solar cell can be retrieved by operating at the \( P_{mpp} \). By Ohm’s law, \( R = \frac{V}{I} \), the correlative \( V_{mpp} \) and \( I_{mpp} \) correspond to the characteristic ohmic load resistance of the solar cell at maximum power point. Connecting a load directly to the solar cell will strongly influence the performance. The electrical resistance of the load will be dictating the operating point of the cell and will rarely be close to the solar cells characteristic resistance analogous to the \( P_{mpp} \). Thus, the cell will not be used as efficiently as possible. Additionally, the variance in irradiance, ambient temperature, age and solar cells temperature affects the characteristic current-voltage and power-voltage curve and subsequently the \( P_{mpp} \) and thus the correlative characteristic resistance of the solar cell.

To obviate these potential negative effects, calls for a dynamical controller that forces the solar cell to operate at the \( P_{mpp} \). This principle can be realized by the algorithm of maximum power point tracking. The algorithm manages the electrical impedance seen by the solar cell, for any arbitrary load, to match the characteristic resistance of the cell (and keeping it there) regarding the current-voltage and power-voltage curve at that moment. This procedure helps the solar cell to operate close or preferably at the maximum power point. Maximum power point algorithm is integrated in power converters such as solar inverters and solar converters that apply voltage or current conversion. These devices are implemented between the solar cell (module) and the load for extracting the maximum available power from the source under any circumstances. Some maximum power point tracking algorithms are based on fine tuning the operating voltage to match the \( V_{mpp} \) (Fixed voltage method, fractional open circuit voltage, perturb and observe, incremental conductance method [37, 41]), while others work with the power and target the \( I_{mpp} \) (fractional short circuit method, perturb and observe [42–44]).

Technologies
Table 2.1 displays three main solar cell technologies used in the solar industry, namely crystalline solar cells (1\textsuperscript{st} generation), thin film solar cells (2\textsuperscript{nd} generation) and new emerging technologies, e.g. multi junction solar cell (3\textsuperscript{rd} generation). Any type of the aforementioned solar cells can be connected in various strings to create solar modules. In turn, connection of multiple solar modules in parallel and/or series connections result in a solar array.

First generation
In the category of 1\textsuperscript{st} generation technology, the crystalline solar modules can be divided into mono-crystalline and poly-crystalline. Both are single-junction devices. These modules are mostly used in residential installations. Commercially available mono-crystalline modules have an efficiency of 16-21% and poly-crystalline modules have an efficiency of 15-17%. Mono-crystalline modules are made from the mono-crystalline silicon ingot that is made by the Czochralski [45] or float zone method [46] using highest-grade silicon. Poly-crystalline modules are made from the cubic shaped multi-crystalline ingot that is created by melting and solidifying highly purified silicon in the silicon casting method.
This difference in fabrication method makes that the mono-crystalline requires less space than poly-crystalline to produce the same amount of power but with the disadvantage that it is more expensive.

**Second generation**

Modules based on the 2\textsuperscript{nd} generation technology use the same principle of single-junction, but aim to reduce the material utilization, while maintaining the efficiencies of 1\textsuperscript{st} generation modules and thus reducing cost. Primarily available commercial modules are amorphous silicon (a-Si), micro-crystalline silicon (μc-Si) tandem cells, Cadmium Telluride (CdTe) and Copper Indium Gallium Selenide (CIGS). These types of modules are used in small solar systems, solar power stations and integrated into buildings (roof, facade). Disadvantage of these modules is the low efficiency, 7-14\%, compared to 1\textsuperscript{st} generation modules. Although, their flexibility makes them interesting for many application, such as a car roof.

**Third generation**

The 3\textsuperscript{rd} generation technology focuses on the implementation of (complex) multi-junction solar modules. In a multi-junction module, different semiconducting materials are used in layers, from the one with the lowest energy band-gap (bottom cell) to the one with the highest band-gap, each absorbing a different part of the solar spectrum \[47\]. This way the thermal losses, due to non-absorption, can be diminished and higher efficiencies can be reached. The currently available commercial tandem cells have an efficiency of 30\%, but the majority is still in the research phase.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Mono-Crystalline</th>
<th>Poly-Crystalline</th>
<th>Thin-Film</th>
<th>Multi-Junction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Generation</td>
<td>1\textsuperscript{st}</td>
<td>1\textsuperscript{st}</td>
<td>2\textsuperscript{nd}</td>
<td>3\textsuperscript{rd}</td>
</tr>
<tr>
<td>Efficiency</td>
<td>16-21%</td>
<td>15-17%</td>
<td>7-14%</td>
<td>30%</td>
</tr>
<tr>
<td>Temperature</td>
<td>-20°C to 70°C</td>
<td>-20°C to 70°C</td>
<td>-25°C to 90°C</td>
<td>-20°C to 70°C</td>
</tr>
<tr>
<td>Application</td>
<td>Residential</td>
<td>Residential</td>
<td>Building Integration</td>
<td>Research</td>
</tr>
</tbody>
</table>

\[2.2.\ \textbf{Electrochemical Energy}\]

This section explains the fundamentals of the conversion of electrical energy into electrochemical energy and the conversion back to usable electrical energy.

\[2.2.1.\ \textbf{Electrolysis}\]

**Fundamentals**

For the conversion of electricity into electrochemical energy the principle of electrolysis is applied. Electrolysis is a technique that uses direct current. The process of electrolysis is the exchange of atoms and ions by externally applying a voltage and an electric current to an electrolyzer. The simplest form of an electrolyzer has two parallel metal electrodes, an electrolyte, current collectors (not shown here) and a power source, see figure 2.5. Both electrodes are charged by applying an external voltage between the submerged electrodes. The potential has to be larger than the electrical potential difference of the metals. One of the electrodes is negatively charged (cathode) and the other positively (anode). Whether an electrode is positive or negative solely depends on the direction of the current flow determined by the poles of the power supply. The electrolyte contains both positively (cations) and negatively (anions) charged ions that carry the current. Crucial role of the electrolyte is to facilitate charge carrier transport. Now the negatively charged ions (anions) are attracted to the positive
electrode (anode) and are oxidized, while the positively charged ions (cations) are being reduced at the negative electrode (cathode). Both the reduction and oxidation process occurs at the same time and change the charged ions into neutral elements or molecules. The ionic charge transport through the electrolyte is compensated by electron transport via the external circuit. Electrolysis is often used as a method for creating new aqueous solutions, as a deposition method for metals from a solution, battery charging or to decompose a solution into gasses.

A well known principle of decomposition by electrolysis is the splitting of water into hydrogen and oxygen gas, also called water electrolysis. Electrolysis is a non-spontaneous process and thus requiring a minimum amount of energy (237.2 kJ/mol electricity and 48.6 kJ/mol heat) at the standard conditions of 1 bar and 25°C to dissociate water into hydrogen and oxygen molecules [51], as characterized by eq. 2.3. In water electrolysis, the electrolyte is a solution containing free positive and negative ions in an acidic or basic environment. The electrolytic process starts by applying an external voltage potential able to overcome the electrical potential between the electrodes to initiate the non-spontaneous process. In an acidic solution electric current enters the anode, decomposes the water molecule into oxygen gas, ionic charge carriers and free electrons. Electrons travel via the external circuit towards the cathode, while the acidic charge carriers travel via the electrolyte towards the cathode. At the cathode the charge carriers and the free electrons are recombined and hydrogen gas is formed.

$$2\text{H}_2\text{O}(l) + \text{Electricity} + \text{Heat} \rightarrow 2\text{H}_2(g) + \text{O}_2(g)$$  \hspace{1cm} (2.3)

Technologies
The different types of electrolyzers can be categorized based on the implemented electrolyte. There are electrolytes that are liquid solution and others are solid. Dependent of the type of electrolyte, a different charge carrier travels between the anode and the cathode. Subsequently, a different charge carrier means different half reactions, as can be seen in table 2.2, at the anode and cathode. Nevertheless, the overall net equation of electrolysis is equal to eq. 2.3 for all types. Three major types of electrolyzers are researched and applied in the industry, a Solid Oxide Electrolyzer Cell (SOEC), an Alkaline Electrolyzer Cell (AEC) and a Proton Exchange Membrane Electrolyzer Cell (PEMEC). Figure 2.6 and table 2.2 displays a quick overview of the three different fuel cell technologies.
**Solid Oxide Electrolyzer Cell**

Solid Oxide Electrolyzer Cell is also known as a Solid Oxide Regenerative Fuel Cell (SORFC). After all a SOEC is actually a Solid Oxide Fuel Cell (SOFC) running in regenerative mode. Theoretically speaking all types of fuel cells can be run in regenerative mode operating as an electrolyzer, but they are not designed that way. A SOFC is especially designed this way to be able to operate efficiently in electrolysis and fuel cell mode. The electrolyte of a SOEC is a solid ceramic zirconium oxide (ZrO$_2$) stabilised with yttrium oxide (Y$_2$O$_3$) with doubly ionized oxygen (O$^{2-}$) as the charge carrier. In electrolysis mode the charge carrier moves from the anode to the cathode and in fuel cell from the cathode to the anode, see figure 2.6 and table 2.2. The cathode is mostly made of a Nickel doped Yttria-stabilized zirconia (Ni-YSZ) or as the anode made of Perovskite-type lanthanum strontium manganese (LSM). Operating temperature range is about 800$^\circ$C to 1000$^\circ$C with efficiencies around 60%. Advantages of a SORFC is the capability of operating in both electrolysis and fuel cell mode and the high operating temperature removes the need for precious-metal catalyst and solid electrolyte. Disadvantages are the long start-up time, shutdown time and thermal expansion of components due to high temperature operation. Additional disadvantage is the requirement of a competent stabilized oxidation for ceramic solid electrolyte. At the moment SORFC are used in distributed generation, carbon dioxide recycling and on the Mars 2020 rover mission [52].

**Alkaline Electrolyzer Cell**

An alkaline electrolyzer contains a basic solution of potassium hydroxide (KOH) or sodium hydroxide (NaOH) and water. The solution KOH contains potassium ion (K$^+$) and hydroxide ion (OH$^-\$) and NaOH contains sodium ion (Na$^+$) and hydroxide ion (OH$^-\$). The charge carrier for an alkaline electrolyzer is the negative hydroxide ion (OH$^-\$) travelling via the electrolyte from the cathode to the anode, see figure 2.6 and table 2.2. In the electrolyte, there is a thin porous foil, referred to as diaphragm and made of Zirfon, that prevents electrons passing through and thus prevent short circuit. Electrodes are mainly composed of mild metals with the non-noble and cheap Nickel as a catalyst layer. Efficiency of an alkaline electrolyzer is 65-75%, the operating temperature range is 80$^\circ$C to 90$^\circ$C [53]. Advantages of an AEC is that it is a mature technology, cheap component cost due to non-noble Nickel metals and higher durability due to an exchangeable electrolyte. Disadvantages are low current density operation, relatively high operating temperature for residential use and low purity hydrogen produced compared to PEM electrolyzers. Alkaline electrolyzers are used in small stand-alone systems and large scale systems in combination with other chemical process. Also, often used in MW systems due to their relative low investment costs.

**Proton Exchange Membrane Electrolyzer Cell**

Electrolyte used in a Proton Exchange Membrane Fuel Cell (PEMFC) is a solid in the form of a thin permeable sheet of perfluorosulfonic acid (PFSA). The membrane has the ability to only allow positive ions, hydrons (H$^+$), pass through the membrane from the anode to the cathode, see figure 2.5 and table 2.2. The electrons are porous carbons containing a platinum catalyst on the cathode side and iridium on the anode side of the membrane. Efficiency is about 50-70% and the operating temperature range is 60$^\circ$C to 80$^\circ$C [54]. The low operating temperature decreases the startup time and enhances the system response. Furthermore, the solid electrolyte is crack and leakage resistant. Another advantages are higher current density handling, high pressure operations and higher purity of produced hydrogen. Disadvantages are the use of expensive platinum catalyst, low efficiency, high components cost, acidic environment and up-scaling. PEMEC are mostly used in grid-balancing management and stand-alone residential systems [55].
Table 2.2: Overview of three major electrolyzer technologies: Alkaline Electrolyzer Cell (AEC), Proton Exchange Membrane Cell (PEMEC) and Solid Oxide Electrolyzer Cell (SOEC) [53–57].

<table>
<thead>
<tr>
<th></th>
<th>AEC</th>
<th>PEMEC</th>
<th>SOEC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Anode Reaction</td>
<td>$4OH^- (aq) \rightarrow 2H_2O(l) + 4e^- + O_2(g)$</td>
<td>$2H_2O(l) \rightarrow O_2(g) + 4H^+ (aq) + 4e^-$</td>
<td>$2O^2^- (aq) \rightarrow O_2(g) + 4e^-$</td>
</tr>
<tr>
<td>Cathode Reaction</td>
<td>$4H_2O(l) + 4e^- \rightarrow 4OH^- (l) + 2H_2(g)$</td>
<td>$4H^+ (aq) + 4e^- \rightarrow 2H_2(g)$</td>
<td>$2H_2O(l) + 4e^- \rightarrow 2H_2(g) + 2O^2^- (aq)$</td>
</tr>
<tr>
<td>Charge Carrier</td>
<td>$OH^-$</td>
<td>$H^+$</td>
<td>$O^2-$</td>
</tr>
<tr>
<td>Electrolyte</td>
<td>Aqueous solution of KOH</td>
<td>Solid Nafion membrane</td>
<td>Solid Yttria stabilized zirconia</td>
</tr>
<tr>
<td>Operating Temperature Range</td>
<td>80°C to 90°C</td>
<td>60°C to 80°C</td>
<td>800°C to 1000°C</td>
</tr>
<tr>
<td>Efficiency</td>
<td>65-75%</td>
<td>50-70%</td>
<td>60%</td>
</tr>
<tr>
<td>Produced Hydrogen Purity</td>
<td>99.5-99.998%</td>
<td>99.9-99.9999%</td>
<td>99.9%</td>
</tr>
<tr>
<td>Stack size</td>
<td>1kW-100kW</td>
<td>5W-250kW</td>
<td>1kW-2MW</td>
</tr>
<tr>
<td>Stack lifetime</td>
<td>60000-90000 hour</td>
<td>20000-60000 hour</td>
<td>&lt;10000 hour</td>
</tr>
<tr>
<td>Initial Cost</td>
<td>1000-1200 €/kW</td>
<td>1860-2320 €/kW</td>
<td>&gt;2000 €/kW</td>
</tr>
<tr>
<td>Applications</td>
<td>Stand-alone systems, MW installation</td>
<td>Grid-balancing, Stand-alone systems</td>
<td>CO₂ recycling, Mars 2020 rover</td>
</tr>
</tbody>
</table>

Figure 2.6: Illustrative operation of an Alkaline Electrolyzer Cell, Proton Exchange Membrane Electrolyzer Cell and a Solid Oxide Electrolyzer Cell [58].
2.2.2. Fuel Cell Fundamentals

Converting electrochemical energy back to electricity requires a combustion device such as a fuel cell. Electrochemical reaction in a fuel cell is a spontaneous oxidation-reduction reaction and thus exothermic. Any type of combustible fuel can be used to release the chemical potential energy into usable direct current electricity for a load [59]. The structure of a fuel cell is similar to an electrolyzer accommodating two electrodes (anode and cathode) and an electrolyte as shown in 2.7. Similar to electrolysis, the oxidation takes place at the anode and the reduction at the cathode while the electrolyte functions as a carrier for the electrical positively charged ions between the electrodes. The fuel is inserted at the anode and through a catalyst it is oxidized into free electrons and free positive ions. Simultaneously, oxygen or another oxidizing agent is inserted at the cathode. An anode in favor of oxidization and a cathode in favor of reduction results in a difference of electron concentration between the two electrodes. This potential difference can be utilized as source voltage to power DC appliances. Free electrons travel externally to the cathode and deliver current to the load, while the positive ions travelling through the electrolyte are all recombined with the inserted air into water(vapor) and residual gasses. External electron flow from the anode to the cathode for this exothermic process correlates to a positive cathode and a negative anode. Analogous to the electrolysis process, the electrolyte has the key role to only permit charged ions between electrodes that do no disrupt the chemical reactions. Different kind of fuel cells exist in the industry, but the basic fundamentals explained so far are applicable for all of them. A more detailed overview of fuel cell technology can be found in [60].

The opposite of water electrolysis that consumes hydrogen and oxygen gas instead of producing is a hydrogen fuel cell. In such a cell hydrogen gas and oxygen gas are mixed and produce clean usable electricity of 237.2 kJ/mol for one mole of hydrogen with water(vapor) and heat 48.6 kJ/mol as byproducts at the standard conditions (1 bar and 25°C). Hydrogen gas enters the anode and is oxidized. This results in free electrons and positive ionized hydrogen atoms (protons). The electrons travel through the external circuit and provide current to the load while the protons move through the solid or liquid electrolyte in an acidic solution. At the cathode the oxygen is inserted and is reduced by the electrons that travelled externally and the protons into water molecules. The characteristic equation is given in eq. 2.4 and the generated heat is a useless byproduct unless somehow utilized within the system.
2.2. Electrochemical Energy

\[ 2H_2(g) + O_2(g) \rightarrow 2H_2O(l) + Electricity + Heat \]  

(2.4)

Technologies

Distinguishing between types of fuel cells is primarily determined by the employed electrolyte inside the cells. Electrolytes can be liquids, salts or solids. Each type of electrolyte allows different charge carriers to travel between the anode and cathode and thus different half reactions at the anode and cathode. The overall chemical reaction, as given in eq. 2.4, is equal for all types of fuel cells. Currently different types of fuel cells are being researched, developed and employed in the energy industry, e.g. Solid Oxide Fuel Cell (SOFC) explained in section 2.2.1, Molten Carbonate Fuel Cell (MCFC), Phosphoric Acid Fuel Cells (PAFC), Alkaline Fuel Cells (AFC), Proton Exchange Membrane Fuel Cell (PEMFC), Protonic ceramic fuel cells (PCFC) and Direct Methanol Fuel Cell (DMFC). Since this thesis focuses on stand-alone residential energy systems, only AFC and PEMFC will be explained in detail. These two types are mainly used in small scale systems, households and transport due to their low operating temperatures (60°C to 100°C) in contrast to SOFC (800-1000°C) and MCFC (600°C), clean “combustion” of pure hydrogen instead of hydrocarbons (in contrast to MCFC, SOFC and DMFC) and no use of liquid phosphoric acid damaging the environment (in contrast to PAFC) [62]. Figure 2.2.2 and table 2.3 display a quick overview of the three different fuel cell technologies currently being researched and developed.

Alkaline Fuel Cell

The electrolyte in AFC is similar to the liquid electrolyte of the Alkaline Electrolyzer Cell, namely a solution of water and potassium hydroxide (KOH). This is a basic environment where the charge carrier is the hydroxide ion (OH⁻) travelling from the cathode to the anode via the electrolyte, see figure 2.8a and table 2.3. Electrodes are porous metals such as platinum. Efficiency of an alkali fuel cell is about 60% and the operating temperature range is 70°C to 100°C for low temperature AFC and 100°C to 250°C for high temperature AFC [62, 63]. Because of the expensive platinum electrodes, high efficiency and high temperature range these are mostly used in Apollo missions and space shuttles to provide electricity and water [64]. The AFC with low temperature range is suitable for households due to fast startup time. Disadvantages are possible leakages of corrosive liquid electrolyte, expensive platinum, low current density, low dynamic operation and possible carbon dioxide poisoning if air is used instead of pure oxygen.

Proton Exchange Membrane Fuel Cell

Electrolyte used in a Proton Exchange Membrane Fuel Cell (PEMFC) is similar to the Proton Exchange Membrane Electrolyzer Cell. It is a solid in the form of a thin permeable sheet with the ability to only allow positive ions, hydrons (H⁺), pass through the membrane from the anode to the cathode, see figure 2.8b and table 2.3. The electrons are porous carbons containing a platinum catalyst on both sides of the membrane. Efficiency is about 40-50% and the operating temperature range is 60°C to 80 °C [62]. The low operating temperature enables short startup time, rapid system response and the solid, flexible electrolyte is crack and leakage resistant. These advantages makes them suitable for residential use, portable implementations and hydrogen cars [64]. Thin solid membrane and carbon electrodes facilitates high power density for low weight and volume compared to other fuel cell technologies. Disadvantages are the use of expensive platinum catalyst, low efficiency, high components cost, acidic environment and sensitivity to hydrogen fuel impurities that can cause carbon monoxide poisoning.
Table 2.3: Overview of applied fuel cell technologies: Alkaline Fuel Cell (AFC), Proton Exchange Membrane Fuel Cell (PEMFC) and Solid Oxide Fuel Cell (SOFC) [57, 62, 63, 65, 66].

<table>
<thead>
<tr>
<th></th>
<th>AFC</th>
<th>PEMFC</th>
<th>SOFC</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Anode Reaction</strong></td>
<td>$2H_2(g) + 4OH^-(aq) \rightarrow 4H_2O(l) + 4e^-$</td>
<td>$2H_2(g) \rightarrow 4H^+(aq) + 4e^-$</td>
<td>$2H_2(g) + 2O^2- - (aq) \rightarrow 2H_2O(l) + 4e^-$</td>
</tr>
<tr>
<td><strong>Cathode Reaction</strong></td>
<td>$O_2(g) + 2H_2O(l) + 4e^- \rightarrow 4OH^-(aq) + 4e^-$</td>
<td>$O_2(g) + 4H^+(aq) + 4e^- \rightarrow 2H_2O(l)$</td>
<td>$O_2(g) + 4e^- \rightarrow 2O^2- - (aq)$</td>
</tr>
<tr>
<td><strong>Charge Carrier</strong></td>
<td>$OH^-$</td>
<td>$H^+$</td>
<td>$O^2-$</td>
</tr>
<tr>
<td><strong>Electrolyte</strong></td>
<td>Aqueous solution of KOH</td>
<td>Solid Nafion membrane</td>
<td>Solid Yttria stabilized zirconia</td>
</tr>
<tr>
<td><strong>Operating Temperature Range</strong></td>
<td>25°C to 75°C, 100°C to 250°C</td>
<td>60°C to 80°C</td>
<td>800°C to 1000°C</td>
</tr>
<tr>
<td><strong>Efficiency</strong></td>
<td>40-70%</td>
<td>40-50%</td>
<td>60%</td>
</tr>
<tr>
<td><strong>Required Hydrogen Purity</strong></td>
<td>99.5-99.9998%</td>
<td>99.9-99.99999%</td>
<td>99.9</td>
</tr>
<tr>
<td><strong>Stack size</strong></td>
<td>1kW-100kW</td>
<td>5W-250kW</td>
<td>1kW-2MW</td>
</tr>
<tr>
<td><strong>Stack lifetime</strong></td>
<td>7000-100000 hour</td>
<td>20000-400000 hour</td>
<td>&lt;10000 hour</td>
</tr>
<tr>
<td><strong>Initial Cost</strong></td>
<td>1000-1200 €/kW</td>
<td>2300-4000 €/kW</td>
<td>1800-2300 €/kW</td>
</tr>
<tr>
<td><strong>Applications</strong></td>
<td>Military, Space, Portable</td>
<td>Transport, Stationary, Distribution</td>
<td>CO₂ recycling, Mars 2020 rover</td>
</tr>
</tbody>
</table>

Figure 2.8: Illustrative operation of (a) An Alkaline Fuel Cell (b) A Proton Exchange Membrane Fuel Cell (c) A Solid Oxide Fuel Cell [62].
2.3. Electrochemical Storage

In this subsection two methods of electrochemical storage are explained, namely electrochemical storage in a battery and electrochemical storage in the form of chemical hydrogen bond.

2.3.1. Battery

Fundamentals

The fundamental principle of a battery being charged is similar to an electrolyzer, whereas a battery being discharged is similar to a fuel cell, both with subtle differences. A battery is a direct current component similar to an electrolyzer and fuel cell. A major difference is the storage method of the electrical energy into electrochemical energy. In a battery, the energy is stored chemically inside the battery in the electrolyte and electrodes while an electrolyzer and fuel cell require external components for storing the produced and consumed hydrogen. Moreover, the capacity of a battery is limited by the electrodes and the electrolyte whereas an electrolyzer and fuel cell can operate infinitely as long as water or the products decomposed into (hydrogen and oxygen) are available. The principle of both the charging and discharging process of the battery is illustrated by figure 2.9.

\[
\text{Figure 2.9: Simple illustration of battery charging and discharging (Modified by author) [67].}
\]

Electrolytic Cell

Electrolytic process of battery charging consists of two dissimilar metallic electrodes and an acidic or basic electrolyte solution of solvents (positive and negative ions freely to move) and is also known as electrolytic cell. An externally applied voltage is required to overcome the electrical potential between the two metallic electrodes and forces the anode to reduce electrons. The positive ions (cations) are adopted by the negative ions (anions) present in the solution. Electrons travel externally and are oxidized with the positive ions of the other metallic electrode that are present in the solution and close to the cathode. This process, characterized by eq. 2.5, continues till the metallic layer on the anode is entirely consumed while a metallic layer is formed on the cathode resulting in a fully charged battery. The finite metallic materials in the solution and electrodes define the battery capacity. More detailed information on electrolytic cells can be found in [68, 69]

\[
M_1(s) + M_2^{2+}(aq) \rightarrow M_2(s) + M_1^{2+}(aq) \tag{2.5}
\]
Voltaic Cell
Discharging a battery is also known as a voltaic cell which is the opposite of an electrolytic cell and delivers the potential chemical energy in the form of electrical energy. The structure is similar and contains again two dissimilar metallic electrodes and an acidic or basic electrolyte. Connecting a load to the voltaic cell helps the metallic electrode with the most negative standard electrode reduction potential to be oxidized more easily and therefore acts as the anode. The less reactive metal attracts positive ions from the electrolyte. The electrons travel externally and power the load while the positive metal ions dissolved in the electrolyte travel to the cathode and are recombined there with the electrons. Discharging of the battery as characterized by eq. 2.6 continues till the metallic layer on the anode is entirely consumed while a metallic layer is formed on the cathode resulting in a fully discharged battery. The finite metallic materials in the solution and electrodes define the battery capacity. Only now the anode is negatively charged and the cathode positively. More detailed information on voltaic cells can be found in [68, 69]

\[ M_2(s) + M_2^{2+}(aq) \rightarrow M_1(s) + M_1^{2+}(aq) \]  

Technologies
Categorization of batteries can be done based on gravimetric and volumetric energy density. Figure 2.10 displays the established and emerging main battery technologies in the energy industry.

![Figure 2.10: Energy density of main battery technologies.](image)

In the category of established technologies the Lithium-ion (Li) battery is the one with the best gravimetric and volumetric energy density whereas Lead-Acid batteries have the worst energy capacities. Discussing all types of battery technology is out of the scope of this thesis. Instead, only lithium and lead-acid battery technology will be explained in detail because of the fact that both are well researched and adopted technologies on the market. For a stand-alone energy system the storage method is a crucial and cost essential part of the system and therefore a comparison between two majorly adopted battery technologies is essential. Implementation of lithium battery can lead to a more compact energy system whereas lead-acid can lead to a cheaper system [71]. Figures 2.11, 2.12 and table 2.4 display a quick overview of the two major battery technologies.
### Table 2.4: Overview of battery technologies: Lead-Acid Battery and Lithium Iron Phosphate Battery [2, 71, 72].

<table>
<thead>
<tr>
<th></th>
<th><strong>Lead-Acid</strong></th>
<th><strong>Lithium Iron Phosphate</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Overall</strong></td>
<td>(2\text{PbSO}_4(s) + 2\text{H}_2\text{O}(l) \rightarrow \text{Pb}(s) + \text{PbO}_2(s) + 4\text{H}^+(aq) + 2\text{SO}_4^{2-}(aq))</td>
<td>(\text{LiC}_6(s) + \text{CoO}_2(s) \leftrightarrow \text{C}_6(s) + \text{LiCoO}_2(s))</td>
</tr>
<tr>
<td><strong>Charging</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Anode Reaction</td>
<td>(\text{PbSO}_4(s) + 2\text{H}_2\text{O}(l) \rightarrow \text{PbO}_2(s) + \text{SO}_4^{2-}(aq) + 4\text{H}^+(aq) + 2\text{e}^-)</td>
<td>(x\text{FePO}_4 + (1-x)\text{LiFePO}_4 \rightarrow \text{LiFePO}_4 + x\text{Li}^+ + xe^-)</td>
</tr>
<tr>
<td>Cathode Reaction</td>
<td>(\text{PbSO}_4(s) + 2\text{e}^- \rightarrow \text{Pb}(s) + \text{SO}_4^{2-}(aq))</td>
<td>(6\text{C}(s) + \text{Li}^+(aq) + \text{e}^- \rightarrow \text{LiC}_6)</td>
</tr>
<tr>
<td><strong>Discharging</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Anode Reaction</td>
<td>(\text{Pb}(s) + \text{SO}_4^{2-}(aq) \rightarrow \text{PbSO}_4(s) + 2\text{e}^-)</td>
<td>(\text{LiC}_6(s) \rightarrow 6\text{C}(s) + \text{Li}^+(aq) + \text{e}^-)</td>
</tr>
<tr>
<td>Cathode Reaction</td>
<td>(\text{PbO}_2(s) + \text{SO}_4^{2-}(aq) + 4\text{H}^+(aq) + 2\text{e}^- \rightarrow \text{PbSO}_4(s) + 2\text{H}_2\text{O}(l))</td>
<td>(\text{FePO}_4 + x\text{Li}^+ + xe^- \rightarrow x\text{LiFePO}_4 + (1-x)\text{FePO}_4)</td>
</tr>
<tr>
<td><strong>Charge Carrier(s)</strong></td>
<td>(\text{SO}_4^{2-} &amp; \text{H}^+)</td>
<td>(\text{Li}^+)</td>
</tr>
<tr>
<td>Electrolyte</td>
<td>Aqueous solution of (\text{H}_2\text{SO}_4)</td>
<td>Liquid (\text{LiClO}_4) in an organic solvent</td>
</tr>
<tr>
<td>Gravimetric Energy Density</td>
<td>30-50 Wh/kg</td>
<td>90-110 Wh/kg</td>
</tr>
<tr>
<td>Volumetric Energy Density</td>
<td>60-110 Wh/l</td>
<td>250-693 Wh/l</td>
</tr>
<tr>
<td>Operating Temperature Range</td>
<td>-20°C to 60°C</td>
<td>0°C to 45°C</td>
</tr>
<tr>
<td>Charge/Discharge Efficiency</td>
<td>50-90%</td>
<td>80-90%</td>
</tr>
<tr>
<td>Lifetime cycles @ 80% DoD</td>
<td>300-500</td>
<td>1000-2000</td>
</tr>
<tr>
<td>Cost</td>
<td>0.3 €/kWh/cycle</td>
<td>0.7 €/kWh/cycle</td>
</tr>
<tr>
<td>Self-discharge per month</td>
<td>3-5%</td>
<td>5-10%</td>
</tr>
<tr>
<td>Depth of Discharge</td>
<td>50-80%</td>
<td>90-100%</td>
</tr>
<tr>
<td>Applications</td>
<td>Stand-alone systems, Gasoline Vehicle, Load levelling</td>
<td>Portable, Stationary, Load levelling, Electrical Vehicles</td>
</tr>
</tbody>
</table>
**Lead-Acid battery**

A Lead-Acid battery operates in an acidic environment. The electrolyte of a Lead-Acid battery is a diluted solution of sulfuric acid (H\(_2\)SO\(_4\)) containing sulfate ions (SO\(_{4}^{2-}\)) and hydrogen ions (H\(^+\)). The negative electrode is made of lead (Pb) and the positive electrode is made of lead dioxide (PbO\(_2\)). see figure 2.11 and table 2.4. A microporous membrane or absorbed glass mat (AGM) is used as a separator between the negative and positive electrode preventing possible short circuit.

![Figure 2.11: Illustration of the charging and discharging process of Lead-Acid battery [73].](image)

In a voltaic lead-acid cell, i.e. discharging, the lead electrode is the more negative standard electrode potential and thus is oxidized as the anode into free lead ions (Pb\(^{2+}\)) and electrons (e\(^-\)). The positive metal ions react with the negative sulfate ions (SO\(_{4}^{2-}\)) in the aqueous solution and stick as a precipitate of lead sulfate (PbSO\(_4\)) to the negative anode while the electrons travel via an external circuit to the cathode. At the positive cathode the lead dioxide (PbO\(_2\)) metal electrode, the free hydrogen ions (H\(^+\)), free sulfate ions (SO\(_{4}^{2-}\)) and the externally travelled electrons are reduced to lead sulfate (PbSO\(_4\)) and water. In an electrolytic cell, i.e. charging, the reverse process occurs. By applying a voltage potential, the positive electrode that initially contained lead dioxide is forced to oxidize the precipitate of lead sulfate into lead dioxide (PbO\(_2\)), free hydrogen ions (H\(^+\)), free sulfate ions (SO\(_{4}^{2-}\)) and electrons and thus acts as the anode. Once again the electrons travel externally and the ions via the electrolyte to be recombined at the negative cathode where the precipitate of the lead sulfate is reduced to lead (Pb) and sulfate ions (SO\(_{4}^{2-}\)).

