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Engineering

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Hydrogen Systems Modelling, Analysis and Optimisation

MPhil Thesis

September 2009

Table of contents

List of figures

List of tables

Abstract

The hydrogen economy is regularly presented as the means to solve both global warming and depletion of fossil fuel resources. However hydrogen technologies are still immature with performance disappointing when compared to conventional systems, which is a major obstacle to the widespread deployment of hydrogen as a viable solution for the future. Computer simulation can help to improve the performance of hydrogen technologies and move what is still a research area towards technical and commercial reality.

To this end, this thesis is concerned with the development of computer models to assist engineers in the design and implementation of hydrogen energy systems. Four typical hydrogen systems have been developed on the TRNSYS [1] platform:

- Stand-alone power system
- Low power application
- Energy buffering system for large wind farms
- Filling station

These models allow the user to perform the following actions:

- Design and simulate the system
- Optimise the size and configuration of the system
- Analyse the technical and economic performance of the system

The models developed on TRNSYS are highly detailed with large numbers of components and parameters; subsequently, these are suitable for expert users only. To assist in the diffusion of modelling technology into the hydrogen community, user-friendly interfaces have been developed for each model that present a simplified view of each model, with only selected parameters available for manipulation. Further, the interface also presents results from the simulations in an integrated and easily understandable form.

In the future these models can be used as a platform to simulate a large variety of hydrogen energy systems. They combine the technical capabilities of the TRNSYS software with an economic model, made available to any user thanks to the user-friendly interface.

The models have been tested and validated using a combination of theoretical and experimental results and have also been successfully applied to the analysis of the wind/hydrogen hybrid system on the Island of Utsira in Norway. This case study illustrated how computer modelling can help improving the design of hydrogen systems and therefore increase their performance.

The work described in this thesis was undertaken as part of a collaborative project between SgurrEnergy and the University of Strathclyde in Glasgow.

A. Introduction and presentation of the project

1. Hydrogen economy

The term "hydrogen economy" has different definitions, but in its purest sense, it represents an energy scheme relying exclusively on renewable energies for its primary resource and hydrogen for energy storage. The term was first used during the energy crisis of the 1970's to describe an energy infrastructure based on hydrogen produced from non-fossil primary energy sources. [2]

As providing efficient responses to human-induced climate change becomes more and more critical, the so-called hydrogen economy with the energy systems associated with it are often proposed as the means to solve both global warming and depletion of fossil fuel resources. Consequently, there has been extensive research interest in the topic, leading to the development of numerous demonstration projects such as the HARI project in Loughborough [3] and the PURE project on Unst [4].

However the performance of many hydrogen technologies is disappointing when compared to conventional systems [5] and further development (technical and economic) is necessary to allow the widespread deployment of hydrogen as an energy vector.

2. Project rationale

The work described here has been undertaken as part of a two-year knowledge Transfer Project (KTP) between the University of Strathclyde and SgurrEnergy Ltd. This project arose from the participation of the two organisations in the International Energy Agency's Hydrogen Implementing Agreement (IEA-HIA) Research Annex 18, modelling the performance of hydrogen energy systems. This research indicated that 1) the performance of many hydrogen energy systems was poor, mainly due to inadequate design, 2) computer modelling was not used in the design process and 3) there was a lack of readily accessible hydrogen systems models and associated methods to allow engineers to test and optimise their designs.

The aim of this KTP project was therefore to develop a hydrogen energy "toolkit" comprising software, models and techniques to allow engineers and designers to optimise the performance and cost of hydrogen energy systems. As both the technical and economic performance would be examined, the development of both technical and complementary cost-benefit models would be required. The specific objectives of the project were defined as:

- Develop a library of generic, technical hydrogen systems models for use with an energy simulation tool enabling the simulation of hydrogen systems performance in different operational contexts.
- The models should support optimisation of the configuration and properties (e.g. components size, capacity) of these systems.
- Develop a cost-benefit analysis model to complement the technical models allowing integrated techno-economic analysis of hydrogen systems.
- Develop an overall methodology for assessing and optimising the operation of any energy system based on hydrogen.

B. Technological review and market analysis

Before starting any modelling activity and in order to assist in the selection of the models to be developed, a review of existing and future hydrogen technologies was carried out. The main objective of this review was to become familiar with the different technology options available on the hydrogen market. The review ends with an analysis of the opportunities for the hydrogen economy and the selection of the hydrogen systems that are to be developed as models.