Adoption of lead-acid batteries in the energy industry is primarily due to their low cycle cost of 0.3 €/kWh/cycle, being a well-known and mature technology, the possibility to deliver high current at an instant and a wide operating temperature range of -20°C to 60°C [72, 74]. This makes them applicable in cars but also in stationary systems at residential level where the cost is an important decision making variable. However, the low gravimetric and volumetric energy density (30-50 Wh/kg and 60-110 Wh/l respectively) along with the limited 50-80% Depth of Discharge (DoD), temperature and DoD dependence life cycle hinders them from being implemented in tied up spaces and portable applications. More disadvantages of lead-acid batteries are the maintenance every 3-6 months (levelling the acidic electrolyte) with a self-discharge rate of 3-5% a month and the impact of the acidic electrolyte on the environment upon disposal [2].
Electrochemical Storage

2.3. Lithium-ion battery

Similar to a lead-acid battery, contains a lithium-ion battery a positive and a negative electrode, an electrolyte and a Solid Electrolyte Interface (SEI) separator to only allow lithium ions to pass, see figure 2.12 and table 2.4. However, major difference between lead-acid and lithium-ion in terms of dynamical (dis)charging behavior is the change in electrode/electrolyte. In lead-acid batteries, the electrode concentration remains constant while the electrolyte concentrations changes whereas in lithium-ion batteries the opposite is true. The concentration change of electrodes in lithium-ion batteries is also known as insertion and extraction of lithium [75, 76]. In general, the negative electrode is made of lithium graphite (LiC₆) and the positive electrode can either be lithium cobalt oxide (LiCoO₂), lithium iron phosphate (LiFePO₄), lithium manganese oxide (LiMn₂O₄), lithium titanate oxide (Li₄Ti₅O₁₂), lithium nickel cobalt aluminium oxide (LiNiCoAlO₂) or lithium nickel manganese cobalt oxide (LiNiMnCoO₂) [76]. The electrolyte is a liquid solution of lithium salt in an organic solvent and there are many options like lithium hexafluorophosphate (LiPF₆), lithium hexafluoroarsenate monohydrate (LiAsF₆), lithium perchlorate (LiClO₄), lithium tetrafluoroborate (LiBF₄) and lithium triflate (LiCF₃SO₃) [77]. Selection between the types of positive electrode material and electrolyte strongly depends on the application of the lithium-ion battery. In stationary and portable applications majorly lithium iron phosphate batteries are with the lithium iron phosphate electrode material and a liquid electrolyte of lithium perchlorate in a ethylene carbonate–dimethyl carbonate (EC–DMC) organic solvent.

![Figure 2.12: Illustration of the charging and discharging process of a Lithium ion battery](image)

During discharge, the negative electrode acts as the anode and oxidizes the lithium graphite into graphite (C₆), lithium ions (Li⁺) and electrons. The positive ions travel via the electrolyte to the positive electrode (cathode) and the electrons move via an external circuit. At the cathode, the lithium ions are reduced into the lithium iron phosphate in combination with the electrons resulting in lithium iron phosphate. During the charge process, the positive electrode becomes the anode and is oxidized. Consequently the lithium ions are extracted from the lithium iron phosphate, resulting in free electrons to move externally. Simultaneously, the free lithium ions travel via the electrolyte to be reduced back to lithium graphite at the cathode.

The advantages of lithium-ion battery over lead-acid battery is the high gravimetric and volumetric density (90-110 Wh/kg and 250-693 Wh/l respectively) and the high Depth of Discharge (DoD) of 90-100% making them the best suitable established technology for portable systems like laptops, mobile
phones and electrical vehicles [2]. Lithium-ion battery is in contrast to a lead-acid battery maintenance free and thus another argument to be used in portable systems. Although the lithium-ion battery requires no maintenance, it has a high self-discharge rate of 5-10% a month and unfortunately, when charging, only operable above zero degrees, 0°C to 45°C [74]. On the other hand, these batteries are becoming more cost-effective and in combination with the environmental friendly components it is gradually growing in the stationary application. Although, with the current cost of 0.7 €/kWh/cycle (twice the price of lead-acid) it is still not largely adopted in many residential systems [2, 72]. One more disadvantage is the thin solid electrolyte interface separator that is becoming thinner to save cost and pack more energy, but resulting in high risk of ignition and possible explosion due to the flammable electrolyte.

2.3.2. Hydrogen

Fundamentals

The chemical compound of hydrogen is the lightest element of the periodic table and the most abundant element, primarily found in water, on earth. Compared to other known fuels it is carbon-free and adds a new level to the renewable energy industry when combined with renewable energy sources. Unfortunately, hydrogen does not exist as a primary energy source. Yet, it can be retrieved via many process like the aforementioned water electrolysis. The melting and boiling point of hydrogen are -259.2°C and -252.8°C respectively and thus is produced hydrogen via electrolysis at ambient conditions (1 bar, 25°C) a nontoxic, odourless, flammable and colourless gas with a low volumetric density of 0.0813 kg/m³ [79]. Specific energy of hydrogen is larger than the specific energy of all other fossil fuels, e.g. natural gas and methane have the highest specific energy of 55 MJ/kg while hydrogen has a specific energy density of 142 MJ/kg [3, 80]. Another advantage of hydrogen gas is the rapid diffusion into the atmosphere compared to to methane and propane and thus is safer to use in case of any potential leakages in a large space. Yet, because of the wide flammability range of 4-75%, hydrogen is also easily ignited by a simple spark if mixed with air in a closed area [20]. Hydrogen seems promising to be adopted as an energy carrier because of the high energy density. To be adopted as a viable and safe storage medium, it requires superiority concerning the flammability and low volumetric density. Table 2.5 summarizes the properties of hydrogen and figure 2.13 displays the primitive phase diagram for hydrogen.

![Figure 2.13: Primitive phase diagram for hydrogen. Liquid hydrogen only exists between the solid line and the line from the triple point at 21.2 K (-252°C) and the critical point at 32 K (-241°C) [81].](image)
Table 2.5: Properties of Hydrogen molecule [3, 79, 82].

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Formula</td>
<td>H₂</td>
</tr>
<tr>
<td>Molar weight</td>
<td>2.016 g/mol</td>
</tr>
<tr>
<td>Gas density at 1 bar, 25°C</td>
<td>0.0813 kg/m³</td>
</tr>
<tr>
<td>Liquid density at 1 bar, -252.8°C</td>
<td>73.3 kg/m³</td>
</tr>
<tr>
<td>Solid density at 1 bar, -259.2°C</td>
<td>86.0 kg/m³</td>
</tr>
<tr>
<td>Melting point</td>
<td>-259.2°C</td>
</tr>
<tr>
<td>Boiling point</td>
<td>-252.8°C</td>
</tr>
<tr>
<td>Higher Heating Value</td>
<td>142 MJ/kg or 285.8 kJ/mol</td>
</tr>
<tr>
<td>Lower Heating Value</td>
<td>120 MJ/kg or 241.9 kJ/mol</td>
</tr>
</tbody>
</table>

Technologies
Section 2.2 discussed both the production and consumption of hydrogen as an electrochemical energy compound. In contrast to batteries, an external storage method is crucial for a safe and cost-effective hydrogen system. The low volumetric density of hydrogen presents challenges for storing it in a safe and cost-effective method. Hydrogen can be stored as a compressed gas in high pressure cylindrical tanks, as a liquid in dewars and tanks at -253°C, as metal hydrid in metal alloys like Lanthanum Nickel (LaNi₅), adsorbed as gaseous hydrogen in carbon nanotubes, bonded with microporous material like zeolites, microsphere storage consisting of hollow glass spheres, physisorption and other methods [83–86]. The three main technologies currently employed as a viable hydrogen storage are compressed gas storage, liquid storage and solid storage in metal hydrids, as summarized in table 2.6, and will be discussed in this subsection. Other methods are still inefficient, endure difficulties in process or are still in research phase.

Table 2.6: Overview of hydrogen storage methods: Compressed Gas Storage, Liquefied Storage and Metal Hydride Storage [85, 87–89].

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Compressed</th>
<th>Liquid</th>
<th>Metal Hydride (LaNi₅)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Storage Pressure</td>
<td>800 bar</td>
<td>1 bar</td>
<td>2 bar</td>
</tr>
<tr>
<td>Storage Temperature</td>
<td>25°C</td>
<td>-252.8°C to -259.2°C</td>
<td>25°C</td>
</tr>
<tr>
<td>Energy for storage</td>
<td>24 MJ/kg</td>
<td>57 MJ/kg</td>
<td>-</td>
</tr>
<tr>
<td>Energy for release</td>
<td>-</td>
<td>-</td>
<td>36 MJ/kg</td>
</tr>
<tr>
<td>Volumetric density</td>
<td>35 kg/m³</td>
<td>73 kg/m³</td>
<td>120 kg/m³</td>
</tr>
<tr>
<td>Gravimetric density</td>
<td>13 wt.%</td>
<td>100 wt.%</td>
<td>2 wt.%</td>
</tr>
<tr>
<td>Application</td>
<td>Vehicles, Refinery</td>
<td>Rocket fuel, Neutron cooling</td>
<td>Portable, Residential</td>
</tr>
</tbody>
</table>

Compressed Hydrogen Gas Storage
One of the most applied and mature technologies to store hydrogen is compressed hydrogen storage. Hydrogen gas can be stored in tanks by compressing the gas with a compressor at pressure levels of 200 bar and higher, corresponding to a volumetric density of 15.2 kg/m³ and higher. This is done to overcome the issue with the low volumetric density of hydrogen at ambient conditions (0.0813 kg/m³). High pressure stored hydrogen gas has the advantage of being a mature technology and a cost-effective
storage method in applications with limited space. Compressed storage in tanks is also resistant to possible impurities of the stored hydrogen gas. Disadvantages are the cost increasing compressor and high pressure endurance tanks that are required, embrittlement of cylinder material during the charge/discharge cycles and potential gas explosion due to leakages in a closed area. Another limitation of this method is the required compression energy at the expenses of not being able to deliver the load demand, especially in stand-alone energy systems. In fact, about 17% of the higher heating value of hydrogen combustion is required for compression up to 800 bar [87]. High pressure hydrogen tanks are currently adopted in hydrogen vehicles, hydrogen fueling stations and large scale chemical refineries [90, 91].

**Liquefied Hydrogen Storage**

Improving the low volumetric density of hydrogen can be achieved by storing hydrogen in a liquid state at 1 bar. Produced hydrogen gas by electrolysis is first pre-cooled and compressed at high pressure, then cooled down in a heat exchanger till cryogenic temperature of -252.8°C before undergoing an isenthalpic expansion. The required energy for liquefaction is about 40% of the higher heating value of hydrogen combustion [87]. At 1 bar and between -252.8°C and -259.2°C hydrogen is in a liquid state and can take advantage of the high volumetric density of 73.3 kg/m³ [79]. However, the additional heat exchanger to maintain hydrogen at cryogenic state and tanks to handle the extreme low temperatures (liquid hydrogen is highly flammable) add cost to the system. The energy required for the liquefaction at the expenses of providing the load demand and increase of system complexity are more drawbacks of this storage method. Currently liquid hydrogen is used as rocket fuel for rocketry applications, adopted storage method in hydrogen vehicles and also used for cooling down neutrons in neutron scattering studies [92].

**Metal Hydrides Hydrogen Storage**

Liquefied hydrogen and compressed gas hydrogen are physical storage methods. Storage of hydrogen as a solid is a chemical storage method. For this process the repulsive forces of hydrogen are reduced by interacting with metal alloys. An example is Lanthanum Nickel alloy (LaNiₓ) which is added as a powder in a storage tank. As the hydrogen gas flows into the tank, the Lanthanum Nickel metal alloy powder absorbs the hydrogen atoms atomically and results in stable metal hydrides. Metal hydrides are metal cations (M⁺) and one or more hydride anions (H⁻). During this charging process, the pressure in the tank increases and the heat is released from the tank to the environment. Retrieving the hydrogen gas back for usage requires external heat. As the temperature is increased (between 120°C and 200°C), the hydrogen gas is released from the hydride. The required energy for the release is about 25% of the higher heating value of hydrogen combustion [87]. The characteristic equation for the absorption/desorption process is [86]:

\[
M(s) + \frac{x}{2}H_2(g) \leftrightarrow MH_x(s) + \text{Heat} \tag{2.7}
\]

Metal hydrides require less volume compared to gaseous and liquid storage. The volumetric density of a lanthanum nickel metal hydride tank at 2 bar is comparable with a 1800 bar compressed hydrogen gas tank [93]. Also, the risk of accidental leakages and potential explosion is low since the hydrogen is atomically stored within the metal hydride and requires heat for release. Additionally, some metal hydrides are suitable for adsorption and desorption of hydrogen at ambient temperature and pressure which in turn is favorable for portable applications. On the other hand, the requirement of external heat sources induces to additional cost, to an increase of system complexity and possible limited load demand satisfactory. In addition, metal hydrids require high purity hydrogen. Impurities can potentially harm the adsorbance rate of the metal hydrid and therefore decrease the lifetime of the storage tank. The impurities being left behind fill up the spaces in the metal that first was occupied by the hydrogen atoms. Metal hydrids are mainly in the research phase but are gradually being implemented in hydrogen cars, hydrogen adsorption cryocoolers, portable metal hydride compressors and as a safe and reliable storage method in residential energy systems [85].
2.4. Concluding Remarks

The previous sections explained comprehensively the fundamentals behind the generation of electrical energy by PV modules, conversion of electrical energy to electrochemical energy by electrolysis, back conversion of electrochemical energy to electrical energy by fuel cell and the electrochemical storage methods of battery and chemical hydrogen. For the generation of electrical energy the following technologies were elaborately discussed in section 2.1, namely mono- and poly-crystalline (1<sup>st</sup> generation), thin-film (2<sup>nd</sup> generation) and multi-junctions (3<sup>rd</sup> generation). In the technology sector of converting electrical energy to electrochemical energy, the three major electrolyzer types were thoroughly discussed: (1) alkaline electrolyzer, (2) pem electrolyzer and (3) solid oxide electrolyzer. For the back conversion, only the alkaline fuel cell, pem fuel cell and the solid oxide regenerative fuel cell were described due to their low operating temperatures which makes them manageable for residential use. Short term storage in the form of battery can be done with either lead-acid or lithium-ion, since both are well researched and established technologies in the renewable energy industry. Long term storage in the form of hydrogen can be stored as compressed gas in tanks, as a liquid in dwars or atomically in metal hydrides. Considering the discussed fundamentals of each technology and their advantages, disadvantages and limitations regarding efficiencies, lifetime, price, availability and other reasons, suitable main components are adopted for the proposed stand-alone hybrid PV-Electrolyzer-Battery-FC energy system.

For the electricity generation, a mono-crystalline silicon module is used for this thesis research because it currently has the highest efficiency (16-21%) of the available commercial PV modules on the market.

For the production of hydrogen the alkaline electrolyzer is selected. Considering the current technologies, the alkaline electrolyzers are the most efficient (65-75%) type on the market. In addition, the large lifetime (60000-90000 hours) and the low cost (1000 €/kW) makes them advantageous for residential applications where the cost is an important decision variable. The lower produced hydrogen purity compared to PEM (99.5 vs 99.9%) can be neglected if the appropriate method of hydrogen storage is employed.

To convert electrochemical energy back to electricity, a PEM fuel cell is selected. Even though PEM fuel cell has a higher cost than alkaline electrolyzer and solid oxide electrolyzer, the lower operational temperature (60-80°C) and the availability of wide stack size in the range of 5W-250kW encourages the implementation particularly for typical households. Moreover, the stack lifetime (20000-40000 hours) and the fact that there is no chance of carbon dioxide poisoning makes PEM fuel cell favorable over alkaline and solid oxide fuel cells.

Selected battery technology for this thesis as a short term storage method is the lead-acid technology. Lead-acid battery is a mature technology and the ten times lower cost/cycle compared to lithium ion (0.3 €/kWh/cycle vs 0.7 €/kWh/cycle) encourages the adoption primarily for residential stand-alone energy systems where the system cost is still majorly the deciding variable. In addition, the wide temperature range (-20°C to 60 °C), with the ability to be operated at temperatures below zero, and a low self-discharge rate of 3-5% in reference to lithium-ion makes lead-acid favorable.

Selected hydrogen storage method is the mature and cost effective technology of compressed gas cylinders. Although the high pressure tanks have the drawback of being potentially unsafe for residential applications, it is a more efficient storage method compared to liquid and metal hydrides. With just 20% of the lower heating value of hydrogen combustion lost due to this storage method. Being a mature technology, one can assume that current materials used for the tanks can better withstand high pressures (i.e. propane tanks in caravans) and prevent possible leakages and/or explosions. Installing a compressed gas tank in an open area can help the hydrogen easily escape into the atmosphere because of its volatility. Furthermore, the produced hydrogen by the alkaline electrolyzer is, with relatively low purity, a possible contaminant for the metal alloy powder and decrease the lifetime of the tank.
Simulation Model

A simulation model of the proposed stand-alone hybrid PV-Electrolyzer-Battery-FC energy system is designed for behavioural study. First, the used simulation environment for the development of the model is described in section 3.1. Followed by an elaborated and detailed mathematical modelling of the (main) components that are essential for the proposed hybrid energy system in section 3.2. Subsequently, in section 3.3, a schematic overview of the entire simulation model is displayed and the different operation modes of the hybrid energy system are described. Lastly, the economical point of view, based on the Levelized Cost Of Energy, is described in section 3.4.

3.1. TRNSYS Software

The TRNSYS software, with the logo shown in figure 3.1, stands for Transient System Simulation Tool.

![TRNSYS Logo](Image)

The software is developed at the University of Wisconsin and the coding languages used within the software are C++ and Fortran alongside a standard library of approximately 150 component models [94]. Standard models of the components enforce the “black box” component approach of TRNSYS. This implies that the output of a certain component is sent to the input of another component (at each selected timestep). Also known as the successive substitution method solving. This way a transient successive substitution can be done without detailed knowledge of the components in case the main goal of the simulation study is the behaviour of the entire system rather than component base. Additionally, for the more experienced users, the component models can be modified such that not only it complies with the studied system but also to eliminate the “black box” approach if desired. For this master thesis research the TRNSYS17 version is used. Some standard library components are modified to fit the available components in the Photovoltaic Materials and Devices (PVMD) group, while others are developed by the author of this thesis especially for this study. The used timestep (Δt) during the simulations/optimizations, for this study, is 0.1 hour.

3.2. Technical Modelling

In the following section the technical modelling of the implemented components will be explained in detail. The rated power or flow of each component discussed in this section is intentionally undefined except for the PV module. This is done to prevent undesired constraints for the optimization process.
Furthermore, the thermal models of the mono-crystalline PV module, alkaline electrolyzer and PEM fuel cell are taken into account for this study and can be found in respectively appendix A.1, B and C.

3.2.1. Mini DC-grid
For a stand-alone energy system containing a variety of components that operate at different voltage levels, an internal mini grid is essential. The mini DC grid modelled for this system operates at 48V. The mini grid is used to extract energy from and supply energy to the system components in times of deficit and surplus energy. It receives the generated electricity by the PV array, generated energy by the fuel cell and the delivered energy from the battery bank and delivers energy to the battery bank, to the electrolyzer, DC-AC inverter and other required auxiliary components.

3.2.2. Meteorological Data
The weather condition of any location varies throughout the entire year. Fortunately, there are many weather stations that gather this information for future predictions and/or modelling. This chunk of data is also called the meteorological data. These data files contain many parameters that influence the weather conditions, but the noteworthy parameters in the solar energy sector are solar and terrestrial radiation, wind speed, air/ambient temperature and ambient/air humidity [95]. The main parameter for calculating the performance of a PV module is the incident irradiance received by the plane of array (POA) as a function of time. The POA irradiance is calculated by taking into account; position of the Sun, ground reflectivity, array orientation and irradiance components. The POA consist of three parts, namely beam radiation, sky diffuse radiation and ground reflected radiation, see eq. 3.1. Ground reflected irradiance is calculated as a function of the irradiance received on the ground, the reflectivity coefficient (also known as albedo coefficient) and the tilt angle of the surface. Beam irradiance is a function of the direct normal irradiance on the surface corrected for the angle between the Sun’s rays and tilted surface (known as angle of incidence, AOI). In contrast to beam and ground component of the irradiance, different approaches exist for calculating the diffuse irradiance component. The most comprehensive approach is the Perez Sky Diffuse Model. Perez expands the diffuse irradiance model of Hay & Davies [96, 97], containing solar irradiance on surface from sky dome ($G_{Dome}$) and solar irradiance on surface from circumsolar region ($G_{Circumsolar}$), by introducing a third component, the solar irradiance on surface from sky horizon ($G_{Horizon}$) as given by eq. 3.2 [98].

$$G_{POA} = G_{Beam} + G_{Diffuse} + G_{Ground}$$

where:

- $G_{POA}$, plane of array irradiance
- $G_{Beam}$, beam irradiance
- $G_{Diffuse}$, sky diffuse irradiance
- $G_{Ground}$, ground reflective irradiance

$$G_{Diffuse} = G_{Circumsolar} + G_{Dome} + G_{Horizon}$$

The TRNSYS library has a wide ranged comprehensive set of worldwide meteorological data files. The data set is collected by Meteonorm in the periods 1981-1990 and 1991-2010 for global Solar radiation. Other meteorological parameters are collected in the periods 1961-1990 and 2000-2009 [99]. All data sets are averaged over the measured periods to be used for simulations. For this simulation model, the city of Vlissingen (one of the few Dutch locations in the library) in Zeeland is selected. Table 3.1 summarizes the parameters corresponding to the location and figure 3.2 displays the POA irradiance for an entire year for a tilted PV array fixed at the optimal azimuth and altitude for maximum power generation. The approach and determination of the optimal azimuth and altitude for maximum power generation over an entire year are explained in chapters 5 and 6.
Table 3.1: Parameters regarding the location of Vlissingen in The Netherlands [100, 101].

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Latitude</td>
<td>51.45°</td>
<td>(North being 0°)</td>
</tr>
<tr>
<td>Longitude</td>
<td>3.57°</td>
<td>(East being 0°)</td>
</tr>
<tr>
<td>Optimal Azimuth</td>
<td>0.7°</td>
<td>(South being 0° and East being -90°)</td>
</tr>
<tr>
<td>Optimal Altitude</td>
<td>37.8°</td>
<td>(Horizontal being 0° and positive towards the azimuth)</td>
</tr>
<tr>
<td>Albedo</td>
<td>0.7</td>
<td>snow</td>
</tr>
<tr>
<td>Albedo</td>
<td>0.2</td>
<td>no snow</td>
</tr>
</tbody>
</table>

Figure 3.2: Total incident irradiance received by the solar array for the location of Vlissingen.

3.2.3. Solar Panel

In this subsection, the modelling approach will be explained first and then empirically verified with an experimental measurement by illuminating a mono-crystalline PV module. The electrical model of the PV module is described in this subsection and the detailed temperature model of the PV module can be found in appendix A.1.

Modelling

Modelling a PV array requires a good understanding of the electrical performance. Subsection 2.1 explained the fundamentals of electricity generation by the absorption of photons. Also, a typical current-voltage curve of an illuminated silicon crystalline solar cell (similar for a module) was given in figure 2.4. In practical PV modules, the ratio between maximum power point ($P_{mpp}$) and the product of open circuit voltage ($V_{oc}$) and short circuit current ($I_{sc}$), also known as Fill Factor (FF), is strongly influenced by a series resistance, a shunt resistance and additional recombination in the p-n junction. The presented series and parallel resistors are responsible for internal dissipation in the cell [102]. In such cases, the behaviour of a solar cell is explained by an ideal two diode equivalent circuit model as shown in figure 3.3 and characterized by the current-voltage curve equation that describes the ideal diode behaviour of a PV module as follow:

$$I = I_L - I_D \left[ \exp \left( \frac{q}{V \cdot k_B \cdot (T_m + 273.15) \cdot n_s} \cdot (V + I \cdot R_s) \right) - 1 \right] - \frac{V + I \cdot R_s}{R_{sh}} \quad (3.3)$$
where:

- $I_\text{o}$, operating current
- $V_\text{o}$, operating voltage
- $I_L$, photo current generated
- $I_D$, dark diode current
- $q$, elementary charge
- $\gamma$, ideality factor diode corresponding to semiconductor material
- $n$, number of cells in series
- $R_s$, series resistance module
- $R_{sh}$, parallel resistance module
- $k_B$, Boltzmann’s constant
- $T_m$, module’s Temperature

The 5-parameter diode model is mainly selected to study the behaviour of amorphous and thin-film modules, where the slope of the current-voltage curve at the short circuit has a negative value. Therefore, by studying a crystalline silicon module, it is assumed that the opposite is true about the slope of the current-voltage curve at short circuit. Namely, that the slope is either positive or zero. This is justifiable approximation for crystalline modules and thus the 5-parameter diode model can be simplified to the 4-parameter diode model (refer to figure 3.4), where the $R_{sh}$ is infinitely large. For this study, the 4-parameter model introduced by Duffie & Beckman and validated by De Soto is adopted. The 4-parameter diode model circuit includes a current source, a diode and a resistor. The resistor represents the resistance of the current through the emitter and in the metal contacts.

To calculate the characteristic current-voltage curve, as defined by eq. 3.3 with $R_{sh}$ infinitely large, it is crucial to obtain the three unknown parameters of the 4-parameter equivalent circuit; $I_L$, $I_D$ and $R_s$. 
Doing so requires iterative solving of eq. 3.3 at the boundary conditions listed below by the Newton Raphson Method \([102]\) at Standard Test Conditions (STC). The STC values are normally given in the module's data sheet \((G_{m_{STC}} = 1000 \frac{W}{m^2}, T_{m_{STC}} = 25^\circ C)\), where \(\mu_{V_{oc}}\) is the temperature coefficient of the open circuit voltage.

- \(I = I_{sc_{STC}}, V = 0\), Short Circuit Current
- \(V = V_{oc_{STC}}, I = 0\), Open Circuit Voltage
- \(I = I_{mpp_{STC}}, V = V_{mpp_{STC}}\), Maximum Power Point
- The derivative with respect to the power at MPP is zero. \((\frac{\partial P}{\partial V})_{mpp}\)
- Temperature coefficient of the \(V_{oc}\) at Normal Operation Cell Temperature, \(\mu_{V_{oc_{NOCT}}} = \left(\frac{\partial V_{oc}}{\partial T_m}\right)\)

Regarding the found unknown parameters, the characteristic current-voltage curve of a PV module can be determined at Standard Test Conditions (STC). Nevertheless, the characteristic current-voltage curve of a PV module is strongly influenced by the environmental conditions, like the incident irradiance, ambient temperature, and wind speed. All these environmental conditions fluctuate throughout the day and season. The impact of these environmental conditions on the module’s temperature and thus performance (i.e. current-voltage and power-voltage curve) are elaborately explained in appendix A.1.

**Experimental**

In the solar industry the external parameters of a PV module are \(V_{oc}, I_{sc}, P_{mpp}, V_{mpp}\) and \(I_{mpp}\) and are determined by illumination of the PV module at STC \((G_{m_{STC}} = 1000 \frac{W}{m^2}, T_{m_{STC}} = 25^\circ C)\). For this thesis research, a practical mono-crystalline module is selected and fitted within the explained simulation model in the previous subsection. The purpose of doing so, to empirically verify the made assumptions regarding the 4-parameter ideal diode equivalent circuit model and also, to posses a more realistic solar model. To compare the experimental module parameters and the modeling module parameters, the practical PV module is illuminated by the available solar simulator (LASS) operated at Experimental Test Conditions of \(G_{m_{ETC}} = 970 \frac{W}{m^2}\) and \(T_{m_{ETC}} = 30^\circ C\). Unfortunately, the LASS is due to limitations not able to exactly meet the STC of industrial solar simulators. By illuminating the PV module, the external parameters are experimentally measured. Subsequently, this reference point is adopted for the explained modelling equations in the previous subsection and solved for the aforementioned boundary conditions in conjunction with the characteristic coefficients of the PV module tabulated in table 3.2. This way, the external parameters of the practical PV module on the basis of modelling and assumptions are determined. The external parameters, both experimentally measured and iterative determined by the simulation model, are tabulated in table 3.3. Also, the relative error, calculated according to eq. 3.4 is given in table 3.3. Characteristic current-voltage and power-voltage curve of both methods are plotted in figure 3.5.

\[
Error = \frac{|Value_{experiment} - Value_{model}|}{Value_{experiment}} \cdot 100\% \tag{3.4}
\]
Table 3.2: Characteristics SunForte PM096B00 Mono-Crystalline PV module at NOMT [37, 106].

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>NOMT</td>
<td>45°C</td>
<td>Normal Operating Module Temperature</td>
</tr>
<tr>
<td>$\mu_{oc}$</td>
<td>-0.26 %/°C</td>
<td>Temperature coefficient open circuit voltage</td>
</tr>
<tr>
<td>$\mu_{sc}$</td>
<td>0.05 %/°C</td>
<td>Temperature coefficient short circuit current</td>
</tr>
<tr>
<td>$\mu_{P_{mpp}}$</td>
<td>-0.33 %/°C</td>
<td>Temperature coefficient maximum power point</td>
</tr>
<tr>
<td>$\eta_m$</td>
<td>20.6%</td>
<td>Module efficiency</td>
</tr>
<tr>
<td>$A_{mod,: e}$</td>
<td>1.63 m²</td>
<td>Module surface</td>
</tr>
<tr>
<td>$n_s$</td>
<td>96</td>
<td>Number of cells in series</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>1.5</td>
<td>Ideality factor crystalline silicon</td>
</tr>
</tbody>
</table>

Table 3.3: External parameters SunForte PM096B00 335Wp Mono-Crystalline PV module at ECT ($g_{m,\: ETC} = 970 \: \frac{W}{m^2}$ and $T_{m,\: ETC} = 30°C$).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Experimental Value</th>
<th>Modelling Value</th>
<th>Relative Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_{mpp}$</td>
<td>328 W</td>
<td>327 W</td>
<td>0.31%</td>
</tr>
<tr>
<td>$V_{oc}$</td>
<td>64.2 V</td>
<td>64.2 V</td>
<td>0.32%</td>
</tr>
<tr>
<td>$I_{sc}$</td>
<td>6.66 A</td>
<td>6.67 A</td>
<td>0.15%</td>
</tr>
<tr>
<td>$V_{mpp}$</td>
<td>52.9 V</td>
<td>52.8 V</td>
<td>0.19%</td>
</tr>
<tr>
<td>$I_{mpp}$</td>
<td>6.19 A</td>
<td>6.20 A</td>
<td>0.17%</td>
</tr>
</tbody>
</table>

The small error margins can be imputed by the diode ideality factor ($\gamma$). The diode, and thus ideality factor, in the equivalent circuit represents a measure of the junction quantity and the type of the recombination. Although, for modelling purposes, the ideality factor is kept constant, it should be noted that this is not the case during experiments. This could explain the observed error margins reported in table 3.3.

![IV and PV curve](image)

Figure 3.5: Current-Voltage and Power-Voltage curves at ETC.

Studying the plotted characteristic current-voltage and power-voltage curves, the experimentally measured data and the algebraically determined external parameters, it can be concluded that the 4-parameter model is a valuable fitting method if an error margin of 0.31% at $P_{mpp}$ at Experimental Test Conditions (ETC) is acceptable. For the completeness of the study, the extrapolated current-voltage...
and power-voltage curves of the fitted PV module are algebraically determined for various irradiance and temperature levels, whereby the ETC as taken as the reference point, and given in appendix A.2. It should be noted that the current-voltage and power-voltage curves of a single PV module can simply be extrapolated to predict the performance of a PV array in a solar energy system. Furthermore, the power output of this module to the internal DC mini-grid is always equal to the maximum power point at that moment in time. Also, a constant efficiency of 87% is assumed due to the degradation rate at the end of 25 year lifetime [106]. From figure 3.6, it can be observed that the operating temperature of the module for the location of Vlissingen is mainly operating in the temperature range of 10-30°C during summer and in the range of 0-10°C during winter. This is below the typically rated NOMT of 45°C at an incident level of 800 W/m², wind speed of 1 m/s and an air temperature of 20°C. This can be explained due to the fact that, according to the Dutch weather institute KNMI, the ambient air temperature for Vlissingen is about 3-18°C throughout the year and the measured average wind speed is 6.1 m/s [107].

Figure 3.6: SunForte 335Wp PV module temperature for the location of Vlissingen.

Figure 3.7 displays the maximum power output of the fitted PV module for the location of Vlissingen oriented at an azimuth of 0.7° and an altitude of 37.8°. This orientation is the optimal orientation for maximum generation over an entire year for one single PV module. The approach and determination of the optimal azimuth and altitude for maximum power generation over an entire year are explained in chapters 5 and 6. Note that the number of PV modules is determined by the optimization process in this study.
3.2. Technical Modelling

3.2.4. Charge Controller

In the previous section, it is mathematically defined that the output of the PV model equals the maximum power point at that moment in time. The maximum available output power of the PV model is delivered to the internal DC mini-grid without a model of a MPPT charge controller. Instead of a MPPT charge controller, typically used in practice, the master controller (explained in 3.3.1), will act as a charge controller and energy manager for the energy flows throughout the system. Nevertheless, using a MPPT charge controller in practice for the incoming energy flow and tracking the maximum power point of the PV array corresponds to energy losses due to the inefficiency of the charge controller and needs to be taken into account. The efficiency of such a MPPT charge controller is defined by:

\[
\begin{align*}
    P_{out, mppt} &= P_{in, mppt} \cdot \eta_{mppt} \\
    \eta_{mppt} &= \frac{P_{out, mppt}}{P_{out, rated, mppt}} \cdot 100\% 
\end{align*}
\]  

(3.5a)  
(3.5b)

where:

- \(P_{out, mppt}\), mppt charge controller output power
- \(P_{in, mppt}\), mppt charge controller input power
- \(P_{out, rated, mppt}\), rated power mppt charge controller
- \(\eta_{mppt}\), efficiency mppt charge controller

These efficiency losses affect the generated energy by the PV array and thus the rest of the energy flow in the system. To account for the losses and prevent an undersized stand-alone hybrid energy system, an efficiency curve is implemented in the master controller, see figure 3.8. The efficiency curve is constructed by Müller et al. [108].

Figure 3.7: Generated power by SunForte 335Wp PV module for the location of Vlissingen.
## 3.2.5. Electrolyzer

The fundamental principle of an electrolyzer, as explained in chapter 2, can be extended by studying the involved fundamentals of thermodynamics and reaction kinetics. The thermodynamics of electrolysis, regarding the Gibbs free energy, the change in enthalpy and entropy are elaborately explained and can be found in appendix B.1. Thermal model of the adopted PHOEBUS alkaline electrolyzer is described in B.2.

### Reaction Kinetics

Electrolysis of liquid water at the thermoneutral voltage of 1.48V, correlative to the change in enthalpy (refer to eq. B.4 in appendix B.1), is the theoretical point that the single electrolyzer cell is 100% efficient and no waste heat is produced. Yet, in practical applications, the required cell voltage \( V_{\text{cell}_{\text{th}}} \) for electrolysis is higher than the thermoneutral voltage due to irreversibility. This irreversible term of voltage potential is caused by the ohmic overpotential \( V_{\text{ohm}} \), concentration overpotential \( V_{\text{con}} \) and the activation overpotential \( V_{\text{act}} \) according to:

\[
V_{\text{cell}_{\text{th}}} = V_{\text{in}} + \sum V_{rrv} \tag{3.6a}
\]

\[
V_{rrv} = V_{\text{ohm}} + V_{\text{con}} + V_{\text{act}} \tag{3.6b}
\]

The ohmic overpotential \( V_{\text{ohm}} \) is caused by the ohmic losses, such as the electrical resistance of the electrode, current collectors and interconnections. Additionally, the gas bubbles on the electrodes surface, ionic transfer in the electrolyte and the membrane resistivity contribute to the ohmic losses. Concentration overpotential \( V_{\text{con}} \) is caused by the limitations in the mass transport in the form of diffusion and convection. This limitation occurs in the interface between the electrodes and the electrolyte, since the concentration of the charge carriers change throughout the electrolysis [51]. The last term of the irreversible voltage is related to the activation energies of hydrogen and oxygen formation on the surface of the electrodes. At the electrodes, the ionic charge carriers have to overcome an energy barrier to go from the electrolyte to the electrodes and vice versa. This process highly depends on the catalytic properties of the anode and cathode and thus causes the activation overpotential \( V_{\text{act}} \). The higher practical cell voltage due to the overpotentials becomes apparent as waste heat and needs to be taken care of. Figure 3.9 shows the three overpotential terms involved in water electrolysis for processes at 25°C and 80°C.
3.2. Technical Modelling

The displayed current-voltage curve of the electrolyzer’s cell, see figure 3.9, displays the reversible and overpotential voltages as a function of current density. It can be observed that the activation overpotential is highly nonlinear and increases with a logarithmic tendency with increasing current density. Increasing the current density causes a linear increase of the ohmic overpotential and a parabolic increase of the concentration overpotential. Also, as mentioned earlier, increasing the temperature decreases the reversible voltage and as well the overpotentials, refer to figure 3.9. On the other hand, increasing pressure hardly effects the overpotentials as it also did not affect the reversible voltage in figure B.2 [110]. Note that a detailed understanding of the relation between current density and overpotentials is out of the scope of this research and thus is not discussed here. But more profound and elaborated information and equations can be found in [109, 111–113].

Efficiency

As expressed by eq. 3.6, the practical voltage of an electrolyzer cell is higher than the thermoneutral voltage due to irreversibility. This difference in voltage potentials defines the voltage efficiency of a single electrolyzer cell as given by equation 3.7a. If the electrolysis process follows the Faraday law of decomposition [114], the practical produced quantity of hydrogen is correlative to the theoretical possible quantity of hydrogen that can be produced based on the energy input. Thus, the Faraday efficiency, defined by eq. 3.7b, is 100%. Consequently, the electrolyzer efficiency, defined by eq. 3.7c, is equal to the voltage efficiency. Nonetheless, during the process of water electrolysis, several losses can occur resulting in a lower practical produced quantity of hydrogen compared to the theoretical maximum. For example, possible recombination of hydrogen and oxygen gas forming water in the presence of the catalytic materials in the electrodes, gas leakages to the surrounding or possible electrons at the anode leaking through the membrane towards the cathode (instead of travelling external and providing useful work). Taken into account the Faraday efficiency (eq. 3.7b), the electrolyzer efficiency becomes the product of the voltage and faraday efficiency:

\[
\eta_{\text{voltage}_{\text{ely}}} = \frac{V_{\text{tn}}}{V_{\text{cell}_{\text{ely}}}} \cdot 100\% \quad (3.7a)
\]

\[
\eta_{\text{faraday}} = \frac{V_{\text{H}_2,\text{practical}}}{V_{\text{H}_2,\text{theoretical}}} \cdot 100\% \quad (3.7b)
\]

\[
\eta_{\text{ely}} = \eta_{\text{voltage}_{\text{ely}}} \cdot \eta_{\text{faraday}} \quad (3.7c)
\]
where:

- $\eta_{\text{voltage,ely}}$, voltage efficiency electrolyzer
- $\eta_{\text{faraday}}$, faraday efficiency
- $\eta_{\text{ely}}$, electrolyzer efficiency
- $v_{H_2\text{practical}}$, practical quantity hydrogen
- $v_{H_2\text{theoretical}}$, theoretical quantity hydrogen

Another method for calculating the efficiency of the electrolyzer is the ratio between energy of the produced hydrogen and the provided power to the electrolyzer ($P_{\text{ely}}$):

$$\eta_{\text{ely}} = \frac{\phi_{\text{molar,}H_2} \cdot \text{HHV} \cdot 1000}{P_{\text{ely}}} \cdot 100\%$$  \hspace{1cm} (3.8)

where $\phi_{\text{molar,}H_2}$ is the molar flow of produced hydrogen and HHV is the higher heating value of hydrogen (285.8 kJ/mol). The molar flow rate of the produced hydrogen and oxygen ($\phi_{\text{molar,o2}}$) are directly proportional to the electrical current applied to the electrolyzer stack ($I_{\text{ely}}$):

$$\phi_{\text{molar,}H_2} = \frac{I_{\text{ely}} \cdot \eta_{\text{faraday}}}{Z \cdot F}$$  \hspace{1cm} (3.9a)

$$\phi_{\text{molar,o2}} = \frac{I_{\text{ely}} \cdot \eta_{\text{faraday}}}{2 \cdot Z \cdot F}$$  \hspace{1cm} (3.9b)

where the molar flow rate of hydrogen and oxygen is expressed in mass flow rate for consistency purposes:

$$\phi_{H_2} = \phi_{\text{molar,}H_2} \cdot M_{H_2}$$  \hspace{1cm} (3.10a)

$$\phi_{O_2} = \phi_{\text{molar,o2}} \cdot M_{O_2}$$  \hspace{1cm} (3.10b)

Note that the produced molar flow rate is given for a single electrolyzer cell. In the case of multiple cells connected in series in one single stack, the molar flow rate is simply multiplied by the number of cells ($n_e$). The same applies to the thermoneutral and reversible voltage of a single electrolyzer stack with multiple cells in series.

**Electrochemical Model Alkaline Electrolyzer**

The electrolyzer model selected for this research is the empirically verified model of the alkaline electrolyzer implemented in the PHOEBUS system by Meurer and Ulleberg [29, 115]. The alkaline electrolyzer model consists of a single stack with 21 cells in series, a cell area ($A_{\text{cell}}$) of 0.25 m$^2$, a maximum operating temperature ($T_{\text{ely}}$) of 80°C and a maximum allowable current density of 300 mA/cm$^2$ as tabulated in table 3.4. However, it should be noted that the maximum allowable current density and thus rated power of the PHOEBUS alkaline electrolyzer model is disregarded for this study. Instead, this is determined by the optimization process.

As aforementioned, the pressure plays a negligible role in the required cell voltage of an electrolyzer and thus only the temperature effect is considered. Ulleberg empirically defined the constants of the characteristic current-voltage curve of a single cell of the electrolyzer, expressed by eq. 3.6a, and presented the following:
\[ V_{\text{cell}_{\text{ely}}} = V_{\text{tn}} + \frac{r_1 + r_2 \cdot T_{\text{ely}}}{A_{\text{cell}}} \cdot I_{\text{ely}} + s_1 \cdot \log \left( \frac{t_1 + \frac{t_2}{T_{\text{ely}}} + \frac{t_3}{T_{\text{ely}}}}{A_{\text{cell}}} \right) + 1 \] (3.11)

where \( r_1 \) and \( r_2 \) are ohmic resistance coefficients and \( s_1, t_1, t_2, t_3 \) are the overvoltage coefficients on the electrodes. Table 3.4 tabulates the empirically derived coefficients by Ulleberg for the alkaline electrolyzer implemented in the PHOEBUS system. The corresponding characteristic current-voltage curve and voltaic efficiency of the single electrolyzer cell for different temperatures at 1 bar are given in figures 3.10 and 3.11.

Table 3.4: Characteristics and empirically derived coefficients by Ulleberg for the current-voltage curve of the PHOEBUS alkaline electrolyzer [29, 115].

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( r_1 )</td>
<td>8.05e-3 ( \Omega m^2 )</td>
<td>Ohmic resistance</td>
</tr>
<tr>
<td>( r_2 )</td>
<td>-2.50e-7 ( \Omega m^2/°C )</td>
<td>Ohmic resistance</td>
</tr>
<tr>
<td>( s_1 )</td>
<td>0.185 V</td>
<td>Overvoltage on electrodes</td>
</tr>
<tr>
<td>( t_1 )</td>
<td>-0.10 m²/A</td>
<td>Overvoltage on electrodes</td>
</tr>
<tr>
<td>( t_2 )</td>
<td>8.42 m²/°C/A</td>
<td>Overvoltage on electrodes</td>
</tr>
<tr>
<td>( t_3 )</td>
<td>247.27 m²/°C²/A</td>
<td>Overvoltage on electrodes</td>
</tr>
<tr>
<td>( A_{\text{cell}} )</td>
<td>0.25 m²</td>
<td>Electrode area</td>
</tr>
<tr>
<td>( T_{\text{ely}} )</td>
<td>80°C</td>
<td>Maximum electrolyzer temperature</td>
</tr>
<tr>
<td>( n_e )</td>
<td>21</td>
<td>Number of cells</td>
</tr>
</tbody>
</table>

Figure 3.10: Characteristic current-voltage curve of the alkaline electrolyzer model adopted in TRNSYS displayed for 25°C, 40°C, 60°C and 80°C at 1 bar.

The plotted characteristic current-voltage curve of the alkaline electrolyzer implemented in the PHOEBUS system (refer to figure 3.10), represents flawlessly the typical polarization curve of the overpotentials caused by the ohmic and activation losses in figure 3.9. The concentration losses are neglected by Ulleberg since these occur in higher current density regions than the studied alkaline electrolyzer allows.
Figure 3.11: Voltaic efficiency curve of the alkaline electrolyzer model adopted in TRNSYS displayed for 25°C, 40°C, 60°C and 80°C at 1 bar.

The faraday efficiency, expressed by eq. 3.7b, is empirically derived by Ulleberg for the PHOEBUS alkaline electrolyzer and plotted in figure 3.12. As mentioned earlier, the efficiency of the electrolyzer is defined as the product of voltaic and faraday efficiency and is plotted in figure 3.13.

$$\eta_{faraday} = \left( \frac{(I_{ely}/A_{cell})^2}{a_1 + (I_{ely}/A_{cell})^2} \right) \cdot a_2 \cdot 100\%$$  \hspace{1cm} (3.12)

Table 3.5: Empirically derived coefficients by Ulleberg for the faraday efficiency of the PHOEBUS alkaline electrolyzer for 25°C, 40°C, 60°C and 80°C at 1 bar. [115, 116].

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>$T_{ely} = 25^\circ C$</th>
<th>$T_{ely} = 40^\circ C$</th>
<th>$T_{ely} = 60^\circ C$</th>
<th>$T_{ely} = 80^\circ C$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_1$</td>
<td>112.5 $A^2/m^4$</td>
<td>150 $A^2/m^4$</td>
<td>200 $A^2/m^4$</td>
<td>250 $A^2/m^4$</td>
</tr>
<tr>
<td>$a_2$</td>
<td>0.975</td>
<td>0.970</td>
<td>0.965</td>
<td>0.960</td>
</tr>
</tbody>
</table>
Figure 3.12: Characteristic Faraday efficiency curve of the PHOEBUS alkaline electrolyzer model adopted in TRNSYS.

Figure 3.13: Electrolyzer efficiency curve of the alkaline electrolyzer model adopted in TRNSYS displayed for 25°C, 40°C, 60°C and 80°C at 1 bar.

**3.2.6. Fuel Cell**

The fundamental principle of a fuel cell, as explained in chapter 2, can be extended by studying the involved fundamentals of thermodynamics and reaction kinetics. The thermodynamics of electrolysis, regarding the Gibbs free energy, the change in enthalpy and entropy are described in appendix C.1. Thermal model of the adopted PEM fuel cell is given in C.2.

**Reaction Kinetics**

The maximum retrievable electrical energy of a fuel cell, if 100% efficient, is equal to the Gibbs free energy correlative to the reversible voltage of 1.23V at the standard conditions of 1 bar and 25°C (refer
to C.1. Yet, in practical applications, the operational output voltage \( (V_{\text{cell, FC}}) \) of a fuel cell is lower than the reversible voltage due to irreversibility. This irreversible term of voltage potential is caused by the ohmic overpotential \( (V_{\text{ohm}}) \), concentration overpotential \( (V_{\text{con}}) \) and the activation overpotential \( (V_{\text{act}}) \) according to:

\[
V_{\text{cell, FC}} = V_{\text{rev}} - \sum V_{\text{rrv}} \quad (3.13a)
\]
\[
V_{\text{rrv}} = V_{\text{ohm}} + V_{\text{con}} + V_{\text{act}} \quad (3.13b)
\]

The ohmic overpotential \( (V_{\text{ohm}}) \), the concentration overpotential \( (V_{\text{con}}) \) and the activation overpotential \( (V_{\text{act}}) \) causing losses occur both in an electrolyzer and in a fuel cell. In 3.2.5, a brief explanation about these losses is given and thus will not be repeated here again. Nevertheless, it should be noted that a detailed understanding of the losses due to the overpotentials is out of the scope of this research and thus is not discussed here. But more detailed information and equations can be found in [117–119].

The difference between the lower practical output voltage of the fuel cell and the reversible voltage is not converted to useful electrical energy but becomes apparent as waste heat and needs to be taken care of. Figure 3.14 shows the three overpotential terms involved in the “combustion” of hydrogen and oxygen for a single fuel cell.

![Polarization curve of the activation, ohmic and concentration losses defining the practical output voltage of a single fuel cell](image)

The displayed current-voltage curve of the fuel cell, see figure 3.14, displays the reversible and overpotential voltages as a function of current density. The polarization curve of the overpotentials shows that the activation overpotential is highly nonlinear and decreases with a logarithmic tendency with increasing current density. Increasing the current density causes a linear decrease of the ohmic overpotential and a parabolic decrease of the concentration overpotential.

**Efficiency**

As expressed by eq. 3.13, the practical output voltage of the fuel cell is lower than the thermoneutral and reversible voltage due to the ohmic, activation and concentration losses. This difference defines the voltage efficiency of a fuel cell with a single cell as displayed by eq. 3.14a. According to Faraday's
law \[114\], the theoretical minimum consumption rates of hydrogen and oxygen/air in a fuel cell is directly proportional to the transfer rate of electrons to the electrodes. The transfer rate is in turn equivalent to the electrical current in the external circuit. This corresponds to a stochiometric factor equal to one. However, in practical systems, to assure a complete “combustion”, excess hydrogen gas and oxygen are required resulting in a stochiometric factor smaller than one. Hence, the product of the stochiometric ratio of hydrogen ($\eta_{stoch_H_2}$) and the voltaic efficiency defines the fuel cell's efficiency by:

$$\eta_{voltage_{fc}} = \frac{V_{cell_{fc}}}{V_{tn}} \cdot 100\% \quad (3.14a)$$

$$\eta_{stoch_H_2} = \frac{v_{H_2_{theoretical}}}{v_{H_2_{practical}}} \cdot 100\% \quad (3.14b)$$

$$\eta_{stochO_2} = \frac{v_{O_{2_{theoretical}}}}{v_{O_{2_{practical}}}} \cdot 100\% \quad (3.14c)$$

$$\eta_{fc} = \eta_{voltage_{fc}} \cdot \eta_{stoch_H_2} \quad (3.14d)$$

Another method for calculating the efficiency of the fuel cell is the ratio between energy of the consumed hydrogen and the delivered power by the fuel cell ($P_{fc}$):

$$\eta_{fc} = \frac{P_{fc}}{\phi_{molar_{H_2}} \cdot HHV \cdot 1000} \cdot 100\% \quad (3.15)$$

where $\phi_{molar_{H_2}}$ is the molar flow of consumed hydrogen and HHV is the higher heating value. The molar flow rate of the consumed hydrogen and oxygen are directly proportional to the delivered electrical current by the fuel cell stack ($I_{fc}$):

$$\phi_{molar_{H_2}} = \frac{I_{fc}}{z \cdot F \cdot \eta_{stoch_H_2}} \quad (3.16a)$$

$$\phi_{molarO_2} = \frac{I_{fc}}{2 \cdot z \cdot F \cdot \eta_{stochO_2}} \quad (3.16b)$$

where the molar flow rate of hydrogen and oxygen can be expressed in mass flow rate for consistency purposes by the aforementioned eq. 3.10. Note, the consumed molar flow rate is given for a fuel cell with a single cell. In the case of multiple cells connected in series in one single stack, the molar flow rate is simply multiplied by the number of cells ($n_c$). The same applies to the thermoneutral and reversible voltage of a single fuel cell stack with multiple cells in series.

**Electrochemical Model PEM Fuel Cell**

As explained in 2.4, the selected fuel cell technology is a Proton Exchange Membrane fuel cell. Subsequently, for this research, the PEM fuel cell model studied by Amphlett et al. [120] is adopted. The single stack PEM fuel cell consists of 35 cells, an electrode area ($A_{pem}$) of 232 cm$^2$, a membrane thickness ($t_{emb}$) of 0.0118 cm and a temperature set point of maximum 80$^\circ$C, see table 3.6. Maximum rated power of this PEM fuel cell model is determined by the optimization process.
Table 3.6: Characteristics of the adopted PEM fuel cell model of Amphlett et al [120].

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_{pem}$</td>
<td>0.0232 m²</td>
<td>Fuel cell electrode area</td>
</tr>
<tr>
<td>$T_{fc}$</td>
<td>80°C</td>
<td>Maximum electrolyzer temperature</td>
</tr>
<tr>
<td>$\beta$</td>
<td>0</td>
<td>Well hydrated PEM</td>
</tr>
<tr>
<td>$\beta$</td>
<td>1.2</td>
<td>Water deficient PEM</td>
</tr>
<tr>
<td>$n_s$</td>
<td>35</td>
<td>Number of cells</td>
</tr>
<tr>
<td>$t_{memb}$</td>
<td>0.000118 m</td>
<td>PEM thickness</td>
</tr>
</tbody>
</table>

Amphlett defines the output voltage of the fuel cell by:

$$V_{cell_{fc}} = V_{rev} - V_{ohmic} - V_{act}$$  \tag{3.17}

where the reversible voltage can be calculated according to the expressed Nernst equation (eq. B.5), the voltaic ohmic losses, a measure of the IR losses associated with the proton conductivity of the solid polymer electrolyte and electronic internal resistances. These factors are empirically defined by Amphlett. The activation losses, due to the anode and cathode activation over-voltage, are based on theoretical equations from kinetic, thermodynamic and electrochemistry fundamentals. The mass transport losses are incorporated in each of the terms and are not derived separately. In a PEM fuel cell, the hydrogen and oxygen pressure levels are usually kept fairly constant and thus only the temperature variable is taken into account by Amphlett. The theoretically and empirically defined equations by Amphlett of the activation and ohmic overpotentials are given by:

$$V_{ohmic} = \left( \frac{I_{fc} \cdot t_{memb}}{A_{pem}} \right) \cdot \frac{8}{\exp \left[ 3.6 \cdot \left( \frac{T_{fc} + 273}{T_{fc} + 273} \right) \right]} \left[ 1 + \left( 1.64 \cdot \frac{I_{fc}}{A_{pem}} \right) + \left( \beta \cdot \left( \frac{I_{fc}}{A_{pem}} \right)^3 \right) \right]$$  \tag{3.18}

$$V_{act} = 0.95 - \left[ 0.00243 \cdot (T_{fc} + 273) \right] - \left[ 0.000192 \cdot (T_{fc} + 273) \cdot \ln(A_{pem}) \right] + \left[ 0.000192 \cdot (T_{fc} + 273) \cdot \ln(I_{fc}) \right] - \left[ 0.000076 \cdot (T_{fc} + 273) \cdot \ln(c_{o}) \right]$$  \tag{3.19}

The characteristic current-voltage curve and the correlative voltaic efficiency of the modelled PEM fuel cell by Amphlett et al. are plotted in figure 3.15. Voltage of the fuel cell is displayed by the right axis and the voltaic efficiency by the left axis.
3.2. Technical Modelling

As already mentioned, the characteristic current-voltage curve of the fuel cell is empirically and mechanistically determined by Amphlett et al. [120] and the mass transport causing the concentration overpotential is already incorporated in each of the activation and ohmic terms. That could explain the difference in the decreasing slope near the output voltage approaching zero compared to figure 3.14. Furthermore, the studied PEM fuel cell is operating in the lower current density range, whereas according to figure 3.14, the concentration losses occur in the high current density range.

The explained stochiometric efficiency of hydrogen and oxygen in equations 3.14b and 3.14c are not empirical determined in this model but are determined by the author. According to Ulleberg, in [121], typically an excess amount 15% for both gasses is used to assure a complete reaction. This results in a constant stochiometric efficiency ($\eta_{\text{stoch}}$) of 87% for both the hydrogen and oxygen inlet. Hence, the efficiency of the fuel cell is plotted as below.

![Figure 3.15: Characteristic current-voltage curve and correlative voltaic efficiency of the PEM fuel cell model adopted in TRNSYS displayed for 25°C, 40°C, 60°C and 80°C at 1 bar.](image)

![Figure 3.16: Fuel Cell efficiency curve of the PEM fuel cell model adopted in TRNSYS displayed for 25°C, 40°C, 60°C and 80°C at 1 bar.](image)
Thermal Model PEM Fuel Cell
The operating temperature of the fuel cell plays an important role in the operating voltage and efficiency of the fuel cell and is taken into account for the adopted PEM Fuel Cell model of Amphlett. The thermal model is elaborately explained in appendix C.2.

3.2.7. Battery
It has been explained, in section 2.3.1, that a battery is an electrochemical device used to store a surplus of energy or to provide energy in times of need on a short term base. Subsequently, the adoption of lead-acid battery for this study was briefly explained in 2.4. A battery endures, similar to an electrolyzer and a fuel cell (refer to 3.2.5 and 3.2.6), losses due to activation overpotential, concentration overpotential and ohmic overpotential. The charge curve of a typical battery is comparable with figure 3.9, whereas the discharge is comparable with figure 3.14. In the case of charging, a higher voltage is required to overcome the overpotentials and during discharge, the delivered voltage is lower than the steady-state voltage due to the overpotentials. The detailed relationship between voltage, current and internal resistance is out of the scope of this feasibility research study and therefore, the adopted lead-acid battery model here is based on a simple quasi-static energy model. Furthermore, the load is connected to the inverter, which in turn is connected to the internal mini 48VDC grid, instead of directly to the battery(bank). This diminishes the significance of the relation between the battery voltage and the delivered power to the load.

Electrical Model
The simplified quasi-static energy model for the lead-acid battery adopted in this study is proposed by Raszmann et al. [122]:

\[
E_{\text{batt}}(t) = E_{\text{batt}}(t-1) \pm [P_{\text{batt}}(t) \cdot \Delta t \cdot \eta_{\text{batt}}]
\] (3.20)

where:

- \(E_{\text{batt}}(t)\), energy capacity battery at time \(t\)
- \(E_{\text{batt}}(t-1)\), energy capacity battery at time \(t-1\)
- \(P_{\text{batt}}(t)\), Instantaneous power to or from battery at time \(t\)
- \(\Delta t\), timestep
- \(\eta_{\text{batt}}\), round-trip efficiency battery

Consequently, the State of Charge of the lead-acid battery can be calculated at any moment in time, where \(E_{\text{batt,rated}}\) is the rated energy capacity battery and \(SoC_{\text{batt}}(t)\) is the battery State of Charge at time \(t\), according to:

\[
SoC_{\text{batt}}(t) = \frac{E_{\text{batt}}(t)}{E_{\text{batt,rated}}} \cdot 100\%
\] (3.21)

Besides the simplified energy model, it is assumed that the self-discharge rate is negligible and a constant round-trip efficiency \((\eta_{\text{batt}})\) is assumed. The round-trip efficiency is, probably not a surprise, the product of the voltaic efficiency \((\eta_{\text{batt,volt}})\) and the coulombic efficiency \((\eta_{\text{batt,coul}})\):

\[
\eta_{\text{batt}} = \eta_{\text{batt,volt}} \cdot \eta_{\text{batt,coul}}
\] (3.22)

The voltaic efficiency is caused by the aforementioned overpotentials in both charging and discharging. The coulombic efficiency, is comparable with the faraday efficiency during charge and stochiometric efficiency during discharge. Coulombic efficiency describes the ratio of the total charge extracted from the battery related to the total charge put into the battery over a full cycle. These efficiencies, voltaic
and coulombic, are strongly influenced by the charge/discharge current rate (i.e. C-rate), the internal resistance of the battery and the SoC at that time.

Moreover, it is assumed that the charging and discharging characteristics are similar. A charge/discharge rate \( C_{rate} \) of 20\%, in terms of energy, of the initial battery energy capacity is typically suggested for lead-acid batteries to prolong their lifetime [123]. Another method to prolong the lifetime of a battery is to define the maximum and minimum available energy capacity of a battery. The modelled lead-acid battery encloses a maximum and minimum energy capacity battery (respectively \( E_{batt_{max}} \) and \( E_{batt_{min}} \)) determined by the maximum SoC and DoD:

\[
E_{batt_{max}} = SoC_{batt_{max}} \cdot E_{batt_{rated}} \\
E_{batt_{min}} = DoD_{batt_{max}} \cdot E_{batt_{rated}} = (1 - SoC_{batt_{max}}) \cdot E_{batt_{rated}}
\] (3.23a) (3.23b)

In table 3.7, the assumed characteristics of the developed lead-acid battery model are summarized. The voltage of the battery (bank) is defined as the voltage of the internal mini DC grid (48V DC) and the rated energy capacity battery \( E_{batt_{rated}} \) and the initial SoC \( SoC_{batt_{in}} \) are determined by the optimization process in this study.

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( V_{batt} )</td>
<td>48 V</td>
<td>Voltage battery (bank)</td>
</tr>
<tr>
<td>( \eta_{batt} )</td>
<td>78%</td>
<td>Battery efficiency</td>
</tr>
<tr>
<td>( SoC_{batt_{max}} )</td>
<td>100%</td>
<td>Maximum State of Charge</td>
</tr>
<tr>
<td>( DoD_{batt_{max}} )</td>
<td>20%</td>
<td>Maximum Depth of Discharge</td>
</tr>
<tr>
<td>( C_{rate} )</td>
<td>20%</td>
<td>Typical charge/discharge rate</td>
</tr>
</tbody>
</table>

**Thermal Model**

In general, the performance of a battery is strongly influenced by the operating temperature. Temperature decrease of only 5 degrees can lead to an energy capacity decrease of 5\% [123]. However, for simplicity the effect of temperature on this developed model is not taken into account. Therefore, this model is only valid for environments with relatively constant temperatures, like a garage or other indoor places.

### 3.2.8. DC-AC Inverter

PV modules generate DC power whereas majority of household appliances consume AC power. Thus, being able to deliver power to the appliances a DC-AC inverter is required. The AC output power of the inverter is reduced due to inefficiency of the inverter. The inefficiency is defined by the Partial Load Ratio (PLR), which is the ratio between the demanded power by the load and the rated power of the inverter as given by equations 3.24 and 3.25.

\[
P_{out_{AC}} = Pin_{DC} \cdot \eta_{inv}
\] (3.24)

\[
\eta_{inv} = \frac{P_{out_{AC}}}{P_{out_{rated}}} \cdot 100\% = f(PLR)
\] (3.25)
where:

- \( P_{out_{AC}} \), AC output power
- \( P_{in_{DC}} \), DC input power
- \( P_{rated} \), rated power inverter
- \( \eta_{inv} \), efficiency inverter

The inverter model for this research is developed by selecting an average inverter efficiency curve from literature rather than assuming a constant efficiency independent of the PLR. For a most accurate average efficiency curve of an inverter, the research of Aste et al. [125] is employed. Aste et al. investigated 29 inverters and plotted the inverter efficiency as a function of the PLR, see figure 3.17. The employed curve is digitized by OriginPro and curve fitted using the curve fitting tool of Matlab to establish an equation for the average efficiency curve of an inverter as a function of the PLR. Established equation is implemented into the simulation model and the inverter is used to convert the 48VDC power from the internal DC mini-grid to power both the AC household load demands and AC compressor. Selected rated power of the inverter is dependent of the peak demand that is determined by the studied load demands. These characteristics are tabulated in table 3.8. It should be noted that the established efficiency equation for this model is based on an average efficiency curve. In practice each type of inverter has a specific efficiency curve.

![Average efficiency curve inverter][125]

Table 3.8: Characterizations of the adopted DC-AC inverter model.

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( V_{in_{inv}} )</td>
<td>48 VDC</td>
<td>Input voltage inverter</td>
</tr>
<tr>
<td>( V_{out_{inv}} )</td>
<td>230 VAC</td>
<td>Output voltage inverter</td>
</tr>
<tr>
<td>( P_{rated} )</td>
<td>1000-6500 W</td>
<td>Rated inverter power</td>
</tr>
</tbody>
</table>
3.2.9. Compressor

The alkaline electrolyzer produces hydrogen at the ambient conditions of 1 bar and 25°C. Hydrogen gas at 1 bar has a low volumetric density (refer to table 2.5) and needs to be compressed before storage to save space. This requires the adoption of a compressor in this stand-alone hybrid PEBF system. The compressor is activated by the master controller for the case that the produced hydrogen by the electrolyzer needs to be stored. The compressor is an 230VAC appliance and thus is powered by the inverter as an extra AC load. As explained by Bhadori et al. [126], the required work for compression can either be isothermal, adiabatic or polytropic. In an isothermal process, if occurred slowly, there is no change in gas temperature. An adiabatic process has no heat gain or loss to its surrounding, if occurred rapidly, and a polytropic is a process somewhere between these two process [127]. In practice, most expansion and compression processes operate more according to a polytropic process and obey the pV^N = Constant thermodynamic process rather than isothermic or adiabatic [126]. In this study, the compressor model from the standard library of TRNSYS is adopted that is based on an ideal gas model in quasi-equilibrium compression process for an isothermic and adiabatic process.

But, to approach a more realistic behavior, the model is modified and operates according to polytropic compression. The required work for polytropic compression is defined by Bahadori et al.:

\[ P_{\text{comp}} = \frac{\phi_m}{\eta_{\text{poly}}} \cdot \left[ \frac{N \cdot R \cdot (T_{\text{in}} + 273)}{N - 1} \right] \cdot \left[ 1 - \frac{p_{\text{out}}^{(N-1)/N}}{p_{\text{in}}} \right] \]  
(3.26a)

\[ \eta_{\text{poly}} = \frac{\frac{N}{N-1}}{k_{\text{isen}}} \]  
(3.26b)

\[ k_{\text{isen}} = \frac{C_p}{C_v} \]  
(3.26c)

The produced heat due to polytropic compression is [126]:

\[ T_{\text{out}} = \left( T_{\text{in}} + 273 \right) \cdot \left[ \frac{p_{\text{out}}^{(N-1)/N}}{p_{\text{in}}} \right] - 273 \]  
(3.27a)

\[ Q_{\text{comp}} = \phi_m \cdot C_p \cdot (T_{\text{out}} - T_{\text{in}}) \]  
(3.27b)

where:

- \( P_{\text{comp}} \), required compressor power
- \( Q_{\text{comp}} \), produced heat by compression
- \( \eta_{\text{poly}} \), polytropic efficiency
- \( \phi_m \), mass flow
- \( N \), polytropic constant dependent of compressor type
- \( T_{\text{in}} \), input temperature gas
- \( T_{\text{out}} \), input temperature gas
- \( R \), ideal gas constant
- \( p_{\text{in}} \), input pressure gas
- \( p_{\text{out}} \), output pressure gas
- \( k_{\text{isen}} \), isentropic constant dependent of compressed gas
• $C_p$, specific heat ideal gas at constant pressure

• $C_v$, specific heat ideal gas at constant volume

It is assumed that there is no loss in mass flow and thus mass flow in is mass flow out. Isentropic exponent, $k_{isen}$, is gas dependent and is equal to 1.41 [127] for hydrogen gas at 25°C (e.g. air is 1.40) behaving as an ideal gas. The polytropic exponent is experimentally determined for a given type of compressor and ranges from 1.0-1.4 [127]. Since the polytropic exponent changes during the compression process, an average value of 1.2 is assumed for the simulation model in this study. This constant average value corresponds to a polytropic efficiency of 58% by solving eq. 3.26b. Characteristics of the compressor are tabulated in table 3.9.