I. Technological review

Two of the main challenges facing hydrogen are its production and storage. Indeed, in order to be accepted as a realistic and sustainable option for the energy scheme of the future, hydrogen should become a clean, efficient and reliable energy carrier able to supplement electricity. Thus, hydrogen should be produced in a clean and sustainable way. Storing hydrogen should also allow increased flexibility in responding to fluctuations in energy production and demand on a short-term or seasonal basis. [6]

1. Hydrogen production

The first part of this review presents an overview of the existing technologies for hydrogen production. Hydrogen can be produced from diverse resources using a variety of technologies. Hydrogen-containing products such as fossil fuels, water or biomass can be a source of hydrogen. Thermo-chemical processes can produce hydrogen from biomass and fossil fuels. Power generated from renewables and nuclear sources can be used to produce hydrogen through electrolysis. Sunlight can also drive photolytic production of hydrogen from water, using advanced photo-electrochemical and photo-biological processes. Each technology is at a different stage of development and presents different advantages and challenges. The choice and timing of these options will depend on local availability of resources, the maturity of the technology, market applications and demand, policy issues and costs.

Reforming of natural gas, gasification of coal and biomass, water-electrolysis, photo-electrolysis, photo-biological production and high temperature decomposition are the technologies presented in this report. All of them will require significant improvement in plant efficiencies to reduce the capital costs, improve their reliability and increase their operating flexibility.

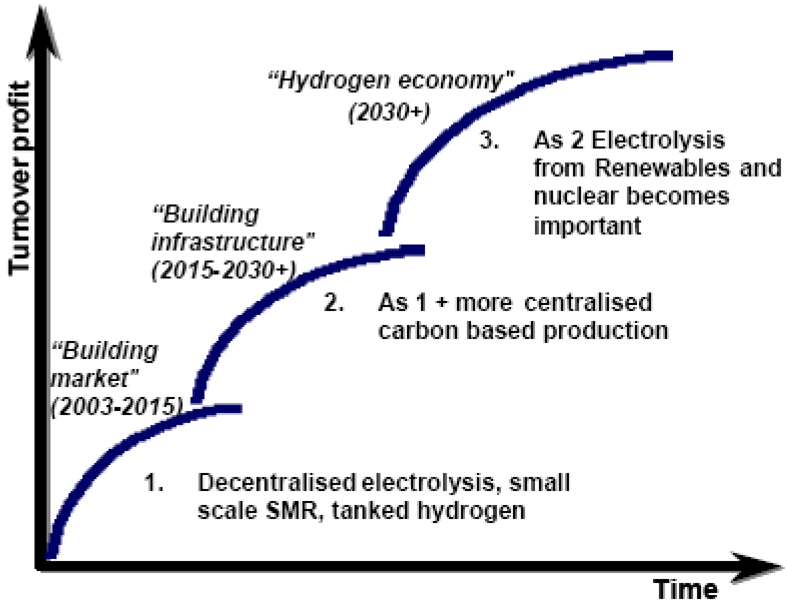


Figure 1: Hydrogen production: the long-term perspective [7]

Several technologies are already available for the industrial production of hydrogen. Electrolysis and fossil-based production are the main sources of hydrogen today [5]. Despite a limited commercial availability, several small-scale natural gas reformers are being tested in demonstration projects (cf. Table 6). Reforming and electrolysis are proven technologies that can be used in the early phases of building a hydrogen infrastructure. However, because of the associated carbon emissions, large-scale hydrogen production based on natural gas cannot be considered as a clean or sustainable supply. Figure 1 illustrates the long-term perspective for hydrogen generation and shows how decentralised production should be followed by large-scale centralised production in order to build the "hydrogen economy".

Other techniques for hydrogen production present severe technical difficulties and are further away from commercialisation and industrial applications. Production from biomass should only be economical at large scale. Photo-electrolysis, photo-biological and high-temperature processes are at a very early stage of development. Material costs and practical issues have to be solved. [8]

a. Hydrogen production from fossil fuels

Hydrogen can be produced from most fossil fuels, especially natural gas and coal. Since CO_2 is produced as a by-product, it should be captured to ensure a sustainable, zero-emission process. The feasibility of the processes will vary with respect to a centralised or distributed production plant.

(i) Hydrogen from natural gas

There are three different chemical processes that allow producing hydrogen from natural gas: steam methane reforming, partial oxidation and auto-thermal reforming.