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_{comp}$</td>
<td>230 VAC</td>
<td>Operating voltage</td>
</tr>
<tr>
<td>$\eta_{poly}$</td>
<td>58%</td>
<td>Overall pump efficiency</td>
</tr>
<tr>
<td>$N$</td>
<td>1.2</td>
<td>Polytropic exponent</td>
</tr>
<tr>
<td>$k_{isen}$</td>
<td>1.41</td>
<td>Isentropic exponent</td>
</tr>
</tbody>
</table>

The compression calculations are based on a single stage compression for simplicity. Yet in practice, multiple stage compression is required, especially for pressure ranges up to 800 bar (common for compressed hydrogen gas cylinders [81]). The output pressure is defined by the present hydrogen gas ($p_{gas}$) in the storage tank. External cooling is not required, since it is assumed that produced heat due to compression is easily lost to the environment.

### 3.2.10. Storage Tank

Compressed hydrogen gas is stored in a cylindrical storage tank. For the tank, the available model from the TRYSNS library is adopted that is developed by Goetzberger [128] and modified. In this model the hydrogen gas stored in the tank obeys the ideal gas law:

$$p_{gas} \cdot V_{gas} = n \cdot R \cdot T_{gas}$$ (3.28)

where:

• $p_{gas}$, pressure of the hydrogen gas in the tank

• $V_{gas}$, volume of the stored hydrogen gas

• $n$, number of moles of the hydrogen gas

• $R$, ideal gas constant

• $T_{gas}$, temperature of the hydrogen gas

The model simply performs a mass balance of the hydrogen gas entering the tank by the compressor, leaving the tank to the fuel cell and/or to the installed hydrogen vehicle and dumping if the tank is full. Remaining hydrogen gas in the tank defines the volume of the gas in the tank. So, the occupied tank level by the hydrogen gas is expressed by eq. 3.29. Furthermore, it is assumed that the inflow and outflow of the hydrogen gas occurs through an isothermal process.
\[
\phi_m(t) = \phi_{m_{in}}(t) - \phi_{m_{out}}(t) - \phi_{m_{dump}}(t) \tag{3.29a}
\]
\[
V_{gas}(t) = V_{gas}(t-1) \pm \left[ \frac{\phi_m(t)}{\rho_{H_2_{350bar,25^\circ C}}} \cdot \Delta t \right] \tag{3.29b}
\]
\[
SoC_{tank}(t) = \frac{V_{gas}(t)}{V_{tank}} \cdot 100\% \tag{3.29c}
\]

where:
- \( SoC_{tank}(t) \), state of Charge hydrogen tank at time \( t \)
- \( V_{gas}(t) \), volume of the stored hydrogen gas at time \( t \)
- \( V_{gas}(t-1) \), volume of the stored hydrogen gas at time \( t-1 \)
- \( \phi_{m_{in}}(t) \), mass flow in at time \( t \)
- \( \phi_{m_{out}}(t) \), mass flow out at time \( t \)
- \( \phi_{m_{dump}}(t) \), mass flow dumped at time \( t \)
- \( V_{tank} \), volume of the storage tank

In chapter 2, it is elaborately explained that it is possible to adopt pressures up to 800 bar [81] for compressed gas tanks to overcome the low volumetric density of hydrogen but it can result in potential safety issues. In this model of the storage tank, the maximum pressure (\( p_{tank} \)) is set to 350 bar to meet the middle path. This way, it can tackle the low volumetric density of hydrogen while maintaining the potential endangerment to a low level. The volume of the hydrogen storage tank (\( V_{tank} \)) and the initial SoC (\( SoC_{tank_{ini}} \)) are determined by the optimization process in this study.

Furthermore, it should be noted that in practice the pressure, temperature and volume of the gas are also influenced by the intermolecular attraction forces between the molecules instead of simply obeying the ideal gas law. Also, in practice, there could be possible losses due to the degradation of the tank caused by the unlimited charging and discharging of the tank. However, these aspects are neglected here.

### 3.2.11. Water Pump

A water pump is required in the system to pump both the cooling and demi-water throughout the entire system. The water pump is activated by the master controller at any time cooling water is needed for the fuel cell or cooling water and demi-water is required for the electrolyzer. Required power for pumping the cooling water and/or demineralized water through the system is calculated according to the following equations:

\[
P_{pump} = \frac{\phi_v \cdot \rho_{H_2O} \cdot \text{height} \cdot g}{\eta_{pump}} \tag{3.30}
\]

where:
- \( \phi_v \), volumetric flow
- \( \rho_{H_2O} \), density water
- \( \text{height} \), maximum height difference system installation
- \( g \), gravitational acceleration
- \( \eta_{pump} \), overall efficiency pump
The developed pump model here assumes a constant overall pump efficiency of 67% [129]. Additionally, for simplicity, a maximum height difference of two meters is assumed between the lowest and highest point of the potential system installation. Moreover, it is assumed that the produced heat, due to the inefficiency is caused by the friction between the fluid and the walls, is perfectly lost to the environment. Hence, there is temperature increase of the water. It is also assumed that the water pump operates at 12VDC and thus requires a buck converter to be powered by the 48VDC internal mini-grid.

3.2.12. DC-DC Converter
Each component implemented in this stand-alone hybrid PV-Electrolyzer-Battery-FC (PEBF) system operates at a different DC voltage. Therefore, several DC-DC converters are required for an operational energy system. There are two buck converters, one to convert the 48V DC power of the internal mini-grid to 12V DC power required by the water pump and another one for the conversion of the 48V DC power to the operating DC voltage power of the electrolyzer. Furthermore, a boost converter is used to convert the output DC voltage power of the fuel cell to 48V DC power of the internal mini-grid. For simplicity and not essential for this research, it is assumed that there is no current or power limitation for the converters and thus able to deliver the required power and current at any given time. However, it should be noted that in practical situations multiple converters are normally required in series and/or parallel to overcome the large voltage increase/decrease and the surpassing current. DC-DC converters have a constant efficiency of 91-97% [130] (type dependent), but here a constant efficiency of 94% is assumed for simplicity. The output power is calculated as follow:

\[ P_{\text{conv, out}} = P_{\text{conv, in}} \cdot \eta_{\text{conv}} \]  

(3.31)

where:
- \( P_{\text{conv, out}} \), dc output power
- \( P_{\text{conv, in}} \), dc input power
- \( \eta_{\text{conv}} \), efficiency converter

3.3. Overview Hybrid System
Up till now, the individual component models required for the simulation of the PV-Electrolyzer-Battery-FC system are described in detail. The theoretical models are mainly based on electrical, thermodynamics, electrochemical and transport phenomena. The PV module, electrolyzer and fuel cell are the most detailed among the major models and are based on empirical derived relationships determining their characteristic current-voltage curves. Figure 3.18 shows an overview of the detailed simulation model of the stand-alone hybrid PV-Electrolyzer-Battery-FC energy system.
3.3. Overview Hybrid System

The irradiation of the Sun received by the PV array is converted into usable power and the MPPT charge controller seeks to extract the maximum available power of the PV array. Consequently, the extracted solar power is either used to fulfill the load demand, to store on a short term base in a lead-acid battery or to store on a long term base in the form of hydrogen gas in a compressed cylindrical gas tank. For the long term storage, the potential excess solar power, together with demineralized water, is fed to the electrolyzer for the production of hydrogen gas. In times of need, the lead-acid battery and/or the fuel cell are used to fulfill the load demand. Overall, the energy management between the load demand(s) and the storage methods will be regulated by the master controller. The master controller, including the different operation modes for the energy management, is described in the next section.
3.3.1. Master Controller  

Energy strategy & management  

A controller for the power management is a necessary component in a complex and autonomous stand-alone energy system. The developed controller for this simulation model acts as the decider and divider of the energy flows throughout the system. Flowchart of the energy strategies is displayed in figure 3.19. The control strategy can operate either in operation mode 1, operation mode 2 or operation mode 3. In all three operation modes the maximum generated power by the PV array \( P_{\text{pv}} \) is extracted whenever solar radiation is available. The master controller, depending on the operation mode, determines the power to the load, the power to/from the battery, the power to the electrolyzer (producing hydrogen), the power from the fuel cell (consuming hydrogen) and the required power for the auxiliary components (e.g. compressor, water pump, converter). Once determined, the power to or from the energy sources are applied to the buck/boost converters and the inverter. For clarity purposes, the energy flow of the PV array enters the system and thus is positive, whereas the energy flow to the load leaves the system and thus is negative. All the other energy flows are all inside the system boundary. Furthermore, it is essential to recognize that \( P_{\text{tank}} \) is not defining the available energy present in the tank. Rather, in the case of filling the storage tank, it represents the consumed power by the electrolyzer and auxiliary components for hydrogen production and storage. In the case of emptying the storage tank (hydrogen “combustion”), \( P_{\text{tank}} \) represents the produced and delivered power by the fuel cell and auxiliary components to the system.

The green circle in the flow chart, named “Battery Management”, adds an additional condition for battery discharge. In times of need, the generated solar power is either not sufficient or not present at all for load fulfillment. Consequently, the required power is primarily extracted from the battery if the following two conditions are met: (1) a \( \text{SoC}_{\text{batt}} \) larger than 20% and (2) at any moment in time that the \( \text{SoC}_{\text{batt}} \) drops below 20%, the controller assures that the battery is first completely charged up to 100%, before it can be discharged again. By applying this extra constraint, it can be prevented that the battery gets stuck in a low energy capacity range, due to a repeatable \( \text{DoD}_{\text{batt}} \) of 80%, affecting the battery lifetime.

The purple colored power, named \( P_{\text{HV}} \), is the power demand of the hydrogen vehicle. The detailed correlation of the consumed hydrogen gas by the vehicle and energy in kWh is explained in chapter 5. \( P_{\text{HV}} \) is only larger than zero in the specific case study that a hydrogen vehicle is connected to the residential house as an extra load demand.
3.3. Overview Hybrid System

Figure 3.19: Flowchart of the energy strategy for the energy management of the stand-alone hybrid PV-Electrolyzer-Battery-FC energy system.
Operation Mode 1
In this operation mode, the generated power by the PV array \( P_{\text{pv}} \) is larger than the load demand \( P_{\text{load}} \), with the inverter efficiency taken into account \( P_{\text{net}} \), and results in a positive net result \( P_{\text{net}} > 0 \). Next, if the \( S\text{oC}_{\text{batt}} \) is below 100\%, the net power is directed towards the battery \( P_{\text{batt}} \) till a \( S\text{oC}_{\text{batt}} \) of 100\% is reached. Then, if there is still excess power \( P_{\text{exc}} > 0 \), the electrolyzer and auxiliary components (e.g. compressor, buck converter and water pump) are activated. Potential remaining power after reaching a hydrogen storage tank level of 100\% \( S\text{oC}_{\text{tank}} \) is dumped \( P_{\text{dump}} \). Note, possible excess power \( P_{\text{exc}} \) is directly sent to the electrolyzer and auxiliary components for hydrogen production or is immediately dumped if the \( S\text{oC}_{\text{tank}} \) is 100\%. Additionally, for the studied case of the hydrogen vehicle, the power demand of the hydrogen vehicle \( P_{\text{hv}} \) is also subtracted to determine the dumped power. The mathematical equations of this operation mode are:

\[
\begin{align*}
    P_{\text{load}} &= \frac{P_{\text{demand}}}{\eta_{\text{inv}}} \quad (3.32a) \\
    P_{\text{net}} &= P_{\text{pv}} - P_{\text{load}} \quad (3.32b) \\
    P_{\text{batt}} &= P_{\text{net}} \quad (3.32c) \\
    P_{\text{exc}} &= P_{\text{net}} - P_{\text{batt}} \quad (3.32d) \\
    P_{\text{aux}} &= P_{\text{pump}} + P_{\text{conv}} + P_{\text{comp}} \quad (3.32e) \\
    P_{\text{ely}} &= P_{\text{pv}} - P_{\text{load}} - P_{\text{batt}} - P_{\text{aux}} \quad (3.32f) \\
    P_{\text{tank}} &= P_{\text{ely}} + P_{\text{aux}} - P_{\text{hv}} \quad (3.32g) \\
    P_{\text{sys}} &= P_{\text{load}} + P_{\text{batt}} + P_{\text{tank}} \quad (3.32h) \\
    P_{\text{dump}} &= |P_{\text{exc}} - P_{\text{tank}}| \quad (3.32i)
\end{align*}
\]

Operation Mode 2
In this operation mode, the generated power by the PV array \( P_{\text{pv}} \) is not sufficient to provide for the load \( P_{\text{load}} \), and results in a negative net result \( P_{\text{net}} < 0 \). Next, if the \( S\text{oC}_{\text{batt}} \) is above 20\% and also meets the constraint of the “Battery Management”, the required net power is extracted from the battery \(-P_{\text{batt}} \). Then, if there is still a shortage of power \( P_{\text{short}} < 0 \), the fuel cell and the auxiliary components (e.g. compressor, boost converter and water pump) are activated and hydrogen is consumed till the load is completely provided or the hydrogen tank is empty. In the case that the \( S\text{oC}_{\text{tank}} \) is empty before the entire load is provided, the deficit power \( P_{\text{def}} \) is calculated. For the studied case of the hydrogen vehicle, the power demand of the hydrogen vehicle \( P_{\text{hv}} \) is also subtracted to determine the deficit power. The deficit power is taken as a positive value for the calculations. The mathematical equations of this operation mode are:

\[
\begin{align*}
    P_{\text{load}} &= \frac{P_{\text{demand}}}{\eta_{\text{inv}}} \quad (3.33a) \\
    P_{\text{net}} &= P_{\text{pv}} - P_{\text{load}} \quad (3.33b) \\
    P_{\text{batt}} &= P_{\text{net}} \quad (3.33c) \\
    P_{\text{short}} &= P_{\text{net}} - P_{\text{batt}} \quad (3.33d) \\
    P_{\text{aux}} &= P_{\text{pump}} + P_{\text{conv}} \quad (3.33e) \\
    P_{\text{fc}} &= P_{\text{load}} + P_{\text{batt}} - P_{\text{pv}} + P_{\text{aux}} \quad (3.33f) \\
    P_{\text{tank}} &= -P_{\text{fc}} - P_{\text{aux}} - P_{\text{hv}} \quad (3.33g) \\
    P_{\text{sys}} &= P_{\text{load}} + P_{\text{batt}} - P_{\text{tank}} \quad (3.33h) \\
    P_{\text{def}} &= |P_{\text{short}} - P_{\text{tank}}| \quad (3.33i)
\end{align*}
\]
Operation Mode 3
This operation mode is comparable to operation mode 2, but now there is no generated power by the PV array at all. The mathematical equations of this operation mode are:

\[ P_{pv} = 0 \] (3.34a)
\[ P_{load} = \frac{P_{demand}}{\eta_{inv}} \] (3.34b)
\[ P_{net} = -P_{load} \] (3.34c)
\[ P_{batt} = P_{net} \] (3.34d)
\[ P_{short} = P_{net} - P_{batt} \] (3.34e)
\[ P_{aux} = P_{pump} + P_{conv\_in} \] (3.34f)
\[ P_{fc} = P_{load} + P_{batt} - P_{pv} + P_{aux} \] (3.34g)
\[ P_{tank} = -P_{fc} - P_{aux} - P_{hv} \] (3.34h)
\[ P_{sys} = P_{load} - P_{batt} - P_{tank} \] (3.34i)
\[ P_{def} = |P_{short} - P_{tank}| \] (3.34j)

System Performance
For a profound understanding of the complex hybrid system, several parameters are discussed here. Such as the ratio of provided energy to the load by energy source (Solar, battery or fuel cell), the loss of load probability, the loss of energy and the overall system round-trip efficiency.

LLP & LOE
Studying the performance of a power system is usually measured in terms of reliability and energy loss indices. Most commonly used methods are the Loss of Load Probability (LLP) and the Loss Of Energy (LOE). The LLP can be defined as the overall probability that the load demand exceeds the available generated PV power and the energy capacity of the storage methods. On the other hand, the LOE is the share of energy that is dumped due to a load demand lower than the generated power by the PV array and/or a fully charged battery and hydrogen tank. Both parameters can be expressed in terms of days/year, hours/year or as a percentage of the energy demand.

The LLP is defined as the ratio between the sum of the deficit power \( P_{def} \) and the sum of the total demanded power \( P_{demand} + P_{aux} \) over a year period. Expressed both in hours/year and as a percentage of the total load demand:

\[ LLP = \sum_{j=1}^{8760} \frac{P_{def\_j} \cdot \Delta t_j}{(P_{demand\_j} + P_{aux\_j}) \cdot \Delta t_j} \cdot 100\% \] (3.35a)
\[ LLP\_h = \sum_{j=1}^{8760} \frac{\Delta t_j P_{def\_j}}{8760} \] (3.35b)

The LOE is defined as the ratio between the sum of the dumped power \( P_{dump} \) and the sum of the generated PV power \( P_{pv} \) over a year period. Expressed both in hours/year and as a percentage of
the total load demand:

\[
LOE = \sum_{j=1}^{j=8760} \frac{P_{\text{dump}} \cdot \Delta t_j}{P_{\text{PV}} \cdot \Delta t_j} \cdot 100\% 
\]  
(3.36a)

\[
LOE_h = \sum_{j=1}^{j=8760} \frac{\Delta t_{\text{f_dump}}}{8760} 
\]  
(3.36b)

**System Performance**

In general, the efficiency of a system is defined by the round-trip efficiency of the energy. The round-trip efficiency is commonly expressed as the product of the required components in series for the generation of energy, for the storage of energy and for the delivery of energy to the load. This method is a simplistic way of defining efficiency of an individual energy path taken to fulfill the load demand at that moment in time. However, this method is inaccurate, if at any moment in time, the load is provided by a combination of two individual energy paths. Therefore, a more accurate method of system efficiency is defined for the studied hybrid system. This method takes into account the total delivered energy to the system, the total generated energy by the PV array and the change in storage capacity of the battery and the hydrogen tank. The practical usable stored energy is the product of the stored capacity and the corresponding efficiency. The system efficiency over a year period can be defined as follow:

\[
\eta_{\text{sys}} = \frac{\sum_{j=1}^{j=8760} P_{\text{SYS}} \cdot \Delta t_j + [\Delta E_{\text{batt}} \cdot \eta_{\text{batt}}] + \left( \frac{\Delta V_{\text{tank}} \cdot \Delta V_{\text{HV}} \cdot P_{\text{hydr}} \cdot \eta_{\text{FC}}}{M_{\text{H}_2}} \right)}{A_{\text{module}} \cdot N_{\text{m}} \cdot \sum_{j=1}^{j=8760} G_{\text{POA}} \cdot \eta_{m_j} \cdot \Delta t_j} \cdot 100\% 
\]  
(3.37)

**Energy Source**

It can also be desirable to understand the performance of a hybrid system per individual energy path, like the PV array, battery bank and the combination of Electrolyzer-Tank-FC. The power delivered to the load by the PV array over a year period is \( P_{\text{PV}_{\text{load}}} \) and the correlative Solar To Load (STL) ratio is defined by:

\[
STL = \sum_{j=1}^{j=8760} \frac{P_{\text{PV}_{\text{load}}} \cdot \Delta t_j}{P_{\text{load}_j} \cdot \Delta t_j} \cdot 100\% 
\]  
(3.38)

The power delivered to the load by the battery bank as the short term storage method over a year period is \( P_{\text{batt}_{\text{load}}} \) and the correlative Battery To Load (BTL) ratio is defined by:

\[
BTL = \sum_{j=1}^{j=8760} \frac{P_{\text{batt}_{\text{load}}} \cdot \Delta t_j}{P_{\text{load}_j} \cdot \Delta t_j} \cdot 100\% 
\]  
(3.39)

The power delivered to the load by the combination of Electrolyzer-Tank-FC as a long term storage method over a year period is \( P_{\text{f}_{\text{load}}} \) and the correlative Fuel Cell To Load (FCTL) ratio is defined by:

\[
FCTL = \sum_{j=1}^{j=8760} \frac{P_{\text{f}_{\text{load}}} \cdot \Delta t_j}{P_{\text{load}_j} \cdot \Delta t_j} \cdot 100\% 
\]  
(3.40)
3.4. Economical Modelling

The economical developed model calculates the levelized cost of energy (LCOE) of the system per kWh provided to the system as follow:

\[
LCOE = \frac{\sum_{d=1}^{\text{d=y}} (I_{cd} + M_{cd} + R_{cd} + F_{cd})}{\sum_{d=1}^{\text{d=y}} \left( \frac{E_{sys}}{(1+r)^d} \right)}
\]

(3.41)

where:

- \( I_{cd} \), investment costs in year \( d \)
- \( M_{cd} \), maintenance costs in year \( d \)
- \( R_{cd} \), replacement costs in year \( d \)
- \( F_{cd} \), fuel costs in year \( d \)
- \( E_{sys} \), energy provided to system
- \( y \), project lifetime
- \( r \), discount rate
- \( d \), year

The total energy provided to the system \( (E_{sys}) \) and the total energy generated by the PV array \( (E_{pv}) \) over a year period are defined as follow:

\[
E_{sys} = \sum_{j=1}^{j=8760} P_{sysj} \cdot \Delta t_j
\]

(3.42a)

\[
E_{pv} = \sum_{j=1}^{j=8760} P_{pvj} \cdot \Delta t_j
\]

(3.42b)

Besides the LCOE per delivered kWh to the system, also the LCOE per generated kWh by the PV array is calculated by simply replacing \( E_{sys} \) in eq. 3.41 by \( E_{pv} \) determined by eq. 3.42b. Table 3.10 displays the economical parameters used for the analysis. In table 3.11, the current and future costs and the lifetime of PV modules, batteries, electrolyzer and fuel cell are given. Additionally, table 3.12 tabulates the investment cost, maintenance cost, replacement cost, fuel cost and lifetime of the other adopted components required for the proposed stand-alone hybrid PV-Electrolyzer-Battery-FC energy system. Investment cost is the first time purchase cost of the component, maintenance cost is a percentage of the investment cost as the reoccurring yearly maintenance. Replacement cost is dependent of the component’s lifetime that is either defined in calendar years (e.g. inverter, storage tank, MPPT), operational hours (e.g. electrolyzer, compressor), charge cycles (battery) or chemically worn out (drierite material). The fuel cost covers the cost of the used fluids and/or gasses. Lastly, an additional installation cost of 10% is assumed over the total system cost.
Table 3.10: Economical parameters. Exchanges rates are dated 03-12-2018.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lifetime project ($y$)</td>
<td>25 years</td>
</tr>
<tr>
<td>Discount rate ($r$)</td>
<td>7%</td>
</tr>
<tr>
<td>Installation rate</td>
<td>10%</td>
</tr>
<tr>
<td>Conversion GBP to EUR</td>
<td>1 : 1.12</td>
</tr>
<tr>
<td>Conversion USD to EUR</td>
<td>1 : 0.88</td>
</tr>
<tr>
<td>Conversion AUD to EUR</td>
<td>1 : 0.65</td>
</tr>
</tbody>
</table>

Table 3.11: Individual investment cost ($I_{c_d}$), maintenance cost ($M_{c_d}$), replacement cost ($R_{c_d}$) and lifetime of PV modules, lead-acid battery, Alkaline electrolyzer and PEM fuel cell in the year of 2020 and 2030. Maintenance and replacement cost are given as a percentage of the investment cost. (X) Assumed by author.

<table>
<thead>
<tr>
<th>Component</th>
<th>$I_{c_d}$</th>
<th>$M_{c_d}$</th>
<th>$R_{c_d}$</th>
<th>Lifetime</th>
</tr>
</thead>
<tbody>
<tr>
<td>PV Module</td>
<td>0.27 €/W$_p$ [131]</td>
<td>0.16 €/W$_p$ [132]</td>
<td>2.8% [133]</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>2020</td>
<td>2030</td>
<td>25 year [134]</td>
<td></td>
</tr>
<tr>
<td>Lead-Acid Battery</td>
<td>0.11 €/Wh [72]</td>
<td>0.07 €/Wh [135]</td>
<td>2% [136]</td>
<td>100% 5 year [137]/500 cycle [138]</td>
</tr>
<tr>
<td>Alkaline Electrolyzer</td>
<td>2.00 €/W [139]</td>
<td>0.70 €/W [65]</td>
<td>2.5% [140]</td>
<td>15% 10000 hour [X]</td>
</tr>
<tr>
<td>PEM Fuel Cell</td>
<td>4.00 €/W [141]</td>
<td>1.00 €/W [142]</td>
<td>2.5% [143]</td>
<td>15% 4000 hour [144]</td>
</tr>
</tbody>
</table>

Several notes about table 3.11 can be made. Current prices are based on the known market prices that are paid now days for kW system sizes, whereas future prices are mainly based on expected cost reduction due to large scale production and implementation according to experts. Lifetime of fuel cell is assumed to be shorter than general (>20000 refer to table 2.3) is the case. This is due the fact that in this study, the effect of accelerated startup-shutdown (occurring repeatedly) on the lifetime of the fuel cell is not taken into account. Therefore, a more conservative lifetime is assumed based on the study of Bae et al. \[144\]. The same argument applies for the assumed shorter lifetime of the alkaline electrolyzer rather than the given lifetime in table 2.2. Replacement period of the lead-acid battery is strongly influenced by the various case studies and thus is replaced either in 5 years or 500 charge cycles. Furthermore, replacement of a battery is performed by disposing the old ones and purchasing new ones. So, the replacement cost of batteries is 100% of the investment cost.
Table 3.12: Individual investment cost ($I_{C_d}$), maintenance cost ($M_{C_d}$), replacement cost ($R_{C_d}$), fuel cost ($F_{C_d}$) and lifetime of the remaining implemented system components and Electrical Vehicle (EV), Hydrogen Vehicle (HV) and Gasoline Vehicle (GV). Price natural gas and gasoline are for 2030 based on increase of oil and gas prices. Maintenance and replacement cost are given as a percentage of the investment cost. (X) Assumed by author.

<table>
<thead>
<tr>
<th>Component</th>
<th>$I_{C_d}$</th>
<th>$M_{C_d}$</th>
<th>$R_{C_d}$</th>
<th>$F_{C_d}$</th>
<th>Lifetime</th>
</tr>
</thead>
<tbody>
<tr>
<td>Charge Controller (MPPT)</td>
<td>0.17 €/W</td>
<td>2%</td>
<td>-</td>
<td>-</td>
<td>25 year [X]</td>
</tr>
<tr>
<td>Storage Tank</td>
<td>87.1 €/m³</td>
<td>1%</td>
<td>-</td>
<td>-</td>
<td>25 year [X]</td>
</tr>
<tr>
<td>AC Compressor</td>
<td>52.7 €/m³</td>
<td>5%</td>
<td>100%</td>
<td>-</td>
<td>40000 hour [149]</td>
</tr>
<tr>
<td>DC Water pump</td>
<td>31.5 €/m³</td>
<td>5%</td>
<td>100%</td>
<td>-</td>
<td>10000 hour [152]</td>
</tr>
<tr>
<td>DC-AC Inverter</td>
<td>0.48 €/W</td>
<td>4%</td>
<td>100%</td>
<td>-</td>
<td>10 year [155]</td>
</tr>
<tr>
<td>DC-DC Converter (3x)</td>
<td>0.18 €/W</td>
<td>-</td>
<td>100%</td>
<td>-</td>
<td>1500000 hour [157]</td>
</tr>
<tr>
<td>Gas Dryer (incl. drierite)</td>
<td>136.4 €/pc</td>
<td>-</td>
<td>8%</td>
<td>-</td>
<td>95 m³ (100% RH) [159]</td>
</tr>
<tr>
<td>AC Heat Pump Boiler</td>
<td>0.57 €/W</td>
<td>4%</td>
<td>100%</td>
<td>-</td>
<td>20 year [162]</td>
</tr>
<tr>
<td>HR Boiler</td>
<td>0.06 €/W</td>
<td>4%</td>
<td>100%</td>
<td>-</td>
<td>17 year [164]</td>
</tr>
<tr>
<td>Electrical Vehicle (Hyundai Ioniq)</td>
<td>29954 €/pc</td>
<td>-</td>
<td>100%</td>
<td>-</td>
<td>10 year [X]</td>
</tr>
<tr>
<td>Hydrogen Vehicle (Hyundai Nexo)</td>
<td>52224 €/pc</td>
<td>-</td>
<td>100%</td>
<td>-</td>
<td>10 year [X]</td>
</tr>
<tr>
<td>Gasoline Vehicle (Hyundai I40)</td>
<td>25754 €/pc</td>
<td>-</td>
<td>100%</td>
<td>-</td>
<td>10 year [X]</td>
</tr>
<tr>
<td>Hydrogen gas</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>12.3 €/kg [166]</td>
<td>-</td>
</tr>
<tr>
<td>DEMI-Water</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>437 €/m³ [167]</td>
<td>-</td>
</tr>
<tr>
<td>Cooling Water</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.95 (incl. taxes) €/m³ [168]</td>
<td>-</td>
</tr>
<tr>
<td>Natural Gas</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.12 €/kWh [169]</td>
<td>-</td>
</tr>
<tr>
<td>Gasoline</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>2.07 €/liter [170]</td>
<td>-</td>
</tr>
</tbody>
</table>
Several notes about table 3.12 can be made. The hydrogen dryer and drierite material are not explained and discussed in the previous technical modelling section. In the simulation model, it is assumed that the produced hydrogen is stored in the compressor without requiring drying to maintain the system complexity low. Yet in practice, a drying unit is required and thus, for the economical analysis, a simple hydrogen dryer with drierite is taken into account. Lifetime of a gas dryer unit (including drierite) is dependent of the absorption capacity of the drierite. Therefore, it is defined as the total volume of hydrogen gas that is fed to the dryer instead of hours or years. Furthermore, due to lack of proper information and for simplicity, all auxiliary components are replaced as an entire product instead of only some parts. Therefore, the replacement cost of the auxiliary components is 100% of the investment cost. Moreover, all fuels are purchased externally and thus are dependent of the current market prices except for the gasoline and natural gas. Both are only implemented in the case studies for the year 2030 and thus the expected future prices are assumed. The price of gasoline is based on the expected 75% price increase, in the year 2030, of crude oil [170] and is assumed to affect the production price of gasoline 1:1. The price of natural gas, in the year of 2030, is based on the announced tax increase of 75% by the Dutch government [169].
This chapter describes briefly the principle of numerical optimization methodology, explains the technical terms used in an optimization problem and clarifies the adopted optimization algorithms Particle Swarm Optimization and Hooke-Jeeves. Section 4.1 discuss the different optimization methods (i.e. intuitive, analytical and numerical) briefly, followed by the standard form of an optimization problem and the description of several numerical optimization methods available for this study. The reader, who is familiar with optimization problems in general and the technical terms, is kindly invited to skip forward to 4.2 for an elaborate explanation of the adopted optimization methods: Particle Swarm Optimization and Hooke-Jeeves. In the last section, section 4.3, is explained how to change a constraint optimization problem into an unconstrained optimization problem.

4.1. General Optimization Theory

Citing Gillet [171]: “The goal of the optimization problem is to find the maximum or minimum value of the objective function subject to the constraints”. Optimization can be done via an intuitive process, analytical or a numerical process. The selected approach depends on many factors, like the researcher’s knowledge regarding optimization techniques, if it is a single or multi dimensional optimization problem, the complexity of the system and the available computational resources. An intuitive approach is based on simplified calculations of the overall system and do not take into account the link between the different subsystems. This can possibly result in an over/under sized system. The analytical approach takes into account all the mathematical calculations and typically finds the exact solution for the optimization problem, but requires an enormous amount of time and effort. Optimization by a numerical approach takes into account all the mathematical calculations and links between the subsystems and attempts to find a good approximation of the solution instead of an exact solution. Today, the majority (over 60% [172]), of optimal system sizing in the renewable energy industry is based on the numerical approach. This is due to the higher accuracy (than intuitive approach) and the simplicity compared to the analytical approach. Potential drawback of the numerical method is the availability of computational power.

4.1.1. Optimization Theory

The standard form of an optimization problem can be described by an objective function, control variables, bound constraints and (in)equality constraints. The objective function determines the optimization problem and the control variables are varied to find the minimum of the objective function. The bound constraints define the domain of the control variables. Also, the inequality and equality constraints have to be met by the solution of the optimization problem. All potential solutions satisfying both the bound and (in)equality constraints set up a space of feasible solutions. The optimal solution exists within this defined space.
min \_x \ f(x) \quad \text{Objective function} \quad (4.1)

\text{s.t. } D_1 \leq x \leq D_2 \quad \text{Bound constraints} \quad (4.2)

h(x) = 0 \quad \text{Equality constraints} \quad (4.3)

g(x) \leq 0 \quad \text{Inequality constraints} \quad (4.4)

It should be noted that the optimization objective is defined as a minimization problem, but can also be approached as a maximization problem:

\max \_x \ f(x) = -\min \_x \ f(x) \quad (4.6)

4.1.2. Numerical Optimization Algorithms

When the complexity of a system increases or multiple criteria are crucial for an optimal system sizing, for example a stand-alone hybrid energy system, then the best optimization approach is numerical. Optimization of a complex stand-alone hybrid system requires a detailed mathematical model for each individual components (refer to chapter 3) and the application of suitable numerical optimization methods. A variety of suitable numerical optimization approaches are gradient free. Gradient free algorithms are typically implemented for optimization problems of systems with either no derivatives or the derivatives are difficult to obtained due to the complexity of the system. This could be the case for extensive hybrid energy systems and for systems whereby the function is discontinuous or discrete. The opposite, gradient based algorithms, attempt to find an optimum using the gradient of the objective function as the search direction. These gradient based algorithms are also known as analytical optimization. Generally speaking, the gradient free algorithms are preferred in hybrid energy systems due to the fact that difficult derivatives do not have to be obtained [173, 174]. However, the drawback is that it has a larger computational time compared to gradient based algorithms [172].

The suitable gradient free optimization algorithm for this study strongly depends on whether the optimization objective function is convex or non-convex. A convex function consists of one global minimum, whereas a non-convex function can have one global minimum or multiple minimums. With one being the global minimum and others the local minimums. Determining whether an objective function is convex or non-convex, can be done by a straightforward numerical method optimization with multiple starting points. Each starting point is a combination of the initial values of the various control variables. If different optimum is found dependent of the initial values, it can be said that the function is non-convex. In all other cases no definite conclusions can be made. As a preliminary assessment, the proposed stand-alone hybrid PV-Electrolyzer-Battery-FC energy system is optimized by the Hooke-Jeeves method. The objective function aims to find an optimal system size for a Loss of Load Probability \leq 1% for the lowest possible Levelized Cost Of Energy. The detailed optimization procedure, control variables and constraints are discussed in the next chapter. Adopting the Hooke-Jeeves optimization algorithm available within TRNSYS and varying the initial starting point, resulted in different found minima for the optimization problem. Therefore, it can be concluded that the objective function for this study is definitely not a convex function. Hence, to reduce the likelihood of getting stuck in a local minimum, it is favorable to solve the optimization problem with a multiple starting point algorithm.

TRNSYS has an optimization functionality, called TRNOPT, which is an implementation of the well-known Generic Optimization Program (GenOpt) within the TRNSYS environment. The Generic Optimization Program is developed by the Lawrence Berkeley National Laboratory and consists of various optimization algorithms for single- and multi-dimensional optimization [175]. Available optimization algorithms implemented in TRNOPT with multiple starting point are the Parametric Runs, PSO and PSO+Hooke-Jeeves. Parametric Runs searches the entire space of the feasible solutions, whereas PSO starts with multiple randomly defined points and thus is more efficient in finding an optimum. The method of PSO+Hooke-Jeeves starts with multiple starting points and therefore reduces the chance of getting stuck in a local minimum. Subsequently, the best found minimum by the PSO is adopted as the base point of the Hooke-Jeeves method. Then, the Hooke-Jeeves method performs a pattern
search, making it possible to find a better minimum than the found minimum, in the case that the found minimum by PSO was a local minimum.

### 4.2. Particle Swarm Optimization & Hooke-Jeeves Optimization

For this study, the hybrid optimization method of PSO+Hooke-Jeeves is adopted and both methods are described in this section.

#### 4.2.1. Particle Swarm Optimization

The Particle Swarm Optimization is introduced by Kennedy, Eberhart and Shi [176, 177] as a method for the optimization of continuous non-linear functions based on the behavior of a swarm of birds. The swarm of birds is on a quest for finding shelter, food or perhaps avoiding predators. To fulfill their quest, the birds share information within the swarm about their location and velocity. Processing the information, gathered by themselves and the swarm, helps them to reach their goal and thus fulfill their quest. The same principles apply to the schools of fish or any other herds of animals that operate together for reaching their goal.

PSO algorithm is adopted in computational science whereby a swarm of birds or schools of fish is called a set of particles. Similar to the individual birds/fishes, each particle has its own location and corresponding velocity. The following PSO explanations are mainly based on the papers of Kennedy and Eberhart [177] and Erdinc and Uzonoglu [173]. Erdinc and Uzonoglu describe the PSO algorithm according to the flowchart given in figure 4.1, by initially generating a random set of particles ($n_o$). Each particle represents a combination of the varied control variables. Additionally, each control variable can be adjusted according to the determined step size within its domain.

The generated set is then randomly scattered throughout the space which is defined by the bound constraint of the control variables. After the first "round" (called generation), the particles share information within the swarm about their current location and velocity. It should be noted that, all particles have a memory containing knowledge about their personal best location ($p_b$) and global best location ($p_g$) within the defined space. Subsequently, the velocity vector and location of each particle is updated for the next generation ($n_o$), according to eq. 4.7 (and visually represented in figure 4.3), by taking into account the shared information and memory of the particles. This iterative process is repeated till the particles converge towards the best solution (i.e. optimum) of the optimization problem.
Particles can share information within the swarm to the other particles by using one of the three neighborhood topology: (1) lbest, (2) gbest and (3) VonNeumann, see figure 4.2. In the lbest topology, each of the particles communicates with only two of it's neighbours. The gbest topology communicates with all other particles present in the defined space and the VonNeumann communicates with the closest four particles in the North, East, South and West. For the PSO, the VonNeumann topology is selected based on the conclusions of Mendens and Wetter. Mendes [178] studied the "Population Structure and Particle Swarm Performance" by applying all three topology and concluded that the VonNeumann topology performs the best. Also, Wetter describes the possibility that gbest topology tends to get stuck in a local minimum.
Mathematical equations for updating the velocity and location vector of each particle and a visual schematic of the equations are respectively given by eq. 4.7 and figure 4.3 for clarity. The cognitive acceleration of the particle ($c_1 \rho_1$) and the social acceleration of the swarm ($c_2 \rho_2$) are uniformly distributed random numbers between 0 and 1 [180] and the effect of these variables on the movement of a particle and thus affecting the search for the optimum is out of the scope of this research.

$$v_i(k + 1) = v_i(k) + c_1 \cdot \rho_1(k) \cdot (p_{b_i}(k) - x_i(k)) + c_2 \cdot \rho_2(k) \cdot (p_{g_i}(k) - x_i(k)) \quad (4.7a)$$
$$x_i(k + 1) = x_i(k) + v_i(k + 1) \quad (4.7b)$$

where:
- $i$, is the particle
- $k$, is the generation
- $c_1 \rho_1$, the cognitive acceleration of the particle itself
- $c_2 \rho_2$, the social acceleration of the swarm
- $p_{b_i}$, personal best position of the particle
- $p_{g_i}$, global best position of the particle
- $x_i$, location of the $i^{th}$ particle
- $v_i$, velocity of the $i^{th}$ particle
Figure 4.3: Illustration of the velocity and location updates in Particle Swarm Optimization [181].

Figure 4.4 displays a contour plot of the Particle Swarm Optimization, with almost all particles converged towards the optimum solution of the objective function: "maximizing the power generation of a single PV module for over a year”. A better representation is given in figure 4.5 that displays the convergence procedure of the particles for several generations.

Figure 4.4: Convergence all generations of the PSO algorithm for finding the optimal Altitude and Azimuth for the maximum generated power by the PV array over a year.

Figure 4.5a shows the first generation of particles, with the azimuth domain being -90° to 90° and the altitude domain being 0-90°. After 30 generations, the particles have completely converged as can be seen in figure 4.5f. Domain of the azimuth is reduced to 0-2° and the altitude domain is reduced to 37.6-38°. The contour plot of the 30th generation presents the optimal found altitude of 37.8° (horizontal being 0°) and azimuth of 0.7° (South being 0°) corresponding to the optimal PV module orientation for maximum power generation in an entire year. Detailed description about the optimization is given in 6.1.
Figure 4.5: Contour plot of convergence for finding the optimal Altitude and Azimuth for the maximum generated power by the PV array over a year by the PSO algorithm. The color bar defines the maximum generated power in kWh. (a) 1st Generation Particles. (b) 5th Generation Particles. (c) 10th Generation Particles. (d) 15th Generation Particles. (e) 25th Generation Particles. (f) 30th Generation Particles.
4.2.2. Hooke-Jeeves Optimization

In 1960 Robert Hooke and T.A. Jeeves [182] introduced a “direct search” optimization method and defined it as: “We use the phrase ‘direct search’ to describe sequential examination of trial solutions involving comparison of each trial solution with the ‘best’ obtained up to that time together with a strategy for determining (as a function of earlier results) what the next trial solution will be”. The Hooke-Jeeves direct search method is a combination of two different operations, namely exploratory moves and pattern moves. The explanation of both operations, is mainly based on the papers of Hooke and Jeeves, the illustrative explanation by Kramer [183] (see figure 4.6), the flowchart studied in the master thesis of Møller [184] (see figure 4.7) and the “Practical Optimization: A Gentle Introduction” chapter by Chinneck [185].

First, a single initial point, also called base point \( x_0 \), is purposefully selected by the user. Similar to the PSO algorithm, the coordinates of the base point corresponds to a combination of the control variables. The base point is evaluated for the objective function of the optimization and followed by an exploratory move. Operation of the exploratory move is to adjust the coordinates of the base point according to the default or user specified step size of the control variables. Adjustment of the base point can either be by increasing (i.e. positive direction) or decreasing (i.e. negative direction) the control variable. It should be noted that the Hooke-Jeeves direct search algorithm is only able to adjust one single variable at a time while performing the exploratory move. If an increase of the control variable results in a better solution of the objective function, the next step is another increment of the control variable. Else, the control variable is decreased and thus evaluated in the negative direction. If the base point shows no more improvement in both the positive and negative direction, the pattern move operation is initiated for the best found point \( x_{best} \) by the exploratory move.

The pattern move starts searching in the direction that was defined as favorable by the exploratory move. Now, the new base point \( x_1 \) is used to generate a new pilot point \( x_2 \) according to:

\[
x_2 = a \cdot x_1 - x_0
\]

where a common choice for \( a \) is equal to two (according to Chinneck [185]). This new pilot point is not evaluated as a solution for the objective function, but instead explored by the exploratory move. After the exploratory move around base point \( x_2 \) is ended, the pilot point is evaluated. If this pilot point presents a better solution for the objective function than base point \( x_1 \), the pattern move is yet another time repeated by generating a new pilot point \( x_3 \). This continues till no improvement is found by the pattern move and thus the operation returns back to the exploratory move for another round of searching till the best solution for the objective function is found. Final step of the Hooke-Jeeves method is to decrease the specified step size, in the event that no improvement is found after completing the entire process of exploratory and pattern move.
4.2. Particle Swarm Optimization & Hooke-Jeeves Optimization

Figure 4.6: Illustrative representation of the Hooke-Jeeves algorithm [183].

Figure 4.7: Flowchart of the Hooke-Jeeves algorithm [184].
4.3. Constraints

In general, any optimization problem can either be an unconstrained problem with only an objective function and bound constraints or a constraint problem by the addition of (in)equality constraints. A constraint optimization problem can be changed to an unconstrained optimization problem by implementing a penalty function. A penalty function can be an interior penalty function (suffer a penalty as the infeasible region is approached) or an exterior penalty function, also called a barrier (suffer a penalty if the constraint is breached). A penalty function can be applied to convert any kind of constraint; inequality, equality or bound constraint. Inequality constraints can be of any form, but commonly are converted to linear or quadratic loss functions:

\[
b(x) = c \cdot \max(0, g(x) - 5)
\]

\[
b(x) = c \cdot \max(0, g(x) - 5)
\]

where \( c \) is the multiplier defining how intense the penalty is. The same applies to equality constraints which are defined as follow:

\[
b(x) = c \cdot (h(x) - 5)^2
\]

\[
b(x) = c \cdot (h(x) - 5)
\]

The given equations are just some examples typically used for minimization problems. The value of 5 included in the equations can have any other value. If the constraint is breached, a value is added to the objective function which increases the solution of the objective and thus pushes the point/particles back to the feasible region. In the case that the optimization problem is a maximization problem, the penalties can be chosen in a way to subtract penalties from the solution.

As already mentioned, the proposed stand-alone hybrid PV-Electrolyzer-Battery-FC energy system in this study is simulated in TRNSYS and optimized by GenOpt with the help of TRNOPT. In TRNOPT, the user has the possibility to select one of the aforementioned optimization algorithm that is suitable for the optimization problem. Furthermore, the user can tune the settings of each optimization method. For example, the step size and domain of the control variables, in both the PSO and Hooke-Jeeves algorithm, can be selected, the base point of the Hooke-Jeeves, the number of particles and generations of PSO and even the social and cognitive acceleration of the particles and swarm as expressed by eq. 4.7. However, the embedded optimization program of TRNOPT, lacks the possibility to include essential inequality and/or equality constraints. To tackle this shortcoming of the TRNOPT program, the objective function is extended by adding an interior penalty function. The augmented objective function is now defined as:

\[
f'(x) = f(x) + b(x)
\]
In section 1.3 several studies showed that a stand-alone hybrid PV-Electrolyzer-Battery-FC system can be more reliable and cost-effective than the typical implemented stand-alone PV-Battery systems, if the systems are optimally sized. By performing a techno-economical optimization for these stand-alone hybrid energy systems, the economical and technical performance of power supply can be significantly improved. The optimization problem for the proposed hybrid energy system will be described in section 5.1 and as well the constraints defining this system optimization. In section 5.2 the various adopted load demands applicable for a typical Dutch household are elaborately described. Subsequently, the different case studies, based on a combination of the various load demands, are described in 5.3. Each case study is optimized to find the optimal system size with respect to the constraints.

5.1. Optimization Approach

This study aims to find the optimal system size of the proposed stand-alone hybrid PV-Electrolyzer-Battery-FC energy system for a typical Dutch household. The proposed hybrid system is elaborately explained in chapter 3 and displayed in figure 3.18. The optimal sizing for this study is defined as: “System size where the Loss of Load Probability (LLP) is \( \leq 1\% \) for the lowest possible Levelized Cost of Energy (LCOE) over a lifetime of 25 years”. The LLP and LCOE are already explained and expressed in chapter 3 by equations 3.35a and 3.41 and therefore will not be repeated here. For the optimization procedure, the hybrid optimization method of Particle Swarm Optimization (PSO) and Hooke-Jeeves, as described in chapter 4, is used. The stepsize \( \Delta t \) of the optimization process is 6 minutes. Objective function for the stand-alone hybrid energy system regarding the Levelized Cost Of Energy is defined by:

\[
f(x) = LCOE(x)
\]  

The objective function of the LCOE can be minimized according to the standard form of optimization expressed by eq. 4.1 in chapter 4.

5.1.1. Inequality Constraints
The determined LLP \( \leq 1\% \) is a clear inequality constraint of the objective function (lowest LCOE) and needs to be taken care of. As explained in the previous chapter, in section 4.3, TRNOPT has not the ability to define inequality constraints. Therefore, the LLP inequality constraint is accounted for by the following interior penalty function (refer to eq. 4.9a for the standard form):

\[
b_{LLP}(x) = c_1 \cdot \max(0, LLP - 1\%)^2
\]  

This interior penalty function for the LLP adds a value to the objective function, because this is a optimization problem for minimizing the LCOE.
5.1.2. Equality Constraints

The optimization procedure is performed for a project lifetime of 25 years. However, to save computational time and the fact that the studied system is a deterministic system, the optimization is executed over an one year period. Although this can lead to an optimal system size that fulfills the LLP requirement for the lowest LCOE, the drawback is that the initial SoC ($SoC_{\text{init}}$) and final SoC ($SoC_{\text{fin}}$) of both storage methods can differ. Resulting in a system size that either has a shortage of energy due to a lower final SoC of the storage methods or has to dump energy due to a higher SoC. In both cases, the found optimal system size for the first year leads to an unsuitable sizing for the remainder of the project lifetime. Thus, the SoC of the storage methods are equality constraints defining the optimization problem. To account for this potential drawback, the SoC of the storage tank and battery are converted in the form of interior penalty functions (refer to eq. 4.10a for the standard form):

\[
b_{\text{batt soc}}(x) = c_2 \cdot (SoC_{\text{batt init}} - SoC_{\text{batt fin}})^2
\]

\[
b_{\text{tank soc}}(x) = c_3 \cdot (SoC_{\text{tank init}} - SoC_{\text{tank fin}})^2
\]

(5.3a)

(5.3b)

Similar to the inequality constraint, the interior penalty functions for the battery and storage tank SoC adds a value to the objective function, because this is a optimization problem for minimizing the LCOE.

5.1.3. Bound constraints

All the control variables, see table 5.1, used by the optimization process are bound constraints. The domain of the bound constraints is defined by a minimum and maximum value.

<table>
<thead>
<tr>
<th>Control Variable</th>
<th>Domain</th>
<th>Stepsize</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Azimuth</td>
<td>-90° to 90°</td>
<td>0.1°</td>
<td>-90° being East</td>
</tr>
<tr>
<td>(2) Altitude</td>
<td>0° to 90°</td>
<td>0.1°</td>
<td>0° being horizontal</td>
</tr>
<tr>
<td>(3) $N_m$</td>
<td>0-21</td>
<td>1</td>
<td>Number of PV modules</td>
</tr>
<tr>
<td>(4) $E_{\text{batt rated}}$</td>
<td>0-140 kWh</td>
<td>50 Wh</td>
<td>Rated energy capacity battery</td>
</tr>
<tr>
<td>(5) $V_{\text{tank}}$</td>
<td>0-2 m$^3$</td>
<td>0.01 m$^3$</td>
<td>Rated volume hydrogen storage tank</td>
</tr>
<tr>
<td>(6) $SoC_{\text{batt init}}$</td>
<td>0-100%</td>
<td>1%</td>
<td>Initial SoC battery</td>
</tr>
<tr>
<td>(7) $SoC_{\text{tank init}}$</td>
<td>0-100%</td>
<td>1%</td>
<td>Initial SoC hydrogen storage tank</td>
</tr>
</tbody>
</table>

All other components required for the stand-alone hybrid energy system, that are not designated as control variables, are not constrained. For example, as mentioned in the modelling chapter 3, both the electrolyzer and fuel cell are able to receive or deliver any amount of power without being restricted by an minimum idle power or maximum rated power. The same applies for the compressor, water pump, gas dryer, DC-AC inverter and DC-DC converters. These are all not restricted in any way regarding their rated powers or flows. Note, the maximum rated power, flow or number of all implemented components of the hybrid energy system and number of panels is taken into consideration for the LCOE as aforementioned in 3.4.

Orientation PV array

The PV array orientation is optimized for the maximum generated energy annually by a single PV module. Both the azimuth and altitude are varied as continuous control variables, according to their defined domains. With the sunrise in the east and sunset in the west, varying the azimuth from -90° to 90° encloses the possible positions of the Sun throughout any day. Varying the altitude, from 0-90°, to account for the change in rising and setting positions of the Sun during the summer and winter periods. In the summer, the Sun rises in the northeast and in the winter, the Sun rises in the southeast.
5.1. Optimization Approach

PV Modules
The maximum number of panels is physically restricted by the available roof surface of a typical Dutch household. Several architectural and solar installation websites estimate that on average a Dutch household has a roof surface area of about 60-70 m² [186-188]. Typically, Dutch households consist of slanted roofs and since the Netherlands is on the Northern Hemisphere, it is more profitable (in terms of maximal power generation) to place PV module(s) on the roof side orientated towards the optimal azimuth orientation. The optimal azimuth for the location of Vlissingen is found to be 0.7° (as is explained and determined in 6.1), with 0° being the South. Consequently, it can be concluded that one side of the slanted roof can be favorable for PV module placement and thus only half of the available roof surface (30-35m²) can be used. This corresponds to roughly 18-21 PV modules of the empirically modelled BenQ 335W PV module with a module area of 1.63m². Note that this applies for roofs where the sides are orientated South to North or East to West. Furthermore, the required spacing between the modules is neglected here. In terms of connection, the PV array is assumed to consist of possible 18-21 panels in parallel. This is assumed for simplicity, whereas in practice different configurations can be implemented dependent of the voltage and current limitations. Moreover, the number of panels is varied as a discrete control variable.

Battery
As already explained, the short term storage method is based on batteries to overcome the daily fluctuation of the Sun. In general, the recommended energy capacity of the battery for a stand-alone energy system is determined by the recommended autonomy days for a certain latitude and the maximum Depth of Discharge ($\text{DoD}_{\text{max}}$) of the battery. For the location of Vlissingen, with a latitude of 51.45°, the recommended autonomy days ($d_a$) are 10-12 according to Smets et. al [37]. Combined with the $\text{DoD}_{\text{max}}$ of 80% (refer to section 2.3.1) and the daily electrical load demand ($E^d$) of 9.3 kWh on average (refer to section 5.2), the rated energy capacity of the battery bank for this study can be calculated according to:

$$E_{\text{batt, rated}} = \frac{d_a \cdot E^d}{\text{DoD}_{\text{batt, max}}}$$ (5.4)

Solving the above equation for 10-12 autonomy days results in a battery bank capacity of approximately 116-140 kWh. Considering the volumetric density of lead-acid batteries, 60-110 Wh/l (refer to table 2.4), corresponds to roughly 1.9-2.3 m³ (for 60 Wh/l) and about 0.95-1.15m³ (for 110 Wh/l) of occupied space. This potential occupied space is comparable with the space that a typical double door American fridge occupies and therefore seems a credible assumption. Moreover, the total energy capacity of the battery bank is varied as a continuous variable for optimization. The number of cells within a battery and number of batteries is neglected.

Hydrogen Storage Tank
As already explained in section 1.2.1, to tackle the seasonal fluctuation of the Sun, a storage method in the form of hydrogen storage is favored. This requires a certain tank volume that can provide the load demand in the winter season when the solar irradiance is minor and the sun hours short. For this study, the adopted annual electrical load demand is 3400kWh and the annual heat demand is 12500kWh. The heat demand is determined by the consumed volume of natural gas and in turn converted to kWh, regarding the specific energy of natural gas. Both are elaborately described in 5.2. The required volume of the hydrogen tank ($V_{\text{tank}}$) to provide the electrical load demand ($E^e$) and/or heat demand ($E^h$) in the winter period can be calculated by:

$$V_{\text{tank}} = \frac{E^e \cdot 3.6}{\rho_{H_2} \cdot HHV \cdot \frac{p_{\text{tank}}}{p_{\text{amb}}}}$$ (5.5)

where the tank pressure ($p_{\text{tank}}$) is determined to be 350 bar (refer to section 3.2.10), the ambient pressure ($p_{\text{amb}}$) is 1 bar and the density of hydrogen at 1 bar and 25°C and the Higher Heating Value of hydrogen are respectively 0.0813 kg/m³ and 142 MJ/kg (refer to table 2.5. For simplicity, the load/heat demand in the winter period is assumed to be half of the annual demand. Solving
the above equation results in a tank volume of approximately 1.5 m$^3$ for the electrical load demand and approximately 5.5 m$^3$ for the heat demand. A storage tank of 1.5 m$^3$ seems more reasonable and credible to be implemented in a typical Dutch family house. Similar to the battery, the occupied space by the storage tank is comparable to a American double door fridge. For the optimization a maximum tank volume of 2 m$^3$ is assumed and with the battery storage this results in a total of roughly 3-3.5 m$^3$ occupied space. This total volume is comparable to a typical bathroom, with dimensions 2.5x2.5x0.5 m, and thus seems plausible.

5.2. Load Demands

In this subsection the electrical and heat demand of a typical household in the Netherlands will be discussed. Likewise, the load profile of a electrical vehicle and a hydrogen vehicle are drawn from available literature studies. Lastly, the fuel consumption of a gasoline fueled vehicle on a yearly basis is explained. It should be noted that the selected electrical and heat demand profiles are average load profiles and thus potential practical individual peak demands are not taken into consideration. For the load profiles of the electrical vehicle, the average available data is taken and applied to a selected brand and thus does not apply to all types of electrical vehicles. Same applies to the hydrogen vehicle and the gasoline fueled vehicle.

5.2.1. Electrical Demand

For the simulation model, a daily load profile curve based on hourly data is used. The curves are obtained by Veldman and Ribeiro [189, 190] for a typical Dutch household with an annual electrical load demand of 3400 kWh (on average 9.3 kWh daily) by collecting load profile data of 400 households in the Netherlands. Digitized data of the load curves are obtained with the software OriginPro, given in appendix B, and redrawn per season as can be seen in figure 5.1. It is assumed that the electrical load profile is similar for weekdays and weekends and thus can result in a small systematic error affecting the optimization results.

![Daily Electrical Demand](image)

Figure 5.1: Daily electrical load demand of a typical Dutch household for Spring (21/03-20/06), Summer (21/06-20/09), Autumn (21/09-21/12) and Winter (22/12-20/03) (Modified by author) [189, 190].

5.2.2. Heat Demand

The heat demand profile is redrawn using the curves established by Veldman [189]. Collected data is based on 400 households in the Netherlands with an annual heat demand of 12500 kWh. The heat demand is determined by the consumed volume of natural gas and converted to kWh, regarding the specific energy of natural gas. Veldman presents, see figure 5.2, the average daily heat demand profile of a typical Dutch household for the 22$^{nd}$ of December, 18$^{th}$ of March and 11$^{th}$ of April with temperatures of -4.5$^\circ$C, 7.2$^\circ$C and 13$^\circ$C respectively.
By studying the average monthly temperature measured in Vlissingen in the last period between 1981-2010, it can be concluded that there are no months that the averaged temperature is below zero. The average temperature is mainly in the range of 3-18°C, as displayed in figure 5.3.

Extrapolating the established heat demand curves by Veldman in figure 5.2 for the monthly average temperatures (given in figure 5.3), results in a more realistic daily heat demand profile for a typical Dutch household correlative to the average temperatures. The given heat demand profiles are assumed to be similar for weekdays and weekends and thus can result in a small systematic error affecting the optimization results.
It should be mentioned that the heat demand can be delivered in a non renewable approach by the use of a gas boiler or in a more environment friendly method by employing an AC heat pump. Both methods will be studied and explained in detail in section 5.3.4. The above shown heat demand profile, if provided by an AC heat pump, is taken care of as an additional AC load demand in the simulation model. Yet, if the heat demand is externally provided by the combustion of natural gas in a gas boiler, the integral over a year period is taken as the total fuel energy consumption.

5.2.3. Vehicles

**Electrical Vehicle**

The daily load demand profile of an average electrical vehicle adopted in a Dutch household for the year 2030 is constructed by Luiten et al. [194] and shown in figure 5.5. Luiten et al. assumed that all electrical vehicle owners prefer charging their vehicle at home and that the plugging happens immediately at arrival. The load profile is assumed to be similar for all seasons for simplicity. This can result in a small systematic error affecting the optimization results.
Luiten performed this study in the year of 2013 and concluded an electricity transfer, per day in 2030, for an average electrical vehicle of 7.2 kWh on a weekday and 5.9 kWh in the weekends, correlative to an average distance of 36 km on a weekday and 29.5 km in the weekends. These results were based on the assumption that an average electrical vehicle can drive 5 km/kWh (250 km with a 50 kWh battery capacity). Therefore, the study by Luiten corresponds to a yearly electricity consumption of 2486 kWh by an average electrical vehicle correlative to a total driven distance of 12430 km. The predicted total driven distance in the future by Luiten et al. is based on the total driven distance in 2013 published by the Central Bureau voor de Statistiek (CBS), the national statistical agency of the Netherlands [196]. By studying the published results of the CBS for the last six years, it can be concluded that the total driven distance is unaltered and thus the assumption of Luiten et al. is still a valid prediction for the year 2030. On the other hand, the currently available electrical vehicles on the market are able to drive 6.4 km/kWh (e.g. Hyundai Ioniq [197]) instead of the assumed 5 km/kWh. The improvement of the driving distance of the Hyundai Ioniq per kWh is taken into consideration and results in the down scaled load profile as displayed in figure 5.6. Like the aforementioned electrical and heat demand profiles, the electrical vehicle load profile is based on hourly data and is taken care of as an additional DC load in the simulation model whenever in operation.

![Daily Demand Electrical vehicle](image)

**Figure 5.6:** Daily load profile of an average Hyundai Ioniq electrical vehicle in 2030.

**Hydrogen Vehicle**

The modelled daily load profile of an average hydrogen vehicle in the Netherlands is given in figure 5.7. Displayed load profile is for an average Hyundai Nexo hydrogen vehicle, in the year 2030, and is assumed to be similar for all seasons for simplicity. This can result in a small systematic error affecting the optimization results.
The displayed load profile of an average Hyundai Nexo is modelled by converting the consumed electricity profile of an average Hyundai Ioniq, as given in figure 5.6, to consumed kilograms of hydrogen. This is done by first converting the consumed electricity to driven kilometers, determined by the ability of the Hyundai Ioniq (6.4 km/kWh), so that the consumed mass of hydrogen is calculated for the same driven distance of 12430 km. Then, by taking the density of the stored hydrogen gas in the fuel tank and the ability to drive a certain distance per liter of compressed hydrogen gas, the consumed kilograms of hydrogen can be calculated according to eq. 5.6. The Hyundai Nexo can drive 5 km/liter of compressed hydrogen gas. The hydrogen gas in the fuel tank of the hydrogen vehicle is stored at 25°C and 700 bar, correlative to a density of 38 kg/m³ [87, 197].

\[
m_{HV} = \frac{E_{EV} \cdot \eta_{EV}}{\eta_{HV}} \cdot \rho_{H_2} \cdot 10^{-3}
\]  

(5.6)

where:

- \( m_{HV} \), consumed mass by hydrogen vehicle
- \( E_{EV} \), consumed energy electrical vehicle
- \( \eta_{EV} \), Driving ability electrical vehicle
- \( \eta_{HV} \), Driving ability hydrogen vehicle
- \( \rho_{H_2} \), hydrogen density

From figure 5.7, it can be concluded that the yearly consumed hydrogen mass is 106 kg for a total driven distance of 12430 kilometers. Moreover, it is assumed that the charging rate of a hydrogen vehicle is similar to an electrical vehicle, whereas in practice the charge time of a hydrogen vehicle is closer to a gasoline fueled vehicle. Lastly, it should be mentioned that the consumed mass of hydrogen is only provided by the available hydrogen gas in the storage tank and is not supplied by direct hydrogen production through electrolysis.

**Gasoline Vehicle**

In contrast to the electrical and hydrogen vehicle, the studied hybrid energy system is not able to provide fuel for the gasoline fueled vehicle. Thus, a detailed model of a gasoline fueled vehicle for the studied hybrid system is unnecessary. However, if a gasoline fueled vehicle is selected over electrical and hydrogen vehicles, it certainly affects the economical analysis and thus should be taken into account in this techon-economical optimization study. To keep a fair comparison to the other two types of vehicle, the total driven kilometers in a year by an average gasoline fueled vehicle is equal to the...
The aforementioned 12430 kilometers assumed for an average electrical vehicle and average hydrogen vehicle. The selected gasoline fueled vehicle is the Hyundai I40 with a driving ability \(\eta_{AV}\) of 18 km/liter [197]. To drive a total distance of 12430 km in a year by an average Hyundai I40 requires 691 liters of gasoline.

5.3. Case Studies

In this section different case studies, based on the various adopted load demands, the bound constraints, inequality constraints and equality constraints, are described. It is intended to find an optimal system size of the proposed stand-alone hybrid PV-Electrolyzer-Battery-FC energy system for each case study. The control variables that will be optimized through the optimization procedure, dependent on the case study, are: (1) azimuth PV array, (2) altitude PV array, (3) number of panels, (4) battery bank capacity, (5) storage tank volume, (6) initial battery capacity and (7) initial volume storage tank.

5.3.1. PV Array Orientation

The goal in this case study is to find the optimal PV array orientation for the stand-alone system throughout the year. To do so the azimuth and altitude, see table 5.2, are varied throughout the optimization process for finding the maximum generated energy \(E_{PV}\), as defined by eq. 3.42a, for an entire year by a single PV module. This is an unconstrained optimization problem with the following objective function that is maximized:

\[
\max_x f(x) = - \min_x f(x) \tag{5.7a}
\]

\[
f(x) = \sum_{i=1}^{8760} E_{PV_i} \tag{5.7b}
\]

Table 5.2: Characteristics maximizing generated solar power for one year period.

<table>
<thead>
<tr>
<th>Control Variable</th>
<th>Domain</th>
<th>Stepsize</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(x_1) Azimuth</td>
<td>-90° to 90°</td>
<td>0.1°</td>
<td>-90° being East</td>
</tr>
<tr>
<td>(x_2) Altitude</td>
<td>0° to 90°</td>
<td>0.1°</td>
<td>0° being horizontal</td>
</tr>
</tbody>
</table>

Consequently, the found optimum azimuth and altitude are used as the fixed panel orientation for the following case studies unless otherwise stated.

5.3.2. PV-Battery System in 2020

For this case study, the aim is to find the optimal system size of a traditionally stand-alone energy system, containing PV modules and battery, for an annual electrical demand of 3400kWh of a typical Dutch household (refer to figure 5.1). The characteristics of the control variables are tabulated in table 5.3. The augmented objective function of the optimization problem is the combination of the LCOE objective function combined with the interior penalty functions for the LLP and \(SoC_{batt_{init}}\). The augmented objective function is defined by:

\[
\min_x f''(x) = \min_x [f(x) + b_{LLP}(x) + b_{batt}(x)] \tag{5.8a}
\]

\[
f(x) = LCOE(x) \tag{5.8b}
\]
Table 5.3: Characteristics minimizing the LCOE for a LLP ≤ 1% for the PV-Battery system.