The steam reforming process is a leading technology today (about 95% of the hydrogen produced today in the US is made via steam methane reforming [8]). It converts methane and water vapour into hydrogen and carbon monoxide in an endothermic reaction:

$CH_4 + H_2O + heat = CO + 3H_2$ Equation 1

The heat required is generally supplied from the combustion of some of the methane feed-gas. A temperature of 700 to 850°C and a pressure of 3 to 25 bar are required for the reaction to occur. The CO produced can be further converted to CO_2 and hydrogen through the water-gas shift reaction:

$CO + H_2O = CO_2 + H_2 + heat$ Equation 2

In the process of partial oxidation of natural gas, hydrogen is produced through the partial combustion of methane (propane and methanol can be used alternatively) with oxygen:

$CH_4 + 1/2O_2 = CO + 2H_2 + heat$ Equation 3

The reaction being exothermic, no external heating of the reactor is needed and a more compact design is possible. The CO produced is further converted into hydrogen as previously described.

Finally, auto-thermal reforming is a combination of both steam reforming and partial oxidation. The temperature is in the range of 950 to 1100°C, and the gas pressure can reach 100 bar. Again, the CO produced is converted to H_2 through the water-gas shift reaction. [9]

Each of these processes presents some benefits and challenges summarised in Table 1:

	Steam methane reforming	**Auto-thermal reforming and partial oxidation**
Advantages	High efficiency Low emissions Costs for large units	Smaller size Costs for small units Simple system
Challenges	Complex system Sensitive to the quality of natural gas	Lower efficiency H_2 purification High emissions

Table 1: Comparison of technologies for H_2 production from natural gas [7]

(ii) Hydrogen from coal

Although it is viewed as a dirty fuel due to its high greenhouse emissions, coal can be used to produce clean hydrogen. Coal could then become a major source of clean hydrogen. While resources of coal will largely outlast oil and natural gas resources [10], the development of clean coal technologies may lead to high energy conversion efficiencies and low emissions compared to conventional coal power plant [11].

A typical reaction for the production of hydrogen from coal is given in the following equation, in which carbon is converted to carbon monoxide and hydrogen.

$C(s) + H_2O + heat = CO + H_2$ Equation 4

Since this reaction is endothermic, additional heat is required. Once more, the CO is further converted to CO_2 and hydrogen through the water-gas shift reaction.

Hydrogen production from coal is commercially mature but more complex than the production from natural gas. The cost is therefore higher (almost twice [11]), but since coal is present in large quantities in many parts of the world like developing countries (e.g. India and China possess about 20% of the proven reserves at end 2007 [10]) and will probably be used as an energy source regardless, it is worthwhile to develop clean technologies to use it.

Some research focuses on advancing the technologies producing hydrogen from coal-derived synthesis gas and to build zero emissions, high-efficiency co-production power plants that would produce hydrogen along with electricity [11]. Partial oxidation of coal is a promising technology that uses integrated gasification combined-cycle technology. It combines coal, oxygen and steam to produce synthesis gas that is cleaned of impurities. For example, the FutureGen project in the US is a 10-year, $1-billion initiative to demonstrate the world's first coal-based, near-zero atmospheric emissions power plant to co-produce electricity and hydrogen [12].

(iii) Capture and storage of CO_2

Although hydrogen from natural gas and coal are certainly viable near-term options, they are not viewed as long-term solutions because they do not help to solve the greenhouse gas or energy security issues [13]. The first point could be solved with carbon sequestration measures.

CO_2 is a major by-product in all production of hydrogen from fossil fuels. To obtain clean production of hydrogen, this greenhouse gas must be captured and stored: a process known as de-carbonisation. There are three different techniques to capture CO_2 in a combustion process: post-combustion, pre-combustion and oxyfuel-combustion. Once captured, the CO_2 can be stored in geological formations like oil and gas fields or in aquifers. However the feasibility of permanent CO_2 storage has not been proven yet and commercialisation is not expected in this decade. [14]

The choice of the transportation system for the CO_2 (pipeline, ship) will also be important for the economic viability of the technology. It should mainly depend on the sites chosen for the production plant and for storage.

b. Hydrogen production from electrolysis

For economic reasons current hydrogen production processes favour the conversion of fossil fuels; but the interest for alternative sustainable techniques from renewable energy resources, which are commonly associated with reduced carbon emissions, is increasing. This section briefly describes the production of hydrogen from the splitting of water: water electrolysis, photo-electrolysis, photo-biological production and high-temperature water decomposition. [15]

(i) Water electrolysis

In the water electrolysis process, water is split into hydrogen and oxygen through the application of electrical current.

$H_2O + electricity = H_2 + 1/2O_2$ Equation 5

Water electrolysis is relatively efficient (>70%) [7], but because it needs electricity the hydrogen produced is expensive (4 times higher than steam reforming for large units [11]). However, it is possible to generate cheaper hydrogen from hydropower [16]. Moreover, the electricity required for electrolysis decreases with the process temperature, so high-temperature electrolysis may be preferable when waste heat from other processes is available (e.g. nuclear plants).