<table>
<thead>
<tr>
<th>Control Variable</th>
<th>Domain</th>
<th>Stepsize</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x_3$ $N_m$</td>
<td>0-21</td>
<td>1</td>
<td>Number of PV modules</td>
</tr>
<tr>
<td>$x_4$ $E_{B_{\text{rated}}}$</td>
<td>0-140 kWh</td>
<td>0.5 kWh</td>
<td>Rated energy capacity battery</td>
</tr>
<tr>
<td>$x_6$ $S_{C_{\text{bat_{initial}}}}$</td>
<td>0-100%</td>
<td>1%</td>
<td>Initial SoC battery</td>
</tr>
</tbody>
</table>

5.3.3. PV-Electrolyzer-FC System in 2020

In contrast to the previous case, the system here contains PV modules, electrolyzer and fuel cell to fulfill the annual electrical demand of 3400 kWh as presented in figure 5.1. Control variables and their characterization is tabulated in table 5.4. The augmented objective function of the optimization problem is the combination of the LCOE objective function combined with the interior penalty functions for the LLP and $S_{C_{\text{tank_{initial}}}}$:

$$\min_x f'(x) = \min_x [f(x) + b_{LLP}(x) + b_{tank}(x)]$$  \hspace{1cm} (5.9a)

$$f(x) = LCOE(x)$$  \hspace{1cm} (5.9b)

Table 5.4: Characteristics minimizing the LCOE for a LLP ≤ 1% for the PV-Electrolyzer-FC system.

<table>
<thead>
<tr>
<th>Control Variable</th>
<th>Domain</th>
<th>Stepsize</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x_3$ $N_m$</td>
<td>0-21</td>
<td>1</td>
<td>Number of PV modules</td>
</tr>
<tr>
<td>$x_5$ $V_{\text{tank}}$</td>
<td>0-2 m$^3$</td>
<td>0.01 m$^3$</td>
<td>Rated volume hydrogen storage tank</td>
</tr>
<tr>
<td>$x_7$ $S_{C_{\text{tank_{initial}}}}$</td>
<td>0-100%</td>
<td>1%</td>
<td>Initial SoC hydrogen storage tank</td>
</tr>
</tbody>
</table>

5.3.4. Hybrid System

In the following cases that are described in this section, the goal is to find a techno-economical optimal system size of the proposed stand-alone hybrid PV-Battery-Electrolyzer-FC energy system fulfilling the annual energy demand of a typical Dutch household. This requires the following control variables: number of modules, battery bank capacity, volume storage tank, the initial SoC of the battery and the initial SoC of the storage tank. The control variables and their characteristics are tabulated in table 5.5. The augmented objective function is defined by:

$$\min_x f'(x) = \min_x [f(x) + b_{LLP}(x) + b_{\text{batt}}(x) + b_{\text{tank}}(x)]$$  \hspace{1cm} (5.10a)

$$f(x) = LCOE(x)$$  \hspace{1cm} (5.10b)
Table 5.5: Characteristics minimizing the LCOE for a LLP ≤ 1% for the PV-Battery-Electrolyzer-FC system.

<table>
<thead>
<tr>
<th>Control Variable</th>
<th>Domain</th>
<th>Stepsize</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x_1$ $N_m$</td>
<td>0-21</td>
<td>1</td>
<td>Number of PV modules</td>
</tr>
<tr>
<td>$x_2$ $E_{batt_{rated}}$</td>
<td>0-140 kWh</td>
<td>0.5 kWh</td>
<td>Rated energy capacity battery</td>
</tr>
<tr>
<td>$x_3$ $V_{tank}$</td>
<td>0-2 m$^3$</td>
<td>0.01 m$^3$</td>
<td>Rated volume hydrogen storage tank</td>
</tr>
<tr>
<td>$x_4$ $SoC_{batt_{ini}}$</td>
<td>0-100%</td>
<td>1%</td>
<td>Initial SoC battery</td>
</tr>
<tr>
<td>$x_5$ $SoC_{tank_{ini}}$</td>
<td>0-100%</td>
<td>1%</td>
<td>Initial SoC hydrogen storage tank</td>
</tr>
</tbody>
</table>

Electrical Demand in 2020
For this case, the optimal system is sized to fulfill the annual electrical load demand of 3400 kWh as profiled by figure 5.1. The prices of the (main)components are based on the current prices as aforementioned and tabulated in tables 3.10, 3.11 and 3.12.

Electrical Demand in 2030
Here, the system size is again optimized for the annual electrical load demand of 3400 kWh, but based on the expected future prices of the main components in the year 2030 as tabulated in table 3.11.

Electrical and Heat Demand in 2030 (I)
For this case, the goal is to find an optimal system size fulfilling the electrical load demand by the standalone hybrid system and the heat demand externally in terms of natural gas consumption. Providing the heat demand by natural gas, in combination with a gas boiler, is simply added to the total cost of the system and thus influences the LCOE. Yet again, the expected future prices in the year of 2030 are used for the main components.

Electrical and Heat Demand in 2030 (II)
In this case the hybrid system is optimized to fulfill both the annual electrical and heat demand of respectively 3400 kWh and 12500 kWh in the form of electrical energy with the help of a heat pump. The load profiles are given by figures 5.1 and 5.4. Expected future prices of the main components in the year 2030 are used.

Electrical and Mobility Demand in 2030 (I)
For this case study, the system is optimal sized to fulfill the annual electrical load demand of 3400 kWh (refer to figure 5.1) and the addition of a gasoline fueled vehicle (fed externally by fossil fuels). Hence, the cost of the petrol is simply added to the total system cost and thus influences the LCOE of the system. Based on expected future prices in 2030 for the main components and the current vehicle prices are considered.

Electrical and Mobility in 2030 (II)
Similar to the previous case, but now the gasoline fueled vehicle is replaced by an electrical vehicle. The load demand profile of the electrical vehicle is determined by figure 5.6 and is assumed as an additional electrical load demand of 2486 kWh. The total annual load demand becomes 5886 kWh.

Electrical and Mobility in 2030 (III)
Here, the electrical vehicle is replaced by a hydrogen vehicle which is fueled directly from the hydrogen storage tank. The load demand profile of the hydrogen vehicle, in terms of mass flow, is given in figure 5.7. The total load demand is the annual electrical load demand of 3400 kWh and the annual consumed hydrogen mass of 106 kg. Yet again, the current vehicle prices is used and the expected future prices for the main components.

5.3.5. Hybrid System & Array orientation in 2030
For this case study, the optimal found azimuth and altitude are reset and thus become part of the optimization problem as extra control variables. Hence, the hybrid system size is optimized fulfilling
the annual electrical load demand of 3400 kWh (refer to figure 5.1), according to the characteristics of the seven control variables tabulated in table 5.6. Future prices of the main components are used. The augmented objective function for the optimization is defined by:

$$\min_x f'(x) = \min_x \left[ f(x) + b_{LLP}(x) + b_{batt}(x) + b_{tank}(x) \right]$$

(5.11a)

$$f(x) = LCOE(x)$$

(5.11b)

<table>
<thead>
<tr>
<th>Control Variable</th>
<th>Domain</th>
<th>Stepsize</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Azimuth</td>
<td>-90° to 90°</td>
<td>0.1°</td>
<td>-90° being East</td>
</tr>
<tr>
<td>(2) Altitude</td>
<td>0° to 90°</td>
<td>0.1°</td>
<td>0° being horizontal</td>
</tr>
<tr>
<td>(3) $N_m$</td>
<td>0-21</td>
<td>1</td>
<td>Number of PV modules</td>
</tr>
<tr>
<td>(4) $E_{batt\text{rated}}$</td>
<td>0-140 kWh</td>
<td>0.5 kWh</td>
<td>Rated energy capacity battery</td>
</tr>
<tr>
<td>(5) $V_{tank}$</td>
<td>0-2 m$^3$</td>
<td>0.01 m$^3$</td>
<td>Rated volume hydrogen storage tank</td>
</tr>
<tr>
<td>(6) $SoC_{batt\text{ini}}$</td>
<td>0-100%</td>
<td>1%</td>
<td>Initial SoC battery</td>
</tr>
<tr>
<td>(7) $SoC_{tank\text{ini}}$</td>
<td>0-100%</td>
<td>1%</td>
<td>Initial SoC hydrogen storage tank</td>
</tr>
</tbody>
</table>
5.3.6. Hybrid System & Future prices in 2050

For this case study, the orientation of the PV array is fixed for the optimal found azimuth and altitude regarding the maximization objective described in section 5.3.1. The goal of the optimization procedure is to find the optimal system size fulfilling the annual electrical load demand of 3400 kWh while varying the prices of PV modules, battery, electrolyzer and fuel cell to reach a LCOE of 0.2 €/kWh. The price of the main components are now added as extra control variables. Characteristics of the control variables are tabulated in table 5.7. Furthermore, the LCOE is not defined as an objective function anymore, but rather an interior penalty function similar to the SoC of the storage methods. The penalty function for the LCOE and the modified augmented objective function becomes:

$$\begin{align*}
\min_x f'(x) &= \min_x \left[ b_{LCOE}(x) + b_{LLP}(x) + b_{batt}(x) + b_{tank}(x) \right] \\
b_{LCOE}(x) &= c_4 \cdot (LCOE - 0.2)^2
\end{align*}$$

(5.12a)  (5.12b)

Table 5.7: Characteristics minimizing the components prices for a LLP of ≤ 1% and a LCOE of 0.2 €/kWh for the PV-Battery-Electrolyzer-FC system.

<table>
<thead>
<tr>
<th>Control Variable</th>
<th>Domain</th>
<th>Stepsize</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_m$</td>
<td>0-21</td>
<td>1</td>
<td>Number of PV modules</td>
</tr>
<tr>
<td>$E_{batt rated}$</td>
<td>0-140 kWh</td>
<td>0.5 kWh</td>
<td>Rated energy capacity battery</td>
</tr>
<tr>
<td>$V_{tank}$</td>
<td>0-2 m$^3$</td>
<td>0.01 m$^3$</td>
<td>Rated volume hydrogen storage tank</td>
</tr>
<tr>
<td>$SoC_{batt ini}$</td>
<td>0-100%</td>
<td>1%</td>
<td>Initial SoC battery</td>
</tr>
<tr>
<td>$SoC_{tank ini}$</td>
<td>0-100%</td>
<td>1%</td>
<td>Initial SoC hydrogen storage tank</td>
</tr>
<tr>
<td>$I_{cpv}$</td>
<td>0.01-0.16 €/Wp</td>
<td>€0.01</td>
<td>Investment cost PV modules</td>
</tr>
<tr>
<td>$I_{battery}$</td>
<td>0.01-0.07 €/Wh</td>
<td>€0.01</td>
<td>Investment cost battery</td>
</tr>
<tr>
<td>$I_{electrolyzer}$</td>
<td>0.01-0.70 €/W</td>
<td>€0.01</td>
<td>Investment cost electrolyzer</td>
</tr>
<tr>
<td>$I_{fuel cell}$</td>
<td>0.01-1 €/W</td>
<td>€0.01</td>
<td>Investment cost fuel cell</td>
</tr>
</tbody>
</table>
Results & Discussion

All the results of the simulation and optimization procedures are discussed in this chapter. For each case study only the essential graphs (regarding the discussions and explanations) are displayed. In 6.1, the optimal orientation of the PV array for maximal energy generation is discussed. Subsequently, section 6.2.1 discusses a PV-Battery system intended to fulfill the electrical demand. A PV-Hydrogen system intended to fulfill the load demand is discussed in 6.2.2. In 6.2.3, optimal design of hybrid systems in the year 2020 and the year 2030, intended to fulfill the electrical demand are described. Hybrid systems optimal designed to fulfill both the electrical and heat demand are discussed in 6.3. Fulfilling the electrical demand and an additional vehicle are described in 6.4. Then, in 6.5, optimal system design of a hybrid system in the year 2030 is studied for varying PV array orientation. Next, required future prices for a competitive optimal hybrid system design are discussed in section 6.6. In section 6.7 the adopted assumptions regarding the simulation and optimization of this research study are discussed. Lastly, in section 6.8, detailed concluding remarks and discussion of the results can be found. The discussed numbers, values and ratios, for each case, in the following chapter can be found in tables 6.3 and 6.4 and diagrams 6.29 and 6.30. A complete overview of the optimal system size and result of the optimization objectives, for each case study, are given in table 6.3. Followed by table 6.4, with the performance factors (e.g. LOE, system efficiency etc) given that corresponds to each studied case. The diagram, see 6.29, displays the ratio of the power delivered to the load by either Solar, Battery or Fuel Cell. Additionally, the cost ratio of the components contributing to the total cost of each studied system can be found in diagram 6.30.

6.1. PV Array Orientation

As defined in the previous chapter by eq. 5.7, the objective function for the PV array orientation is used to find the optimal azimuth and altitude (fixed throughout the year) that corresponds to the maximum generated power by a single SunForte 335Wp PV module, for an entire year, for the location of Vlissingen. Results show that the optimal azimuth and altitude are respectively 0.7° and 37.8°. This corresponds to a maximum generated energy of 377.2 kWh per year for a single SunForte 335Wp PV module. The results are tabulated in table 6.1 and figure 6.1 displays the power output of the SunForte 335Wp module for the found optimal azimuth and altitude.

<table>
<thead>
<tr>
<th>Control Variable</th>
<th>Domain</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( f(x) ) ( \sum_{j=1}^{766} E_{pvj} )</td>
<td>-</td>
<td>377.2 kWh</td>
<td>Maximizing energy generation</td>
</tr>
<tr>
<td>( x_1 ) Azimuth</td>
<td>-90° to 90°</td>
<td>0.7°</td>
<td>-90° being East</td>
</tr>
<tr>
<td>( x_2 ) Altitude</td>
<td>0° to 90°</td>
<td>37.8°</td>
<td>0° being horizontal</td>
</tr>
</tbody>
</table>
6.2. Stand-alone Systems in 2020

In this section three different system designs, namely PV-Battery, PV-Hydrogen and PV-Electrolyzer-Battery-FC, are studied. The intention is to determine the technical and economical feasibility of these system configuration if implemented as a stand-alone energy system for a typical Dutch household. All three configurations are optimal sized with the intention to fulfill the electrical load demand (LLP ≤ 1%) for the lowest LCOE.

6.2.1. PV-Battery System in 2020

For this case study, a battery bank is used as a short term and long term storage method fulfilling the electrical load demand for the lowest possible Levelized Cost of Energy (LCOE) over a lifetime of 25 years. The found optimal system size consists of the maximum number of 21 PV modules (≈7 kWp), the maximum potential battery capacity of 140 kWh and starts wit a $SoC_{batt,ini}$ of 94%. This system sizing corresponds to a LLP of 10.7% for a LCOE of 3.55 €/kWh and exceeds the required LLP of ≤ 1% tremendously.
Figure 6.2 displays the course of the State of Charge of the battery. The SoC of the battery at the start and end of the year is 94%. Large part of the year, the battery SoC is between 85-100% while tackling the daily fluctuation of the Sun. Except for the time period defined by 0-500 hour and 7500-8000 hour representing the winter. In this period, the battery is deeply discharged up to the maximum defined DoD of 80% to fulfill the larger load demand and overcome the low or none solar irradiance. The two depleted regions in the graph, where the battery is not being discharged, is due to the aforementioned battery management (refer to 3.3.1). As aforementioned, the battery management forces to charge the battery up to 100% SoC (after reaching a DoD of 80%) before being discharged again.

The time periods where the battery cannot be discharged results in a power deficit, as displayed in figure 6.3. It can be seen that in the winter period, there is a deficit of power, whereas in the summer period, there is plenty of excess solar power that cannot be stored and thus is dumped. From figure 6.3, it can also be included that during certain time periods the load demand is fulfilled and the battery(bank) is being charged. Therefore, there is no deficit or dumped power.

Regarding the determined bound, inequality and equality constraints for the optimization problem of the PV-Battery system (refer to 5.3.2), the required LLP of ≤ 1% is not met. Thus, the found system size is an infeasible optimal solution of the optimization problem. While the equality constraint
$\text{SoC}_{\text{init}} = \text{SoC}_{\text{fin}}$ is met, the bound constraints of the control variables (number of PV modules and battery capacity) seems to be the limiting factors. Still, it is desired to identify a potential feasible optimal solution for the PV-Battery system that is not restricted by the bound constraints of the battery capacity and/or the number of PV modules. This is managed by dismissing the bound constraints of both the number of PV modules and battery capacity and repeating the optimization.

Found system size corresponds to 61 PV modules ($\approx 20 \text{ kW}_p$), a battery capacity of 105 kWh and a \text{SoC}$_{\text{init}}$ of 95%. This system sizing corresponds to a LLP of 0% for a LCOE of 2.86 €/kWh and a total system cost of €48934. Total electrical load demand is for 48.1% provided by the PV array and for 51.9% by the battery bank. The battery, see figure 6.4, is now only at the end of year deeply discharged up to the maximum 80% DoD. Figure 6.5 displays the dumped and deficit power of the feasible optimal solution. As can be observed, the deficit power is zero (LLP=0%) and the plotted dumped power represents a LOE of 81%.

![Figure 6.4: Battery State of Charge of the feasible PV-Battery energy system size. SoC$_{\text{init}}$ = 95% and SoC$_{\text{fin}}$ = 95%.

![Figure 6.5: Dumped and Deficit power of the stand-alone feasible PV-Battery energy system size.](image)

The found system size meets the inequality and equality constraints and thus is a feasible optimal solution. However, the found system size has an impractical size (in terms of PV modules) to be installed for a typical Dutch household. The found number of 61 PV modules is larger than the 21
that in practice can be installed for a typical Dutch household (refer to 5.1.3) and thus is not practical. Moreover, the electricity bought from the grid in the Netherlands is currently 0.2 €/kWh in contrast to the 2.86 €/kWh. Hence, it can be concluded that a stand-alone PV-Battery system is both technically and economically an inapplicable and noncompetitive energy system for a typical Dutch household in the year of 2020. In general, an autonomous system configuration, purely based on PV modules and battery, is not a realistic option for locations at higher latitudes.

In the next subsection, it is studied if the use of hydrogen as a short and long term storage method can be a better system configuration for a typical Dutch household.

### 6.2.2. PV-Electrolyzer-FC System in 2020

The next pressing question is whether the use of hydrogen, due to the higher energy density compared to batteries, can be a feasible system configuration in 2020 for a typical Dutch household. The feasibility is studied in terms of technical (sizing) and economical (LCOE) feasibility. The electrical load demand of a typical Dutch household is purely provided for by a PV array and the production (electrolyzer) and consumption (fuel cell) of hydrogen. The hydrogen gas is used as a short term and long term storage method. Found optimal system size consists of the maximum number of 21 PV modules (∼7 kW$_p$), the maximum potential tank volume of 2 m$^3$ and starts with a $SoC_{tank,init}$ of 100%. This system sizing corresponds to a LLP of 0% for a LCOE of 2.28 €/kWh.

Figure 6.6 displays the course of the State of Charge of the hydrogen tank. The hydrogen tank starts completely filled and is emptied in the beginning of the year up to a $SoC_{tank}$ of about 45%. Subsequently, the PV array manages to fill the tank with hydrogen in the summer. Next, it is once again emptied at the end of the year up to a $SoC_{tank,fin}$ of 2% fulfilling the load demand. As the load demand is entirely met and the $SoC_{tank}$ neither reaches 100% or 0% SoC after the beginning of the year, both the deficit and dumped power are equal to zero.

![Figure 6.6: Storage tank State of Charge of the infeasible PV-Electrolyzer-FC energy system size. $SoC_{tank,init} = 100\%$ and $SoC_{tank,fin} = 2\%$.](image)

In figure 6.7 both the power to the electrolyzer and the power from the fuel cell are plotted. It can be observed that the fuel cell is operated throughout the year to provide energy to the load, whereas the electrolyzer is mainly operated in the summer period converting the excess solar power into hydrogen and to store it as such. Rated power of the electrolyzer and fuel cell are found to be respectively 5.7 kW and 0.8 kW, see table 6.4.
Although the found optimal system size meets the LLP $\leq 1\%$ requirement within the boundary constraints of the maximum number of panels and tank volume, it certainly does not meet the equality constraint $SoC_{tank_{ini}} = SoC_{tank_{fin}}$. Consequently, the tank is not able to provide for the load demand at the beginning of the second year since it was almost completely emptied at the end of the first year. Therefore, the LLP of the second year will exceed the required $1\%$. Therefore, it can be said that the found optimal system size is an infeasible optimal solution of the optimization problem. For finding a feasible optimal solution, the bound constraints of the number of PV modules and tank volume are dismissed and the optimization is repeated.

The new found optimal system size corresponds to 30 PV modules ($\approx 10 \text{ kW}_p$), a tank volume of 1.80 m$^3$ and a $SoC_{tank_{ini}}$ of 42%. This system sizing corresponds to a LLP of 0% for a LCOE of 2.87 €/kWh and a total cost of €55546. Total electrical load demand is for 43.6% provided by the PV array and for 56.4% by the hydrogen tank. Course of the SoC of the tank, see figure 6.8, shows that $SoC_{tank_{ini}}$ and $SoC_{tank_{fin}}$ are both 45% and thus accede the equality constraint. The new found system size is a feasible optimal solution for the optimization problem as both the inequality and equality constraints are met.
The time period in autumn (6000-6500 hour), where the SoC of the tank is kept at about 100%, indicates that there is potential excess energy that cannot be stored and thus is dumped. This indeed corresponds to the plotted dumped power (LOE of 1.3%) in figure 6.9. Furthermore, the plot of the power to the electrolyzer and power from the fuel cell is comparable to figure 6.7 with a subtle difference. Due to the increase of PV modules, the power to the electrolyzer and thus its rated power ($P_{el}$) is increased to 8.5 kW. Rated power of the fuel cell is unchanged since this is purely set by the load demand profile.

Note that both the optimal found number of 30 PV modules exceeds the physical restriction of 21 modules as determined in 5.1.3. Therefore, the found optimal system size is impractical to be implemented for a typical Dutch household. Also, compared to the electricity price for the grid in the Netherlands (0.2 €/kWh), a stand-alone PV-Electrolyzer-FC system is economically (2.87 €/kWh) not competitive. So, as with the PV-Battery system, a stand-alone PV-Electrolyzer-FC is both technically and economically an inapplicable and noncompetitive energy system for a typical Dutch household in the year of 2020.

The PV-Electrolyzer-FC energy system is competitive with the previously discussed PV-Battery system as both have a comparable LCOE. However, the total cost of stand-alone PV-Electrolyzer-FC system (€55546) is more expensive than an old-fashioned stand-alone PV-Battery system (€48934). Larger total cost is mainly due to the additional auxiliary costs (e.g. water pump, compressor, converters, fuels) for the PV-Electrolyzer-FC system as shown in bar diagram 6.30. Also, the optimal PV-Battery system has a LOE of 80.9% in contrast to the 1.3% LOE of the PV-Hydrogen system. Both the lower total cost and the larger LOE (if put to good use) make the PV-Battery system more beneficial in comparison to the PV-Hydrogen system.

Now the question arise if a combination of a battery bank and usage of hydrogen can help towards a feasible system configuration. Such a hybrid system utilizes a battery bank to tackle the daily fluctuations and the combination of Electrolyzer-FuelCell-Tank to tackle the seasonal fluctuation. The next subsection discussed the feasibility of an autonomous hybrid energy system that adopts a battery bank as a short term storage method and the use of hydrogen as a long term storage method.

### 6.2.3. Hybrid System in 2020

For this case study, the electrical load demand of a typical Dutch household is provided for by a PV array, a battery bank for short term storage and the use of hydrogen as the long term storage method. Optimal system size consists of 19 PV modules ($=6.4 \text{ kW}_p$), a battery capacity of 28.5 kWh, a tank volume of 1.18 m$^3$, $SoC_{tank_{ini}}$ of 40% and a $SoC_{batt_{ini}}$ of 74%. This sizing meets the inequality and equality constraints and thus is a feasible optimal solution of the optimization problem. The electrical load demand is entirely fulfilled (LLP = 0%) for a LCOE of 2.16 €/kWh and a total cost of €38200.
6.2. Stand-alone Systems in 2020

Figure 6.10 displays the course of the State of Charge of both the battery bank and the storage tank. It can be noticed that the SoC of the battery fluctuates throughout the year to tackle the daily shortcomings. While the storage tank is mainly emptied in the winter period and refilled with hydrogen during the spring/summer period to fulfill the energy demand at the end of the year. Therefore, acting as the long term storage method and tackling the seasonal fluctuation. Total electrical load demand is for 41.9% provided by the PV array, for 42.9% by the battery bank and for 15.2% by the hydrogen tank as presented by 6.29. An explanation for the high ratio “battery to load” compared to “fuel cell to load” is the fact that, the aforementioned master controller (refer to 3.3.1), is prioritized to first discharges the battery before the hydrogen tank in times of need. This is also emphasized by the plotted power to the electrolyzer and power from the fuel cell in figure 6.11. Rated power of the electrolyzer and fuel cell are respectively 5.2 kW and 0.8 kW.

Figure 6.10: Tank and battery State of Charge of the feasible hybrid energy system size in 2020. \( \text{SoC}_{\text{tank,ini}} = 40\% \) and \( \text{SoC}_{\text{tank,fin}} = 40\% \) & \( \text{SoC}_{\text{batt,ini}} = 74\% \) and \( \text{SoC}_{\text{batt,fin}} = 74\% \).

Figure 6.11: Power to electrolyzer and from fuel cell of the stand-alone feasible hybrid energy system size in 2020. \( P_{\text{ely}} = 5.2 \) kW and \( P_{\text{fc}} = 0.8 \) kW.

Potential excess power that cannot be stored in either the tank or battery, between the time period 5500-6500 hours, is dumped. Graphical presentation of this occurrence is given by figure 6.12 and corresponds to LOE of 9.8%.
The found optimal system size meets inequality and equality constraints and thus is a feasible optimal solution. As the physical restrictions of the modules, battery and tank volume are not exceeded, it can be concluded that the optimal system size is technically applicable for a typical Dutch household. This hybrid system is advantageous over the PV-Battery and PV-Electrolyzer-FC because it is technically applicable and cheaper. Both the total cost of the hybrid system (€38200) and the LCOE (2.16 €/kWh) are lower compared to the other two system design, refer to table 6.3. Nevertheless, in the end, the price per kWh is still much larger than buying the electricity from the grid. Therefore, a stand-alone hybrid PV-Electrolyzer-Battery-FC energy system is technically applicable but economically not viable for a typical Dutch household in the year of 2020.

Although the hybrid system is feasible from a technical point of view, it is currently still not competitive in terms of LCOE. Therefore, in the following subsection the technical and economical feasibility of the hybrid system is assessed, regarding expected future prices in 2030 of the main components.

### 6.2.4. Hybrid System in 2030

Here, the PV-Electrolyzer-Battery-FC system is again optimized but now with the expected future prices of the main components in 2030: PV modules, electrolyzer, fuel cell and battery (refer to chapter 3, table 3.11). Found optimal system sizing contains 19 PV modules (≈6.4 kWp), a battery capacity of 25.5 kWh, a tank volume of 1.24 m³, SoC_{tank,final} of 43% and a SoC_{batt,final} of 73%. As expected, this sizing fulfills the load demand completely for a LCOE of 1.04 €/kWh and a total cost €18401. Similar to the hybrid system in the year of 2020, the found optimal size is a feasible optimal solution of the optimization problem and technically applicable for a typical Dutch household. It was observed that the shape of the graphs of the SoC of the storage methods, power to electrolyzer and power from fuel cell and dumped power are comparable with respectively figures 6.10, 6.11 and 6.12. As expected, the optimal system size of the hybrid system in 2030 is not significantly changed, whereas the total cost is reduced down to €18401. This is mainly due to the price decrease of the main components. Yet, with a LCOE of 1.04 €/kWh, it is clear that even in 2030 a stand-alone hybrid PV-Electrolyzer-Battery-FC is economically not viable for a typical Dutch household.

An interesting observation can be made regarding the found optimal hybrid system size in 2030. The bar diagram, displayed by 6.30, shows that the ratio of the total cost determined by the fuel cell and electrolyzer is decreased, whereas the ratio of the total cost determined by the battery bank is hardly changed. The cost ratio of the electrolyzer is decreased from 34% to 25% and the cost ratio of the fuel cell is decreased from 14% to 7%. This can be explained by the assumptions made that electrolyzer price is decreased to 0.7 €/W and fuel cell price is decreased to 1 €/W in the year 2030 (refer to table 3.11). This invites to investigate if a hybrid system with an unconstrained tank volume can lead to a
system size fulfilling the load demand for a lower LCOE. So, the optimization procedure is repeated and the following optimal system size is found: 21 PV modules (≈7 kWp), battery capacity of 7.0 kWh, tank volume of 2.35 m³, SoC\textsubscript{tank\textsubscript{init}} of 34% and a SoC\textsubscript{batt\textsubscript{init}} of 91%. Corresponding to a LLP of 0% for a LCOE of 0.97 €/kWh and a total cost of €17552. As a consequence of the larger tank volume, the ratio of hydrogen providing the load is increased from 15.6% up to 25.2% while the ratio of the battery is decreased from 42.5% down to 33.4%. Note, plots of the SoC of the battery and the tank, power to the electrolyzer and power from the fuel cell and the dumped power show similar trends as shown in figures 6.10 and 6.11 and thus are not displayed again. However, it should be mentioned that due to more PV modules and larger tank, the rated power of the electrolyzer is increased up to 5.9 kW.

An interesting observation is that by dismissing the tank volume constraint, not only a lower LCOE (0.97 vs 1.04 €/kWh) is found but also the LOE is decreased from 9.7% down to 0%. Therefore, it can be beneficial to study the implementation of a large scale hydrogen utility. For such a case, the hydrogen storage can be centralized for both storage and consumption purposes and thus is not limited to the physical constraint of 2 m³ per household. Doing so can direct towards stand-alone systems that can consume and produce hydrogen and feed it to the centralized storage tank. The implementation of a centralized hydrogen tank can reduce the essential number of PV modules required for the fulfillment of the electrical load demand of a single household since in deficit times hydrogen can be used. In turn, the available roof area can be completely covered by PV modules to contribute to the centralized tank in times of excess energy. This is emphasized by the found number of 21 PV modules for this scenario. Additionally, the battery capacity can be reduced to only address the daily fluctuations and thus further decrease the system costs. As it is established by the reduction of the battery capacity from 25.5 kWh to 7 kWh.

6.3. Electrical and Heat Demand in 2030

The found hybrid system size, discussed in 6.2.4, is still not limited by the assumed constraints regarding the PV modules, battery bank and hydrogen storage tank. Hence, it can be interesting to assess the technical and economical feasibility of the hybrid system by adding an additional heat demand profile (refer to figure 5.4). In this section, two different system configurations are studied. Firstly, the additional heat demand is provided by a traditional gas boiler by the consumption of natural gas. Secondly, the additional heat demand is provided by a heat pump that is powered by an optimal autonomous hybrid system size. Both configurations are optimal sized with the intention to fulfill the electrical and heat demand ( LLP ≤ 1%) for the lowest LCOE.

6.3.1. Electrical and Heat Demand in 2030 (I)

For this case study, it is intended to both fulfill the electrical and heat demand. A gas boiler is added to provide for the supplementary heat demand. The gas boiler is fed by natural gas obtained from industry. Found optimal system sizing for electrical load demand is unchanged compared to the hybrid system in 2030 (refer to 6.2.4), but the total cost of the system and thus LCOE are increased up to respectively €27200 and 1.68 €/kWh. This is due to the additional cost of the gas boiler and the consumed natural gas during the total lifetime of the project. Since the optimal system sizing is unchanged, the course of the battery, tank, power to electrolyzer and power from fuel cell and dumped power are the same as figures 6.10, 6.11 and 6.12.

6.3.2. Electrical and Heat Demand in 2030 (II)

For this case study, it is intended to fulfill the supplementary heat demand in a sustainable matter with a heat pump instead of a gas boiler. Additionally, this method is more advantageous than a gas boiler since it is not dependent of any external energy source except for the Sun. Optimal system size containing the maximum number of 21 PV modules (≈7 kWp), maximum battery capacity of 140 kWh, a storage tank of 2 m³, SoC\textsubscript{tank\textsubscript{init}} of 100% and a SoC\textsubscript{batt\textsubscript{init}} of 100% cannot fulfill both the electrical and heat demand. From figures 6.13 and 6.14, it can be observed that the storage tank and battery are immediately emptied at the beginning of the year. Subsequently, after being charged in the summer period, battery up to a 100% SoC and tank up to 55% SoC, both are again immediately emptied. Resulting in a high deficit power (LLP of 67.5%) as can be seen in figure 6.15. Clearly, both the inequality and equality constraints are not met for this system sizing and thus is an infeasible
optimal solution of the optimization problem.

Figure 6.13: Tank and battery State of Charge of the infeasible Hybrid energy system size providing for the electrical and heat demand. \( \text{SoC}_{\text{tank ini}} = 100\% \) and \( \text{SoC}_{\text{tank fin}} = 0\% \) & \( \text{SoC}_{\text{batt ini}} = 100\% \) and \( \text{SoC}_{\text{batt fin}} = 99\% \).

Figure 6.14: Power to electrolyzer and from fuel cell of the stand-alone infeasible Hybrid energy system size providing for the electrical and heat demand. \( P_{\text{ely}} = 5.9 \text{ kW} \) and \( P_{\text{fc}} = 6.2 \text{ kW} \).
6.3. Electrical and Heat Demand in 2030

Nevertheless, there is a system size that can be feasible if the bound constraints of the number of PV modules, battery capacity and tank volume are dismissed. Found feasible system sizing contains 550 PV modules (≈184 kWp), a battery capacity of 200 kWh, a tank volume of 30 m³, SoC_{tank_{ini}} of 79% and a SoC_{batt_{ini}} of 79%. This sizing corresponds to a LLP of 0.8% for a LCOE of 3.63 €/kWh and a total cost of €281231.

Several notes have to be made regarding figure 6.16 and the found system size. It can be noticed that the storage tank is barely emptied at the beginning of the year, but rather at the end of the year. This can be explained by the 550 PV modules that are able to provide for the electrical and heat demand and even refill the hydrogen tank in the month of December (time period > 8000 hours). The oversized PV array and the fact that the tank is only emptied at the end of the year could question the large tank volume of 30 m³. While the total annual load demand (15900 kWh) is only about five times the annual electrical demand (3400 kWh), both the tank volume and PV array are about 30 times enlarged compared to the hybrid system discussed in 6.2.4. Therefore, it is safe to say that the found system sizing is clearly not an optimal system sizing. The immense found system oversize for this case study can be explained by: (1) higher peak demand of the combined heat and electrical demand profile...
Results & Discussion

compared to individual electrical demand profile and (2) insufficient convergence of the particles in the Particle Swarm Optimization. The heat demand profile holds a peak demand that is about 8 times the electrical demand profile by comparing the aforementioned figures 5.1 and 5.4. Calculated standard deviation of the PSO algorithm for this case study, see table D.2 in appendix D, is insufficiently converged towards a minimum in the last generation. The last generation still has a standard deviation of 81 PV modules for the PV array and 15 m$^3$ for the tank volume. Yet, an autonomous hybrid system fulfilling combined electrical and heat demand can be intuitively sized. An intuitive sizing of the tank volume can be done based on the required cubic meters of hydrogen for the additional annual heat demand. The additional heat demand of 12500 kWh, taking into account the energy density (142 MJ/kg) and specific density (28.45 kg/m$^3$) of hydrogen at 350 bar corresponds to 12 m$^3$ of hydrogen gas. The PV array size can be intuitively sized to overcome the higher peak demand of the combined electrical and heat demand. Referring to figures 5.1 and 5.4, it is observed that the combined peak demand is 10 times the electrical demand. Thus the PV array size is most probably in the range of 200 PV modules. Hence, from this intuitively sizing, it can be simply concluded that an autonomous hybrid system for the combined electrical and heat demand is technically infeasible. From an economical point of view, this hybrid system is economically not feasible. While the combined load demand is 5 times the electrical demand, the total system size (and thus cost) is enlarged by more than 5 times. So, the LCOE will increase compared to a hybrid system that solely fulfills the electrical demand and the heat demand with a gas boiler (LCOE is 1.68 €/kWh). Without a doubt, it can be concluded that fulfilling the heat demand by a stand-alone hybrid system is not viable at the moment compared to a stand-alone system with an old-fashioned gas boiler. Neither is it competitive with the current systems where the electrical demand is provided for by the grid (0.2 €/kWh) and the heat demand by the consumption of natural gas (0.12 €/kWh). In other words, a stand-alone PV-Electrolyzer-FC fulfilling both the electrical and heat demand is technically and economically an inapplicable and noncompetitive energy system for a typical Dutch household in the year of 2030.

A potential solution can be to adopt the optimal hybrid system, as discussed in 6.2.4, and install as many PV modules as possible on the roof area. Doing so can provide for the electrical load demand and fuel the centralized hydrogen tank. Then, hydrogen can be used from the central storage tank for the additional heat demand.

6.4. Electrical and Mobility Demand in 2030

The found hybrid system size, discussed in 6.2.4, is still not limited by the assumed constraints regarding the PV modules, battery bank and hydrogen storage tank. Hence, it can be interesting to assess the technical and economical feasibility of the hybrid system by adding an additional mobility demand profile. In this section, three different system configurations are studied. Firstly, a gasoline fueled vehicle is added to the system that is fueled by fossil fuel. Secondly, an electrical vehicle is added to the system and it is intended to fulfill the combined electrical and mobilty demand on an optimal autonomous hybrid system size. Lastly, a hydrogen vehicle is added and it is again intended to fulfill the combined electrical and mobilty demand by an optimal autonomous hybrid system size. All configurations are optimal sized with the intention to fulfill the electrical and heat demand (LLP ≤ 1%) for the lowest LCOE.

6.4.1. Electrical and Mobility in 2030 (I)

In this case study, a gasoline fueled vehicle is added to the stand-alone hybrid system and it is intended to fulfill the electrical demand by the stand-alone hybrid system and fulfill the fuel consumption of the vehicle energy produced via fossil fuels. Yet again, the optimal system sizing for the electrical load demand is unchanged compared to the hybrid system in 2030 (refer to 6.2.4), but the total cost of the system and thus LCOE are increased up to respectively €72242 and 1.27 €/kWh. The considerable increase in the total cost is due to the purchase and maintenance of a gasoline fueled vehicle and the LCOE is solely increased by the fuel cost for the provided primary energy value of the gasoline. Since the optimal system sizing is unchanged, the course of the battery, tank, dumped power and power to electrolyzer and power form fuel cell are the same as figures 6.10, 6.11 and 6.12.
6.4.2. Electrical and Mobility in 2030 (II)
Here, an electrical vehicle is added to the stand-alone hybrid system and it is intended to fulfill both the electrical demand and the electrical load consumption of the vehicle. Found optimal system sizing corresponds to the maximum of the 21 PV modules (=7 kWp), a battery capacity of 140 kWh, a tank volume of 2 m³, SoC\textsubscript{tank\textsubscript{ini}} of 100% and a SoC\textsubscript{batt\textsubscript{ini}} of 100%. This corresponds to a LLP of 0% for a LCOE of 1.72 €/kWh and a total cost of €100626. However, from figure 6.17 it can be observed that the SoC of the battery and the tank at the end of the year do not match the initial SoC and thus the equality constraint is not met. Hence, this is an infeasible optimal solution of the optimization problem. There is no dumped or deficit power.

As can be concluded from figures 6.17 and 6.18, the hydrogen tank is emptied at the beginning of the year (time period 0-1500 hour), topped off during spring/summer (time period 2500-7000 hour) and emptied again at the end of the year.

Figure 6.17: Tank and battery State of Charge of the infeasible Hybrid energy system size providing for the electrical demand and electrical vehicle. SoC\textsubscript{tank\textsubscript{ini}} = 100% and SoC\textsubscript{tank\textsubscript{fin}} = 16% & SoC\textsubscript{batt\textsubscript{ini}} = 100% and SoC\textsubscript{batt\textsubscript{fin}} = 88%.

Figure 6.18: Power to electrolyzer and from fuel cell of the stand-alone infeasible Hybrid energy system size providing for the electrical demand and electrical vehicle. P\textsubscript{el} = 5.6 kW and P\textsubscript{fc} = 1.5 kW.
For finding a potential feasible optimal solution, the bound constraint of the number of PV modules and battery capacity (since an electrical vehicle is practically an extra battery) are dismissed and the optimization process is repeated. The found optimal system size consists of 35 PV modules (≈11.7 kW), battery capacity of 170 kWh, a tank volume of 1.37 m³, \(SoC_{\text{tank ini}}\) of 39% and a \(SoC_{\text{batt ini}}\) of 83%. This system size meets both the inequality (LLP = 0%) and equality constraints for a LCOE of 2.15 €/kWh and a total cost of €112446. Thus, the new optimal system size is a feasible optimal solution of the optimization problem. Course of the SoC of both the storage methods is displayed in figure 6.19.

This optimal system size has a larger battery capacity and a larger PV array. The system is oversized and results in a LOE of 31.7% as displayed in figure 6.20. Course of the power to the electrolyzer and power from fuel cell is similar to figure 6.18 with the subtle difference that the rated power of the electrolyzer is increased to 9.7 kW.

The advantage of this optimal system size is that it is an entirely stand-alone system. But it is not applicable for a typical Dutch household due to the larger battery capacity and PV array. Moreover, as
expected, the larger hybrid system size increases the LCOE from 1.04 €/kWh (discussed in 6.2.4) up to 2.15 €/kWh. Found LCOE of 2.15 €/kWh clearly states that a stand-alone PV-Electrolyzer-FC fulfilling the electrical demand of both a household and an electrical vehicle is both technically and economically an inapplicable and noncompetitive energy system for a typical Dutch household in the year of 2030.

In terms of total cost (system + vehicle), even in the year of 2030 (with gasoline prices of 2.07 €/liter [170]) it is still more beneficial purchasing a gasoline fueled vehicle, which is fueled by energy produced via fossil fuels, rather than an electrical vehicle ‘fueled’ by the hybrid system. The system plus gasoline vehicle costs €72242 and the hybrid system plus electrical vehicle costs €112446. Although, a different approach can perhaps influence the decision. A different strategy can be to adopt the hybrid system and the electrical vehicle but obtain the electrical consumption of the electrical vehicle via a charging station at a cost of 0.2 €/kWh. This results in a total cost of €85319 for the hybrid system with an electrical vehicle. In comparison, the total cost of a hybrid system plus a gasoline fueled vehicle is €72242. Thus, adopting a hybrid system plus an electrical vehicle or a gasoline fueled vehicle are both less expensive than a completely stand-alone system. Drawback is that in such a case, both the vehicles are fulfilled by energy produced via fossil fuels.

Another type of vehicle that can be fueled by such a hybrid system is a hydrogen vehicle. These type of vehicles are currently almost twice the cost of an electrical vehicle (€52224 vs €29904). But up till now, it is observed that a hybrid system utilization the full potential of hydrogen production and consumption can lead to a reduction in LCOE. Hence, perhaps the same observation can be applied to an autonomous hybrid system with an added hydrogen vehicle rather than an electrical vehicle.

### 6.4.3. Electrical and Mobility in 2030 (III)

Similar to the previous case study but now the electrical vehicle is replaced by a hydrogen vehicle. Once again, the maximum number of 21 PV modules (≈7 kWp), a battery capacity of 140 kWh, a tank volume of 2 m³, SoC\textsubscript{tank,init} of 100% and a SoC\textsubscript{batt,init} of 100% is an optimal system size. This sizing corresponds to a LLP of 52.7% for a LCOE of 1.34 €/kWh and a total cost of €138350. So, the inequality constraint is not met and neither are the equality constraints regarding the SoC of the storage methods, see figure 6.21. Therefore, the found system size is an infeasible optimal solution.

![Figure 6.21](image)

Figure 6.21: Tank and battery State of Charge of the infeasible Hybrid energy system size providing for the electrical demand and hydrogen vehicle. SoC\textsubscript{tank,init} = 100% and SoC\textsubscript{tank,fin} = 0% & SoC\textsubscript{batt,init} = 100% and SoC\textsubscript{batt,fin} = 94%.

From figure 6.22, it is interesting to observe that although the tank is emptied after the time period > 5000 hour, the electrolyzer is still producing hydrogen. However, the produced hydrogen is directly used for the hydrogen consumption of the vehicle and not the electrical load. Otherwise the fuel cell would be operating as well. Nevertheless, this system sizing is not capable to fulfill both the electrical demand and the hydrogen vehicle consumption. Resulting in deficit power after 5000 hours as can be
seen in figure 6.23.

Figure 6.22: Power to electrolyzer and from fuel cell of the stand-alone infeasible Hybrid energy system size providing for the electrical demand and hydrogen vehicle. $P_{\text{sty}} = 5.8 \text{ kW}$ and $P_{\text{fc}} = 0.8 \text{ kW}$.

Figure 6.23: Dumped and Deficit power of the stand-alone infeasible Hybrid energy system size providing for electrical demand and hydrogen vehicle.

For finding a potential feasible optimal solution, the bound constraint of the number of PV modules and tank volume (since an hydrogen vehicle is practically an extra storage tank) are dismissed and the optimization process is repeated. The found optimal system size consists of 40 PV modules ($\approx 13.4 \text{ kW}$), battery capacity of 72.5 kWh, tank volume of 1.86 m$^3$, $\text{SoC}_{\text{tank}}$ of 38% and a $\text{SoC}_{\text{batt}}$ of 89%. This system size meets both the inequality (LLP = 0%) and equality constraints for a LCOE of 0.95 €/kWh and a total cost of €135547. The course of the SoC of both the storage methods is displayed in figure 6.24.
It can be seen that the equality constraints are met and that there is a brief period of excess energy that is dumped (LOE of 0.5%) around the time period of 6000-6400 hours as displayed by figure 6.25. Power to the electrolyzer and power from the fuel cell are plotted in figure 6.26. It can be observed that the fuel cell is again put to use at the end of the year due to abundant energy in the tank. The larger PV array and tank volume result in a higher rated power of the electrolyzer ($P_{ely} = 11.7$ kW) compared to the infeasible optimal solution.
Although the found optimal system size is a stand-alone system, it is unfortunately not applicable for a typical Dutch household due to the limited roof area for the found PV array size. As hoped for, the larger hybrid system size decreases the LCOE from 1.04 €/kWh (discussed in 6.2.4) down to 0.95 €/kWh. The found LCOE is more comparable to the LCOE of 0.97 €/kWh for the hybrid system in 2030 with an enlarged storage tank. This result emphasizes once again that a larger tank volume can be more beneficial to be centralized. Besides the larger tank, the PV array is doubled and the battery capacity is fivefolded and still results in a lower LCOE. Nevertheless, found LCOE of 0.95 €/kWh still states that a stand-alone PV-Electrolyzer-FC fulfilling the electrical demand of both a household and an electrical vehicle is both technically and economically an inapplicable and noncompetitive energy system for a typical Dutch household in the year of 2030.

In terms of total cost (system + vehicle), even in the year of 2030 (with gasoline prices of 2.07 €/liter [170]) it is still more beneficial purchasing a gasoline fueled vehicle, which is fueled by energy produced via fossil fuels, rather than a hydrogen vehicle ‘fueled’ by the hybrid system. The system plus gasoline vehicle costs €72242 and the hybrid system plus hydrogen vehicle costs €135547. Although, a different approach can perhaps influence the decision. A different strategy can be to adopt the hybrid system and the hydrogen vehicle but obtain the hydrogen consumption (annual 106 kg) of the vehicle via a charging station at a cost of 12.3 €/kg [166]. This results in a total cost of €113667 for the hybrid system with a hydrogen vehicle. In comparison, the total cost of a hybrid system plus a gasoline fueled vehicle is €72242. Thus, adopting a hybrid system plus a hydrogen vehicle or a gasoline fueled vehicle are both less expensive than a completely stand-alone system. Drawback is that in such a case, both the vehicles are fulfilled by energy produced via fossil fuels.

Referring to table 6.3, an interesting observation can be made regarding the LCOE of the hybrid system plus a vehicle. Previously mentioned, for the calculation of the LCOE, the costs (investment, replacement and maintenance) of the vehicles are taken out of the equation. An interesting observation is that the LCOE of a stand-alone system with a hydrogen vehicle is lower than the LCOE of a stand-alone system with an electrical vehicle (0.95 vs 2.15 €/kWh). Therefore, in terms of LCOE, it is more beneficial to adopt a stand-alone hybrid system, unrestricted by PV array size and tank volume to fulfill the hydrogen consumption of a hydrogen vehicle rather than a hybrid system fulfilling the electrical consumption of an electrical vehicle. Such a stand-alone hybrid system is also less expensive (0.95 €/kWh) than the hybrid system (discussed in 6.2.4) plus a gasoline fueled vehicle (1.27 €/kWh). Hence, without a doubt, it can be said that a hybrid system unlimited by the size of the tank and the PV array size can become even cheaper than in the case that only the tank volume is not limited. Once again, a centralized storage tank and a completely covered roof area of each household with PV modules can be the solution towards centralization in a sustainable matter.
6.5. Hybrid System & Array orientation in 2030

So far, all the case studies are optimized regarding the found optimal PV array orientation in section 6.1. The found optimal orientation corresponds to the maximum energy generation by a PV module over a year period. However, it can be more beneficial to orientate the PV array in such a way that the generated energy meets the energy demand. Doing so can lead to smaller system sizes (e.g. less PV modules, smaller battery capacity and/or smaller storage tank) and thus lower system costs. Therefore, in this case study, it is intended to find the optimal system size fulfilling the electrical demand for varying PV array orientations.

The found optimal consists of 18 PV modules (∼6 kWp), battery capacity of 23 kWh, tank volume of 1.20 m³, SoC_{tank,init} of 40%, SoC_{batt,init} of 63%, azimuth of 19° and an altitude of 45°. This results in a LLP of 0% for a LCOE of 1.01 €/kWh with a total cost of €17851. The course of the SoC of the storage methods and the dumped (LOE of 2.8%) and deficit power are plotted in respectively figures 6.27 and 6.28. Both the inequality and equality constraints are met and thus the found system size is a feasible optimal solution of the optimization problem.

Figure 6.27: Tank and battery State of Charge of the feasible Hybrid energy system size providing for the electrical demand by changing PV array orientation. SoC_{tank,init} = 40% and SoC_{tank,fin} = 40% & SoC_{batt,init} = 63% and SoC_{batt,fin} = 63%.
The found optimal system size is directed more towards the Southwest (28°) instead of towards the South (0.7°) as determined in 6.1. It seems that for the studied electrical load profile, where the demand is higher as the evening starts, orientating the PV array towards the Southwest (to receive the last available daily Sun hours) is more beneficial than the found optimal orientation corresponding to maximum energy generation by the PV array. Resulting in a smaller PV array size compared to the discussed hybrid system in 6.2.4. Number of PV modules is decreased from 19 to 18. Also, studying diagram 6.29, it can be seen that the energy provided by the PV array is unchanged (“STL” is about 42%), even though the number of PV modules is decreased. Indicating that this found PV array orientation is better abiding the daily fluctuations of the Sun. Being less abiding of the daily fluctuations can also lead to energy being used more directly rather than being stored before usage. This can also be concluded by the fact that the energy from the “BTL” is decreased from 42.5% to 41.1% (see table 6.29), and the fact that the battery capacity is slight decreased from 25.5 kWh to 23 kWh. The found altitude of 45° is more favorable for the winter period and thus results in a larger energy generation in the winter. Consequently, the load can be provided more directly via the PV array and thus requires a smaller storage tank. The tank volume is decreased from 1.24 m³ to 1.20 m³. Logically, a smaller tank volume results in a higher ratio of “FCTL” (increased up to 16.9%) as can be seen in diagram 6.29.

Conclusively, it can be said that the found orientation for the particular studied electrical load demand, displayed by figure 5.1, results in a smaller system size compared to the hybrid system discussed in 6.2.4. As a consequence, the total system cost decreases from €18401 to €17851 and the LCOE decreases from 1.04 €/kWh to 1.01 €/kWh.

6.6. Hybrid System & Future prices in 2050
Up till now, it is observed that an autonomous hybrid PV-Electrolyzer-Battery-FC energy system can only fulfill the electrical load demand of a typical Dutch household within the technical limitations. However, it is an infeasible system, in terms of a LCOE of 1.04 €/kWh, and not competitive with the current electricity price of 0.2 €/kWh. Even though the expected future prices will drop down to 0.16 €/Wp for PV, 0.07 €/Wh for battery, 0.7 €/W for electrolyzer, 1 €/W for fuel cell and 0.08 €/kWh for the storage capacity. So, the question arise what the future prices have to be for a feasible autonomous hybrid energy system, from a technical and economical point of view. Hence, in this case study, it is intended to find the optimal system size and the optimal prices of the main components in the year 2050 or later to make the stand-alone hybrid system economically competitive with the current price of 0.2 €/kWh for electricity.
6.6. Hybrid System & Future prices in 2050

Found optimal system size consists of 18 PV modules (≈6 kWp), a battery capacity of 39 kWh, a tank volume of 1.1 m³, SoC\text{tank} of 34% and a SoC\text{batt} of 76%. The found optimal price are 0.01 €/Wp for the PV module, 0.01 €/Wh for the battery bank, 0.01 €/W for the electrolyzer and fuel cell and 0.08 €/kWh for the tank capacity. This system size and the optimal prices correspond to a LLP of 0.8% for a LCOE of 0.28 €/kWh and a total cost of €4922. Plots of the SoC of the storage methods, power to electrolyzer and power from fuel cell and dumped power show similar trends as shown in figures 6.10, 6.11 and 6.12. It seems that even with almost free main components, the stand-alone hybrid system is not cost competitive with the electrical grid. However, from diagram 6.30, it can be observed that the total system cost is now mainly due to the battery bank and auxiliary components (e.g. pump, compressor, inverter, converters, fuels). Compared to the hybrid system in 2030, the contribution of the battery bank to the total system cost is decreased from 29% to 23% and the auxiliary components is increased from 27% to 73%. While the electrolyzer, fuel cell and PV array are decreased to about 1-3%. Therefore, it can be viable to move towards a more centralized storage tank for hydrogen storage. Doing so can help reduce the battery capacity (to only address the daily fluctuation) and thus reducing the total cost of the system and subsequently reducing the LCOE. Eventually, it is desired to provide energy, produced via renewable energy systems, for a LCOE of 0.2 €/kWh to suppress the energy production via fossil fuels. A potential solution can be to upscale the hybrid energy system to a hybrid energy economy. In such an energy economy, each household is completely covered by PV modules and a minimum battery capacity to tackle the daily fluctuations. All the excess energy is fed to the hydrogen refinery where hydrogen is produced by an electrolyzer and stored. In times of need, the hydrogen is consumed by a fuel cell and fed as electricity to the households. Doing so can help to reduce the infrastructure costs (e.g. auxiliary components) by scattering it over all the consumers.

Finally, by adopting a centralized hydrogen refinery (or economy) and installing only PV modules and a battery bank for each household, regarding the found optimal prices of the main components, the LCOE of a typical Dutch household is reduced down to 0.19 €/kWh for energy that is purely produced via renewable energy sources. The found optimal prices are 0.01 €/Wp for the PV module, 0.01 €/Wh for the battery bank, 0.01 €/W for the electrolyzer and fuel cell and 0.08 €/kWh for the tank capacity,
Table 6.3: Results of the optimization process regarding system size, loss of load probability, total cost and levelized cost of energy. LCOE of the hybrid system with a vehicle, defined by \([X]\), are based on the total system cost but left out the investment, maintenance and replacement cost of the vehicle.

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Note: \(Az=19^\circ\ & Al=44.5^\circ\)

\([X]\) \(€0.01W\)/Wh/W
Table 6.4: Performance factors regarding optimal found system size. LCOE\(_{\text{gen}}\), of the hybrid system with a vehicle, defined by \([X]\), are based on the total system cost but left out the investment, maintenance and replacement cost of the vehicle.

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<th>LOE [%]</th>
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<td></td>
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<td></td>
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<tr>
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<td></td>
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<tr>
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<td>9.7</td>
<td>810</td>
<td>0.58</td>
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<td>73</td>
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<tr>
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Note: Costs are €0.01 per W/Wh
Figure 6.30: Ratio of total system cost for the feasible optimal solutions. Auxiliary cost of the PV-Battery consists of inverter and installation costs. Auxiliary cost of the PV-Hydrogen and Hybrid system consists of inverter, installation, pump, compressor, converter, fuels. A potential heat source or vehicle is also accounted for in the auxiliary costs. (1) PV-Battery year 2020. (2) PV-Hydrogen year 2020. (3) Hybrid year 2020. (4) Hybrid year 2030. (5) Hybrid year 2050, enlarge tank. (6) Electrical & Heat (I), gas boiler. (7) Electrical & Heat (II), heat pump (8) Electrical & Mobility (I), gasoline vehicle. (9) Electrical & Mobility (II), electrical vehicle. (10) Electrical & Mobility (III), hydrogen vehicle. (11) Hybrid year 2030, orientation. (12) Hybrid year 2050.
6.7. Remarks Regarding Assumptions

In this study several assumptions were made to simplify the simulation and optimization problems. Some of the major assumptions, that can affect the found results either in a positive way or a negative way, are discussed below.

Note that the defined optimization objective for this research study is: “System size where the Loss of Load Probability (LLP) is \( \leq 1\% \) for the lowest possible Levelized Cost of Energy (LCOE) over a lifetime of 25 years”. Yet, studying table 6.3, it can be concluded that most of the found system sizes corresponds to a LLP of 0\% rather than a LLP of 1\%. While the system size with the lowest LCOE is most probably close to a LLP of 1\%. Therefore, it can be concluded that the found system size for each case study is the local minimum of the optimization problem instead of the global minimum. Although the global minimum is not found, it should be noted that even a system size that corresponds to a LLP of 1\% (and thus lower LCOE) is an infeasible system size from an economical point of view. Since, neither of the found sizing is close to the current electricity price of 0.2 €/kWh.

Furthermore, the adopted penalty function for the equality constraints of the SoC of the battery and storage tank strongly influences the system size. Because, due to the equality constraint \( \text{SoC}_{	ext{ini}} = \text{SoC}_{	ext{fin}} \), for both storage methods, there is still energy left at the end of the year and thus also at the end of the 25 year. This applies to the optimal system size of all studied cases. Therefore, it can be interesting to perform an optimization for the entire project lifetime of 25 years. This way, the equality constraint of both storage methods can be dismissed and the \( \text{SoC}_{	ext{fin}} \) can be zero. It can be expected that this approach can lead to a smaller system size and thus a lower LCOE. But, it is not expected to become competitive with the current price of 0.2 €/kWh.

As previously determined, refer to table 3.11, the battery bank is replaced either every 500 charge cycles or 5 calendar years. An interesting fact observed from the results is that the battery bank endures on average 15 charge cycles per year. The battery charge cycles for each feasible optimal solution is given in table D.1 in appendix D. In other words, theoretically speaking, the battery bank requires no replacement during the project lifetime of 25 years. Consequently, the total system cost will drop down and so will the LCOE. Yet, practically speaking, it is common to replace a battery every 5 years due to the sulfation on the electrodes that reduce the battery capacity.

Remember that the calculated maximum power of the PV module is based on a constant degradation rate that corresponds to the 25\textsuperscript{th} year of it’s lifetime. Hence, in practical applications, an optimal sized system will perform better in the first year(s) of the project lifetime and linearly degrade down to the found conservative performance regarding the found optimal system sizes.

6.8. Concluding Remarks & Discussion

The previous sections comprehensively discussed several potential optimal system sizes. Each found optimal system size is designed with the intention to fulfill the total load demand of a typical Dutch household. The load demand is either the electrical demand, the electrical demand with additional heat demand or electrical demand with supplementary load demand corresponding a certain type of vehicle.

In the first section it was found that the optimal orientation of a PV array for the location of Vlissingen corresponds to an azimuth of 0.7° and an altitude of 37.8°. This orientation results in a maximum generated energy of 377.2 kWh by a single PV module in an entire year.

Next, three different system designs, namely PV-Battery, PV-Hydrogen and PV-Electrolyzer-Battery-FC, are optimal sized with the intention to fulfill the electrical load demand \( \text{LLP} \leq 1\% \) for the lowest LCOE. Results showed that both the PV-Battery and PV-Hydrogen systems are technically not applicable for a typical Dutch household. The PV-Battery system requires 61 PV modules and a battery capacity of 105 kWh. PV-Hydrogen system consists of 30 PV modules and a tank volume of 1.8 m\(^3\). Both systems tremendously exceed the maximum number of 21 PV modules. On the other hand, a hybrid PV-Electrolyzer-Battery-FC system with 19 PV modules, a battery capacity of 28.5 kWh and a tank volume of 1.18 m\(^3\) is able to fulfill the load demand within the physical restrictions. As can be observed
from figure 6.10, the battery bank is primarily used as the short term storage method (tackling the daily fluctuation) and the hydrogen tank as the long term storage (tackling the seasonal fluctuation). Unfortunately, the hybrid stand-alone system has a LCOE of 2.16 €/kWh and therefore is economically not a feasible system for a typical Dutch household in 2020 compared to the electricity bought from the grid for 0.2 €/kWh.

Repeating the optimization procedure for the hybrid system with the expected future prices in 2030 resulted in the following sizing: 19 PV modules, a battery capacity of 25.5 kWh and a tank volume of 1.24 m³. This sizing corresponds to a LCOE of 1.04 €/kWh. Yet, compared to the electricity price of 0.2 €/kWh, the stand-alone hybrid system is in 2030 still economically not viable. Moreover, a simulation is performed where the battery bank is not replaced for this hybrid system and the LCOE becomes 0.84 €/kWh. Thus, the hybrid system is economically still not feasible. On the other hand, it is observed that by removing the restriction of the tank volume, a cheaper optimal hybrid system size is found to fulfill the load demand for a LCOE of 0.97 €/kWh. Therefore, a potential centralized storage tank for hydrogen can perhaps be a solution to reduced the system cost even further.

Additionally, the optimal system size to fulfill both the electrical and heat demand solely by the hybrid system, resulted in an infeasible system. Both from a technical and economical point of view. The found system size consists of 550 PV modules, a battery capacity of 200 kWh and a tank volume of 30 m³ for a LCOE of 3.63 €/kWh. It should be noted that this found system size seems implausible due to insufficient convergence of the PSO algorithm. Providing the electrical demand by the technically feasible hybrid system (refer to 6.2.4) and the heat demand by a supplementary gas boiler (fed by fossil fuels) can reduce the LCOE to 1.78 €/kWh. Yet, compared to the electricity bought from the grid (0.2 €/kWh) and the natural gas bought from the grid (0.12 €/kWh), even a hybrid system with a gas boiler is economically not feasible in 2030.

Also, a case study is performed finding an optimal system size to fulfill both the electrical demand and the load demand of an electrical vehicle or a hydrogen vehicle. Found optimal system size for a hybrid system plus an electrical vehicle consists of 35 PV modules, a battery capacity of 170 kWh and a tank volume of 1.37 m³ for a LCOE of 2.15 €/kWh. Replacing the electrical vehicle with a hydrogen vehicle resulted in an optimal system size of 40 PV modules, a battery capacity of 72.5 kWh and a tank volume of 1.86 m³ for a LCOE of 0.95 €/kWh. Both optimal system sizing are neither technically nor economically feasible. A third case, where the discussed hybrid system in 6.2.4 adds a gasoline fueled vehicle (fed by fossil fuels) results in a LCOE of 1.37 €/kWh. Therefore, in terms of LCOE, it is more beneficial to adopt a stand-alone hybrid system, unrestricted by PV array size and tank volume to fulfill the hydrogen consumption of a hydrogen vehicle rather than a hybrid system fulfilling the electrical consumption of an electrical vehicle or a gasoline fueled vehicle. As previously observed, a centralized storage tank and a completely covered roof area of each household with PV modules can be the solution towards centralization in a sustainable matter.

Next, it is intended to find an optimal hybrid system size corresponding to a different orientation than the orientation (azimuth of 0.7° and altitude of 37.8°) found in 6.1. Found system size consists of of 18 PV modules, a battery capacity of 22.5 kWh and a tank volume of 1.20 m³. Corresponding PV array orientation is at an azimuth of 19.5° and an altitude of 42°. It seems that for the studied electrical load profile, where the demand is higher as the evening starts, orientating the PV array towards the Southwest (to receive the last available daily Sun hours) is more beneficial than the optimal orientation corresponding to maximum energy generation by the PV array. This results in a smaller system size and thus in a lower LCOE of 1.01 €/kWh.

Lastly, it is found that the future prices of the main components need to approach 0.01 €/Wₚ, for PV, 0.01 €/W for electrolyzer and fuel cell and 0.01 €/Wh for battery, to become competitive with the current electricity price of 0.2 €/kWh. Regarding these prices, the found optimal system size consists of 18 PV modules, a battery capacity of 39 kWh and a tank volume of 1.1 m³ with a LLP of 0.8% for a LCOE 0.28 €/kWh. For such a scenario, the total cost of the system is mainly composed of auxiliary cost (about 73%). The auxiliary cost is determined by the cost of the water pump, compressor, converters, inverter, demi water and cooling water.
Therefore, to finally reach a point where the LCOE of a renewable energy system equals the current price of 0.2 €/kWh (produced by fossil fuels), a completely centralized hydrogen economy is required. Each household is fully covered by PV modules and contains a battery capacity large enough to tackle the daily fluctuations. Excess energy is fed to the hydrogen refinery for hydrogen production and storage. In times of need, the hydrogen is consumed by a fuel cell in the refinery and fed as electricity to the consumer. By centralizing the hydrogen production, consumption and storage, the infrastructure costs (e.g. auxiliary components) of such a hydrogen economy can be scattered across all the consumers. If such a scenario is fulfilled, then the electricity can be provided in a renewable matter for a LCOE of 0.19 €/kWh.

As a final discussion point, the found LCOE for the proposed hybrid system is compared with the found LCOE’s in literature. The found LCOE 1.04 €/kWh for the hybrid system in this study is higher than the found LCOE’s by Lagorse (0.65 €/kWh [23]), Singh (0.18 €/kWh [31]) and Khemariya (0.19 €/kWh [32]). This can be explained by the fact that these studies are all performed in sunnier locations, like Morocco by Lagorse and India by Singh and Khemariya. Furthermore, the studied load demand profiles in these studies vary from a rural household in Morocco to an university building in an unelectrified village in India. In addition, all three studies have not taken into account the additional systems costs that is determined by the essential auxiliary components. Therefore, a one-to-one comparison of the found LCOE in this study with the LCOE’s found in literature is arbitrary.
Conclusion & Recommendations

In this final chapter, a summary of the interesting observations found in this thesis is provided. Subsequently, several recommendations are introduced and discussed that can guide future research. The aim of this research is introduced in chapter 1 and the following main objective is formulated: “Assess the feasibility of current and future stand-alone hybrid PV-Electrolyzer-Battery-FC energy systems from a techno-economical point of view, based on a numerical optimal system sizing for a typical household”.

7.1. Conclusion & Discussion

This master thesis research is performed to assess the techno-economical feasibility of a stand-alone hybrid PV-Electrolyzer-Battery-FC energy system for residential utilization of a typical Dutch household. Technical feasibility is based on the physical restrictions of the area of a typical average Dutch household, i.e. 21 PV modules, 140 kWh battery capacity and 2 m³ storage tank. Economical feasibility is based on the competitiveness compared to the current electricity price of 0.20 €/kWh produced by fossil fuels. The proposed hybrid system consists of the following main components: (1) PV modules, (2) Alkaline electrolyzer, (3) PEM fuel cell, (4) Lead-Acid battery, (5) Cylindrical storage tank, (6) Master controller and auxiliary components. Lead-Acid battery bank is used as a short term storage method and the chemical product of hydrogen is used as a long term storage method. The studied location is Vlissingen, in the South of the Netherlands.

Firstly, an extended simulation model of the PV-Electrolyzer-Battery-FC energy system is developed within the TRNSYS environment. The theoretical models are mainly based on electrical, thermodynamics, electrochemical and transport phenomena. Electrical model of the PV module is empirically derived by illuminating the mono-crystalline BenQ SunForte 335 Wp module with the LASS in the PVMD lab. The electrochemical and thermal model of the alkaline electrolyzer is based on the studied and empirically verified PHOEBUS electrolyzer by Meurer and Ulleberg [29, 115]. For the conversion of hydrogen to electricity a PEM fuel cell is adopted. The electrochemical and thermal model of the fuel cell is based on the study of Amphlett [120]. For the adopted lead-acid, the battery model studied by Raszmann et al. [122] is used with an assumed constant round-trip efficiency of 78%. Storage of hydrogen is done by the implementation of a high pressure cylindrical tank at 350 bar. Subsequently, a master controller is developed to manage the energy flows between the PV array, load demand, storage methods and Balance of System components.

Secondly, a sub-objective of this thesis project is to find an applicable optimization algorithm for the optimization of the proposed stand-alone hybrid system. TRNSYS has an optimization functionality, called TRNOPT, which is an implementation of the well-known Generic Optimization Program (GenOpt) within the TRNSYS environment. For this study, the optimization method of PSO+Hooke-Jeeves (Particle Swarm optimization and Hooke-Jeeves) is adopted. PSO starts with multiple randomly defined points making it more efficient (in terms of computational power) and reduces the chance of getting stuck in a local minimum. Then, the Hooke-Jeeves method performs a pattern search. Possibly improving the found minimum (i.e. by the PSO algorithm) if it is a local minimum.

The adopted optimization method of PSO+Hooke-Jeeves is used to find the optimal system size of the proposed stand-alone hybrid system for fulfillment of electrical, heat and mobility demand at residential level. For the electrical demand fulfillment the following case studies are studied: (I) electrical demand
fulfillment by (i) a PV-Battery system, (ii) a PV-Electrolyzer-FC system and (iii) a hybrid PV-Electrolyzer-Battery-FC system (based on current and future components prices). Then, the optimal system size is intended to be found for the combined electrical and heat demand. Fulfillment of the heat demand is either realized by an old-fashioned gas boiler or a heat pump. Next, the combined electrical and mobility demand is studied for the cases of a gasoline fueled vehicle, an electrical vehicle and a hydrogen vehicle. Also, it is intended to determine what the benefits are for a PV array oriented corresponding to the load demand profile rather than orientated for the maximum energy generation. Lastly, a case study is performed to establish the future prices of the main components so that the stand-alone hybrid system can be competitive with the current electricity price.

Based on the found results and the gained knowledge, it is established that only the proposed stand-alone hybrid PV-Electrolyzer-Battery-FC is technically feasible to be implemented under specified load demands. It is solely feasible for the fulfillment of the annual electrical demand of a typical Dutch household. The found feasible system size consists of 19 PV modules, battery capacity of 25.5 kWh and a tank volume of 1.24 m$^3$ for a LCOE of 1.04 €/kWh. All other case studies are technically infeasible due to the physical limitations of the area of a typical average Dutch household. In terms of LCOE, all studied cases are economically infeasible in the year of 2030. The found LCOE's tremendously exceed the current electricity price bought from the grid. Additionally, it was observed that an optimal PV array orientation corresponding to the load demand profile is more beneficial than the optimal PV array orientation for maximal energy generation. This leads to a smaller system size and thus lower LCOE.

To determine future potential of hydrogen storage based systems, it is of high importance to understand the limitations, both from a technical and economical point of view. From a technical point of view, the limiting factors seem to be the average number of PV modules that can be installed on the roof and the available space that can be occupied by the hydrogen tank for a typical average Dutch household. From an economical point of view, the limiting factors are the prices of the electrolyzer and fuel cell. Both are mostly still being manufactured and implemented on a small scale basis in comparison to the other two main components: PV modules and lead-acid battery. Therefore, if the prices of the main components: PV modules, battery, electrolyzer and fuel cell drop down (i.e. 0.01 €/W$^p$, for PV, 0.01 €/Wh for battery and 0.01 €/W for electrolyzer and fuel cell), the hybrid system can potentially reach a LCOE of 0.28 €/kWh. So, the proposed system would still be slightly overpriced compared to the current electricity price of 0.2 €/kWh. Hence, it is an infeasible system from an economical point of view. However, sooner or later, a LCOE of 0.17 €/kWh can be realized by renewable energy systems if the following conditions are met: (1) electrolyzer and fuel cell prices should drop to 0.01 €/W, (2) battery price should drop to 0.01 €/Wh, (3) module's price should drop to 0.01 €/W$^p$, (4) fully covered roof area by PV modules and (5) the production, consumption and storage of hydrogen should be centralized to scatter the infrastructure costs over all the consumers. The LCOE can be reduced even further, if it is managed to install large area's full of PV modules that can generate energy and store it as hydrogen in storage tanks. For a centralized large scale utility of hydrogen, a pressurized cylindrical tank at 700 bar with a volume of roughly 45 million m$^3$ is required for the fulfillment of the total annual heat demand of the 8 million households in the Netherlands.

By looking beyond the horizon, it can even be beneficial to use the large solar parks in the “solar belt”, e.g. South America and the Middle East, to store all the generated energy in the form of hydrogen in large tanks. Transfer the hydrogen in liquid form by ships to countries with limited Sun hours (e.g. the Netherlands) and convert the hydrogen back to usable electricity. Although, this approach entails a lot of unanswered question regarding the transfer of hydrogen in large quantities, it can eventually reach a LCOE of 0.05-0.09 /kWh [200]. These large quantity of produced hydrogen can be stored long term and preferably used to fulfill the high heat demand in the winter, whereas the combination of PV modules, a battery bank and centralized storage tanks on site (in the Netherlands) can be used for the electrical demand.

7.2. Future Recommendations

Even though the found results of this thesis research answer the sub-objectives and thus the main objective, the following recommendations can help future research: (I) metal hydrid tanks and lithium-ion battery, (II) constant hydrogen production, (III) adjustable PV array orientation, (IV) peak demand of a specific household and (V) yearly hydrogen stocking.
In this study, a lead-acid battery and a cylindrical storage tank are used for respectively short term and long term storage. However, it can be interesting to study the performance of the proposed hybrid system if other technologies are adopted. Such as replacing lead-acid battery by lithium-ion batteries, since these are becoming mature and thus cheaper in the future and have a larger energy density compared to lead-acid batteries. Additionally, a metal hydrid tank can be used instead of an old fashioned cylindrical storage tank. Metal hydrid tanks have the ability to store roughly four times the amount of hydrogen compared to a pressurized tank of 800 bar (35 kg/m\(^3\) vs 120 kg/m\(^3\)). Also, the hydrogen is stored at atomic level and requires energy to be released and thus a safe storage option. Advantage is that no energy is required for storage but disadvantage is that energy is required for release and it is more expensive than cylindrical storage tank. Adoption of lithium-ion battery and the metal hydrid can tackle the physical restrictions but has a negative effect on the total system cost.

Next, it can be interesting to study the effect of a different energy management strategy. One can study if the performance of the hybrid system and thus system size can be influenced if batteries are not only used as a short term storage method but also to power the electrolyzer during the night. Doing so can help to only activate the electrolyzer for a long run instead of an unlimited on/off cycles. This can help to increase the lifetime of the electrolyzer and the electrolyzer needs fewer replacements during the lifetime of the project. Thus, the total system cost can decrease and as a result the LCOE.

The case study, whereby the optimal found orientation was found regarding the load demand profile, shows that it can be interesting to adopt adjustable PV array orientation that changes throughout the day and year. Whereas the generated energy is decreased by roughly 1.7% due to the smaller PV array size (from 19 to 18 PV modules), the annual electrical load demand is still fulfilled (i.e. LLP is 0%) and the LCOE is decreased by 3%. Besides the PV array size, also the battery bank capacity and tank volume are decreased by respectively 8.0% and 3.2%. Thus, an adjustable PV array orientation can lead to a better match of the generated solar energy and the load demand. As a consequence, the system size is reduced and thereby system costs.

The studied load profiles are average profiles for a typical Dutch household and thus are not representative for a specific Dutch household. Because, in practice, a specific household encounters a higher peak demand on any day than the determined peak demand of 800W shown in figure 5.1. Simply using an oven results in a higher peak demand of about 1500W. Therefore, repeating the optimization for the load demand profile of a specific household can result in a more expensive system due to the higher rated power of the fuel cell and perhaps a larger systems size. Simulations confirmed that by altering the load profile in such a way that, a peak demand of 1500W occurs between 9-11 AM and 8-10 PM, the found optimal hybrid system size (discussed in 6.2.4) is not able to fulfill the LLP inequality constraint. The found LLP corresponds to 4.5% and thus is not an acceptable system size. Future research can focus on a more specified load demand profile whereby multiple peak demands are taken into account.

An interesting next step can be to dismiss the equality constraints of the battery capacity and hydrogen storage tank. Doing so can lead to an optimal system size that is smaller (in terms of battery capacity and storage tank volume) but manages to fulfill the load demand of a typical Dutch household in the first year of the lifetime. Consequently, the found initial SoC of the tank and battery have to be met at the start of each year. This impairs the term “autonomous” but can lead to a lower LCOE.
A.1. Thermal Model PV Module

To account for environmental fluctuations that have a critical impact on the characteristic current-voltage curve of a PV module and determine the corresponding characteristic current-voltage curve at any ambient condition requires the adoption of equations A.1, A.2, A.3 and A.4.

\[ I_L = I_{LSTC} \cdot \frac{G_{POA}}{G_{POASTC}} \]  
\[ T_m = T_{amb} + \left( \frac{T_{NOMT} - 20}{G_{NOMT}} \right) \cdot G_{POA} \cdot \left( \frac{9.5}{5.7 \cdot 3.8 \cdot v_{wind}} \right) \cdot \left( 1 - \frac{\eta_m}{\tau a} \right) \]  
\[ \frac{I_D}{I_{DSTC}} = \left( \frac{T_m}{T_{mSTC}} \right)^3 \cdot \exp \left[ \frac{1}{k} \left( \frac{E_{gSTC}}{T_{mSTC}} - \frac{E_g}{T_m} \right) \right] \]  
\[ E_g = E_{gSTC} - \left( \frac{4.73 \cdot 10^{-4} \cdot T_m}{636 + T_m} \right) \]

where:
- \( G_{POA} \), plane of array irradiance on module
- \( G_{POASTC} \), plane of array irradiance on module at STC
- \( T_{amb} \), ambient temperature
- \( T_{NOMT} \), temperature at normal operation module temperature conditions
- \( G_{NOMT} \), irradiance at normal operation module temperature conditions
- \( E_g \), semiconductor bandgap energy crystalline silicon
- \( E_{gSTC} \), semiconductor bandgap energy crystalline silicon at STC [1.12 eV [37]]
- \( v_{wind} \), wind speed at location
- \( \tau a \), fraction of incident light absorbed by crystalline module [0.9 [103]]
The diode ideality factor and the series resistor are assumed to be independent of irradiance or temperature change [105] where the generated current depends linearly on incident irradiation and the dark diode current and bandgap of the semiconductor material are dependent of the module's temperature. In turn is the module's temperature influenced by the ambient temperature and wind speed with respect to the Normal Operation Module Temperature ($G_{NOMT} = 800 \text{ W/m}^2$, $T_{amb} = 20^\circ \text{C}$, $v_{wind} = 1 \text{ m/s}$).

### A.2. Extrapolated IV and PV curves

![IV curves extrapolated](image)

**Figure A.1:** Extrapolated current-voltage curves at $T_m = 30^\circ \text{C}$.
A. Thermal model & Extrapolated current-voltage and power-voltage curves

Figure A.2: Extrapolated power-voltage curves at $T_m = 30^\circ$C.

Table A.1: PV module parameters at ECT ($G_{\text{m}_{\text{ECT}}} = 970 \frac{W}{m^2}$ and $T_{\text{m}_{\text{ECT}}} = 30^\circ$C).

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<th>$G_m = 500 \frac{W}{m^2}$</th>
<th>$G_m = 800 \frac{W}{m^2}$</th>
<th>$G_m = 970 \frac{W}{m^2}$</th>
<th>$G_m = 1000 \frac{W}{m^2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_{oc}$</td>
<td>57.1 [V]</td>
<td>60.5 [V]</td>
<td>62.3 [V]</td>
<td>64.0 [V]</td>
<td>63.1 [V]</td>
</tr>
<tr>
<td>$V_{mp}$</td>
<td>47.4 [V]</td>
<td>50.1 [V]</td>
<td>51.4 [V]</td>
<td>52.7 [V]</td>
<td>52.0 [V]</td>
</tr>
</tbody>
</table>

A.3. Datasheet
Figure A.3: Datasheet BenQ SunFortesolar module 335Wp.
Thermal Model Electrolyzer

B.1. Thermodynamics

In 2.2.1 is explained that the decomposition of one mole water into hydrogen and oxygen gas requires a minimum of 285.8 kJ energy, majorly electricity and partly heat:

\[ H_2O(l) + Electricity + Heat \rightarrow H_2(g) + \frac{1}{2}O_2(g) \]  \hspace{1cm} (B.1)

Water splitting is done under the assumptions that hydrogen and oxygen gas are ideal gases, that gas and liquid phase are separated and that water is an incompressible fluid [172]. Considering these assumptions the required minimum energy of 285.8 kJ/mol for splitting water into pure hydrogen and oxygen gas at the standard condition of 1 bar and 25°C corresponds to the change in enthalpy, where the electrical energy is defined by the Gibbs free energy (\( \Delta G^o \)) and the thermal energy is defined by the temperature of the process and the entropy change (\( T \Delta S^o \)):

\[ \Delta H^o = \Delta G^o + T \cdot \Delta S^o \]  \hspace{1cm} (B.2)

where:

- \( \Delta H^o \), change enthalpy standard conditions
- \( \Delta G^o \), change internal energy standard conditions
- \( \Delta S^o \), change entropy standard conditions
- \( T \), temperature

The electrical energy defined by the \( \Delta G^o \) is equal to 237.2 kJ/mol and the thermal energy defined by \( T \Delta S^o \) is equal to 48.6 kJ/mol at the standard conditions of 1 bar and 25°C [51]. Changing the pressure and/or the temperature of the electrolysis process affects the enthalpy change (\( \Delta H^o \)), Gibbs free energy change (\( \Delta G^o \)) and the product of temperature and entropy change (\( T \Delta S^o \)) as shown in figures B.1 and B.2. Figure B.1 shows the change in energies at constant pressure of 1 bar for increasing temperature. Increasing the temperature up to 100°C decreases the electrical energy required for electrolysis while the thermal energy increases resulting in a net decrease of the enthalpy change. Further increment of the temperature results in a negligible net increase of the enthalpy change in the gaseous phase by a decrease of electrical energy and an increase of the thermal energy. Note that the latent heat of water vaporization (about 40.8 kJ/mol) is not taken into consideration for the total energy demand (i.e. enthalpy change) for temperature above 100°C. The effect of pressure increase on the enthalpy change, see figure B.2, can be neglected. Even though the electrical energy part increases slightly with a decreasing thermal energy part, the total energy consumption (i.e. enthalpy change) remains practically constant.
It can be concluded from figure B.1 that electrolysis at higher temperatures, hence requiring more thermal and less electrical energy compared to standard condition of 25°C, is more beneficial since producing electrical energy is more costly than producing thermal energy. Especially in combined heat and power systems (cogeneration) where the thermal energy of the electrolysis can be provided by the potential waste heat of the system. This could result in a lower cost of the produced hydrogen. But electrolysis at higher temperatures increases the capital costs because of the more costly materials and ceramics (e.g. electrodes and electrolyte) to endure the high temperatures. On the other hand if it is more straightforward to provide electrical energy rather than thermal energy for electrolysis, increasing the pressure can be an option as figure B.2 displays.

The correlative voltage to apply the electrical energy (i.e. change in Gibss free energy) is known as the reversible voltage and is expressed by:

$$V_{rev} = \frac{\Delta G}{z \cdot F}$$

(B.3)
where:

- $V_{rev}$, reversible voltage
- $z$, number of electrons per hydrogen molecule
- $F$, faraday constant

The reversible voltage potential corresponds to the minimum electrical energy required for initiating the electrolysis process. But as equations B.1 and B.2 express, water electrolysis also requires energy in the form of heat. If the required heat is applied by electrical energy, which is common in commercial electrolyzers, the minimum voltage for water electrolysis is not the reversible voltage but the thermoneutral voltage ($V_{tn}$) and is expressed as:

$$V_{tn} = \frac{\Delta H}{z \cdot F} \quad (B.4)$$

Both the values for the reversible ($V_{rev}^0$) and thermoneutral voltage ($V_{tn}^0$) potentials at standard conditions of 1 bar and 25°C are 1.23V and 1.48V respectively by the Faraday constant ($F = 96485$ coulombs/mole) and the number of electrons ($z = 2$) for splitting one mole of water into one mole of hydrogen and half mole of oxygen gas. The change in temperature affecting the reversible voltage for $F = 96485$ coulombs/mole and the number of electrons $z = 2$, can also be directly calculated by the Nernst equation [202]:

$$V_{rev} = V_{rev}^0 - 0.9e^{-3} \cdot ([T + 273] - 298) + \frac{R \cdot (T + 273)}{z \cdot F} \cdot \ln \left( \frac{p_{H_2} \cdot p_{\frac{1}{2}O_2}}{p_{H_2O}} \right) \quad (B.5)$$

Note that both the reversible voltage and voltage potential due to $T \Delta S$ can differ for other combinations of pressure and temperature as displayed in figures B.1 and B.2. But the thermoneutral voltage will remain practically constant as $\Delta G$ increases and $T \Delta S$ decreases or vice versa.

**B.2. Thermal Model PHOEBUS Electrolyzer**

The temperature of the electrolyzer is determined by a simple quasi-static thermal model using the thermal capacitance of the PHOEBUS electrolyzer as follow:

$$\frac{\partial T}{\partial t} = \frac{\dot{Q}_{net}}{C_{t_{ely}}} \quad (B.6)$$

where $C_{t_{ely}}$ is the thermal capacitance of the electrolyzer and $\dot{Q}_{net}$ is the net difference of the generated heat ($\dot{Q}_{gen}$) lowered by the natural heat loss to the ambient ($\dot{Q}_{loss}$) and auxiliary cooling ($\dot{Q}_{cool}$) expressed as:

$$\dot{Q}_{net} = \dot{Q}_{gen} - \dot{Q}_{loss} - \dot{Q}_{cool} \quad (B.7a)$$

$$\dot{Q}_{gen} = n_z \cdot I_{ely} \cdot (V_{celly} - V_{tn}) \quad (B.7b)$$

$$\dot{Q}_{loss} = \frac{T_{ely} - T_{amb}}{R_{t_{ely}}} \quad (B.7c)$$

$$\phi_{m_{H_2O}} = \frac{\dot{Q}_{cool}}{C_{p_{H_2O}} \cdot (T_{w_{out}} - T_{w_{in}})} \quad (B.7d)$$

where:
• \( \dot{Q}_{\text{net}} \), net heat difference
• \( T_{\text{amb}} \), ambient temperature
• \( C_{t_{\text{ely}}} \), thermal capacitance electrolyzer [625 \cdot 10^3 \text{ J K}^{-1},[115]]
• \( R_{t_{\text{ely}}} \), thermal resistance electrolyzer [0.167 K W\(^{-1}\),[115]]
• \( C_{\text{H}_2\text{O}} \), heat capacity water
• \( T_{\text{w}_{\text{out}}} \), temperature cooling water out
• \( T_{\text{w}_{\text{in}}} \), temperature cooling water in

Subsequently is the model extended to calculate the consumed demi water and cooling water since both influence the system cost and hence the economical analysis:

\[
\phi_{v_{\text{demi}}} = \frac{\phi_{\text{molar}_{\text{DEMI}}} \cdot M_{\text{H}_2\text{O}}}{\rho_{\text{DEMI}}} \tag{B.8}
\]

\[
\phi_{v_{\text{cooling}}} = \phi_{m_{\text{H}_2\text{O}}} \cdot \rho_{\text{H}_2\text{O}} \tag{B.9}
\]

where:
• \( \phi_{v_{\text{demi}}} \), volumetric flow demi water
• \( \phi_{v_{\text{cooling}}} \), volumetric flow cooling water
• \( \phi_{\text{molar}_{\text{H}_2\text{O}}} \), molar flow demi water
• \( \rho_{\text{H}_2\text{O}} \), density water
• \( \rho_{\text{DEMI}} \), density demi-water
• \( M_{\text{H}_2\text{O}} \), molar mass water

It should be noted that it is assumed that the cooling of the electrolyzer is done directly via cooling water and no heat exchanger or any cooling fan is in play. Further is the produced oxygen gas is not stored in any way but released into the atmosphere.
C.1. Thermodynamics

Section 2.2.2 explained the “combustion” of hydrogen and oxygen gas forming water (vapor), heat as useless byproduct (48.6 kJ/mol) and usable electrical energy of 237.2 kJ/mol for one mole of hydrogen at the standard conditions of 1 bar and 25°C:

\[ H_2(g) + \frac{1}{2}O_2(g) \rightarrow H_2O(l) + Electricity + Heat \]  \hspace{1cm} (C.1)

The expressed equation for the change in enthalpy by eq. B.2, under the assumptions that hydrogen and oxygen gas are ideal gases, that gas and liquid phase are separated and that water is an incompressible fluid, is also valid for the fuel cell with a subtle difference that the process delivers energy instead of consuming [172]. Similar to an electrolyzer, the result of operating at higher temperatures leads to a decrease in the change of Gibbs (\( \Delta G \)) free energy and an increase in the product of temperature and entropy change (\( T \Delta S \)) while the change in enthalpy (\( \Delta H \)) remains practically constant. As with the electrolyzer, an increment in pressure can be neglected for the change in energies. Hence a higher operating temperature of a fuel cell results in a smaller \( \Delta G \) and a larger \( T \Delta S \) as useless heat. Only if such fuel cells are used in cogeneration and the byproduct of heat can be utilized, it is favorable to operate fuel cells at higher temperatures. Subsequently, equations B.3 and B.4 can be used to calculate the reversible and thermoneutral voltage of the fuel cell. Both the values for the reversible (\( V_{rev} \)) and thermoneutral voltage (\( V_{th} \)) potentials at standard conditions of 1 bar and 25°C are 1.23V and 1.48V respectively by the Faraday constant (\( F = 96485 \) coulombs/mole) and the number of electrons (\( z = 2 \)) for the combustion of one mole of hydrogen and half mole of oxygen into one mole of water. Again the change in temperature affecting the reversible voltage for, \( F = 96485 \) coulombs/mole and the number of electrons \( z = 2 \), can also be directly calculated by the Nernst equation given in eq. B.5.

C.2. Thermal Model PEM Fuel Cell

Temperature of the fuel cell is determined by a simple quasi-static thermal model using the thermal capacitance of the studied PEM fuel cell as follow:

\[ \frac{\partial T}{\partial t} = \frac{\dot{Q}_{rest}}{C_{tfc}} \] \hspace{1cm} (C.2)

where \( C_{tfc} \) is the thermal capacitance of the fuel cell and \( \dot{Q}_{rest} \) is the net difference of the generated heat (\( \dot{Q}_{gen} \)) lowered by the natural heat loss to the ambient (\( \dot{Q}_{loss} \)), lowered by the evaporation of the
Thermal Model PEM Fuel Cell

water at the cathode ($\dot{Q}_{\text{evap}}$) and auxiliary cooling ($\dot{Q}_{\text{cool}}$) expressed as:

$$
\dot{Q}_{\text{rest}} = \dot{Q}_{\text{gen}} - \dot{Q}_{\text{loss}} - \dot{Q}_{\text{evap}} - \dot{Q}_{\text{cool}} \quad (C.3a)
$$

$$
\dot{Q}_{\text{gen}} = n_s \cdot I_{fc} \cdot (V_{tn} - V_{\text{cell,fc}}) \quad (C.3b)
$$

$$
\dot{Q}_{\text{loss}} = \frac{T_{fc} - T_{\text{amb}}}{R_{tfc}} \quad (C.3c)
$$

$$
\dot{Q}_{\text{evap}} = x_{\text{evap}} \cdot h_{f\text{H}_2\text{O}} \cdot \phi_{\text{m,DEMI}} \quad (C.3d)
$$

$$
\phi_{m_{\text{H}_2\text{O}}} = \frac{\dot{Q}_{\text{cool}}}{C_{p\text{H}_2\text{O}} \cdot (T_{\text{wout}} - T_{\text{win}})} \quad (C.3e)
$$

where:

- $\dot{Q}_{\text{rest}}$, rest heat difference
- $T_{\text{amb}}$, ambient temperature
- $C_{tfc}$, thermal capacitance fuel cell
- $R_{tfc}$, thermal resistance fuel cell
- $C_{p\text{H}_2\text{O}}$, heat capacity water
- $x_{\text{evap}}$, Enthalpy of water vaporization
- $h_{f\text{H}_2\text{O}}$, fraction of demi water vaporized
- $T_{\text{wout}}$, temperature cooling water out
- $T_{\text{win}}$, temperature cooling water in

The thermal capacitance and the thermal resistance are dependent of the geometry of the fuel cell and are calculated according to equations C.4, C.5 and the tabulated characteristics of the fuel cell in table C.1.

$$
R_{tfc} = \frac{L_{frame}}{k_{fc} \cdot A_{fc}} + \frac{1}{h_{\text{air}} \cdot A_{fc}} \quad (C.4)
$$

$$
C_{tfc} = \left( c_{pfc} \cdot \rho_{fc} \cdot n_s \cdot h_{fc} \cdot w_{fc} \cdot t_{fc} \right) + 
\left( 2 \cdot c_{p\text{plate}} \cdot \rho_{\text{plate}} \cdot h_{\text{plate}} \cdot w_{\text{plate}} \cdot t_{\text{plate}} \right) \quad (C.5)
$$
Table C.1: Characterizations of the adopted PEM fuel cell model [120].

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n_s$</td>
<td>35</td>
<td>number of cells in a single fuel cell stack</td>
</tr>
<tr>
<td>$h_{fH_2O}$</td>
<td>0.25</td>
<td>Fraction of demi water vaporized</td>
</tr>
<tr>
<td>$L_{frame}$</td>
<td>0.029 m</td>
<td>Average distance between PEM fuel cell and air</td>
</tr>
<tr>
<td>$A_{fc}$</td>
<td>0.17 m$^2$</td>
<td>Total surface fuel cell</td>
</tr>
<tr>
<td>$k_{fc}$</td>
<td>14.1 W/(m K)</td>
<td>Thermal conductivity fuel cell material</td>
</tr>
<tr>
<td>$t_{plate}$</td>
<td>0.02 m</td>
<td>Thickness end plate</td>
</tr>
<tr>
<td>$w_{plate}$</td>
<td>0.231 m</td>
<td>Width end plate</td>
</tr>
<tr>
<td>$h_{plate}$</td>
<td>0.231 m</td>
<td>Height end plate</td>
</tr>
<tr>
<td>$t_{fc}$</td>
<td>0.005 m</td>
<td>Thickness cell</td>
</tr>
<tr>
<td>$w_{fc}$</td>
<td>0.21 m</td>
<td>Width cell</td>
</tr>
<tr>
<td>$h_{fc}$</td>
<td>0.21 m</td>
<td>Height cell</td>
</tr>
<tr>
<td>$\rho_{plate}$</td>
<td>7850 kg/m$^3$</td>
<td>Density end plate material</td>
</tr>
<tr>
<td>$\rho_{fc}$</td>
<td>2250 kg/m$^3$</td>
<td>Density fuel cell material</td>
</tr>
<tr>
<td>$c_{plate}$</td>
<td>450 J/(kg K)</td>
<td>Heat capacity end plate material</td>
</tr>
<tr>
<td>$c_{pfc}$</td>
<td>710 J/(kg K)</td>
<td>Heat capacity fuel cell material</td>
</tr>
</tbody>
</table>

Subsequently is the model extended to calculate the required cooling water that influences the system cost and hence the economical analysis:

$$\phi_{\nu_{cooling}} = \phi_{m_{H_2O}} \cdot \rho_{H_2O}$$  \hfill (C.6)

It should be noted that it is assumed that the cooling of the fuel cell is done directly via cooling water and no heat exchanger or any cooling fan is in play. Further is the fuel cell assumed to be consuming pure oxygen instead of air extracted from the atmosphere.
## Optimization Results

### D.1. Cycle life battery, electrolyzer and fuel cell

Table D.1: Number of charge cycle of the battery bank and operational hours of the electrolyzer and fuel cell for each case study. Note: only the feasible sizing for each case is given.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
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</thead>
<tbody>
<tr>
<td>PV-Battery year 2020</td>
<td>2</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>PV-Hydrogen year 2020</td>
<td>0</td>
<td>3279</td>
<td>5436</td>
</tr>
<tr>
<td>Hybrid year 2020</td>
<td>8</td>
<td>1120</td>
<td>1284</td>
</tr>
<tr>
<td>Hybrid year 2030 Electrical Demand</td>
<td>12</td>
<td>1123</td>
<td>1325</td>
</tr>
<tr>
<td>Hybrid year 2030 Electrical &amp; Heat (I)</td>
<td>12</td>
<td>1123</td>
<td>1325</td>
</tr>
<tr>
<td>Hybrid year 2030 Electrical &amp; Heat (II)</td>
<td>5</td>
<td>155</td>
<td>208</td>
</tr>
<tr>
<td>Hybrid year 2030 Electrical &amp; Mobility (I)</td>
<td>12</td>
<td>1123</td>
<td>1325</td>
</tr>
<tr>
<td>Hybrid year 2030 Electrical &amp; Mobility (II)</td>
<td>2</td>
<td>555</td>
<td>865</td>
</tr>
<tr>
<td>Hybrid year 2030 Electrical &amp; Mobility (III)</td>
<td>2</td>
<td>2149</td>
<td>381</td>
</tr>
<tr>
<td>Hybrid year 2050 Optimal Orientation</td>
<td>16</td>
<td>1235</td>
<td>1421</td>
</tr>
<tr>
<td>Hybrid year 2050 Optimal Prices</td>
<td>13</td>
<td>1242</td>
<td>1468</td>
</tr>
</tbody>
</table>
### D.2 Standard Deviation Particle Swarm Optimization

Table D.2: Standard Deviations Particle Swarm Optimization per case study. Note: only the feasible sizing per case is given.

<table>
<thead>
<tr>
<th>Case</th>
<th>$N_m$ [-]</th>
<th>$E_{Batt,rated}$ [kWh]</th>
<th>$V_{tank}$ [m$^3$]</th>
<th>$SoC_{batt,ini}$ [%]</th>
<th>$SoC_{tank,ini}$ [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>PV-Battery year 2020</strong></td>
<td>28.5</td>
<td>150</td>
<td>130</td>
<td>29.5</td>
<td>8.30</td>
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<tr>
<td><strong>PV-Hydrogen year 2020</strong></td>
<td>28.6</td>
<td>3.00</td>
<td>1.70</td>
<td>28.9</td>
<td>15.6</td>
</tr>
<tr>
<td><strong>Hybrid year 2020</strong></td>
<td>6.80</td>
<td>38.4</td>
<td>5.80</td>
<td>34.8</td>
<td>3.99</td>
</tr>
<tr>
<td><strong>Hybrid year 2030</strong></td>
<td></td>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Electrical Demand</td>
<td>6.50</td>
<td>40.6</td>
<td>13.7</td>
<td>29.8</td>
<td>7.01</td>
</tr>
<tr>
<td>Electrical &amp; Heat (I)</td>
<td>6.50</td>
<td>40.6</td>
<td>13.7</td>
<td>29.8</td>
<td>7.01</td>
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<tr>
<td>Electrical &amp; Heat (II)</td>
<td>220</td>
<td>89.3</td>
<td>30.1</td>
<td>29.9</td>
<td>7.10</td>
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<tr>
<td>Electrical &amp; Mobility (I)</td>
<td>6.50</td>
<td>40.6</td>
<td>13.7</td>
<td>29.8</td>
<td>7.01</td>
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<tr>
<td>Electrical &amp; Mobility (II)</td>
<td>33.2</td>
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<td>16.5</td>
<td>29.2</td>
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<td>Electrical &amp; Mobility (III)</td>
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<td>45.4</td>
<td>11.2</td>
<td>29.6</td>
<td>2.11</td>
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<td>Hybrid year 2030</td>
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<tr>
<td>Electrical &amp; Heat (I)</td>
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<td>40.9</td>
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<td>Electrical &amp; Mobility (II)</td>
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<tr>
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<td>5.82</td>
<td>38.9</td>
<td>16.2</td>
<td>28.2</td>
<td>19.3</td>
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<td><strong>Optimal Prices</strong></td>
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</table>


[20] The flammable range (explosive range).


[69] Electrochemical cells. [http://hyperphysics.phy-astr.gsu.edu/hbase/Chemical/electrochem.html#c3](http://hyperphysics.phy-astr.gsu.edu/hbase/Chemical/electrochem.html#c3). Accessed 28-02-2019.


[71] H. Keshan; J. Thornburg; T.S. Ustun. Comparison of lead-acid and lithium ion batteries for stationary storage in off-grid energy systems. 4th IET Clean Energy and Technology Conference, (2016).