Of all the hydrogen production technologies, water-electrolysis based on renewable electricity is ideal for a sustainable and clean hydrogen production. Indeed, if renewable energy sources were used for water-electrolysis, not only would the cost be significantly reduced thanks to economies of scale, the result would be a clean hydrogen cycle. Tests are being conducted in different parts of the world using wind, solar and geothermal power (see review of hydrogen systems). However, all of these renewable production methods are still in their preliminary stages.

- **Alkaline electrolysis**

Alkaline electrolysers use an aqueous potassium hydroxide (KOH) solution as electrolyte with good ionic conductivity. They are particularly adapted for stationary applications. Alkaline electrolysis is a mature technology with a significant operating record in industrial applications.

The following reactions take place inside the alkaline electrolysis cell:

Electrolyte: $4H_2O = 4H^+ + 4OH^-$ Equation 6

Cathode: $4\ H^+ + 4e^- = 2H_2$ Equation 7

Anode: $4OH^- = O_2 + 2H_2O + 4e^-$ Equation 8

Sum: $2H_2O = O_2 + 2H_2$ Equation 9

The major R&D challenge for the future of alkaline electrolysers is to design and manufacture equipment at lower cost with higher efficiency. [15]

- **Polymer electrolyte membrane (PEM) electrolysis**

In PEM electrolysers the liquid electrolyte is replaced by a solid polymer membrane which significantly simplifies their design. PEM electrolysers can be designed for operating pressures up to several hundred bars, and can be used for both stationary and mobile applications. However, with relatively high cost, low capacity, poor efficiency and short lifetimes, the products currently available are not as mature as alkaline electrolysers. The limited lifetime of the membranes is their main drawback [17]. Their performance could be improved with further improvements in materials development.

Anode: $H_2O = 1/2O_2 + 2\ H^+ + 2e^-$ Equation 10

Cathode: $2H^+ + 2e^- = H_2$ Equation 11

- **High-temperature electrolysis**

The electrical energy needed to split water decreases at high temperatures thanks to lower electrode polarisation and lower theoretical water decomposition voltage which means that a high-temperature electrolyser can operate at higher efficiencies than regular electrolysers (+30% between 100 and 1000°C).

A typical technology is the solid oxide electrolyser cell, based on the solid oxide fuel cell (SOFC) technology, which normally operates above 700°C. At these high temperatures, the electrode reactions are more reversible, which means that the fuel cell reaction can easily be reversed to an electrolysis reaction. [7]

A possible application is the use of the high-temperature heat from a nuclear reactor. The heat could be supplied to a high-temperature electrolysis plant through an intermediate heat exchanger, providing high efficiency electrolysis while avoiding the use of fossil fuels.

(ii) Photolytic production

Photolytic processes use the energy in sunlight to separate water into hydrogen and oxygen. These processes are in the very early stages of research but offer long-term potential for clean hydrogen production with reduced environmental impact. [7]

- **Photo-biological water splitting**

Photo-biological production of hydrogen, directly inspired by nature, is based on two reactions: photo-synthesis and hydrogen production catalysed by hydrogenases in green algae and cyanobacteria for example (fermentative micro-organism systems) [8]. When these microbes consume water in the presence of sunlight, they naturally produce hydrogen as a by-product of their metabolic process. A major challenge is the fact that the enzyme that triggers the hydrogen production is inhibited by oxygen also normally produced by these organisms. The solution is to generate O_2-tolerant, H_2-producing mutants from photosynthetic micro-organisms. [18]

Photosynthesis: $2H_2O = 4H^+ + 4e^- + O_2$ Equation 12

Hydrogen Production: $4H^+ + 4e^- = 2H_2$ Equation 13

Developing micro-organisms that will ferment sugars or cellulose to hydrogen instead of alcohol is also an idea. This research aims at generating mutants that selectively block the production of waste acids and solvent generated in fermentation reactions to maximise the hydrogen production. Long-term research is needed in this area, but if successful, a long-term solution for renewable hydrogen production could result. Reproducing the two steps using artificial photosynthesis is also an option to consider.

- **Photo-electrochemical water splitting**

In this process, hydrogen is produced from water using sunlight and specialised semiconductors called photo-electrochemical materials. The semiconductor uses light energy to directly dissociate water molecules into hydrogen and oxygen.

Different semiconductor materials work at particular wavelengths of light and energies. Research focuses on finding semiconductors with the correct energies to split water that are also stable when in contact with water. The process is in the very early stages of research (performance, lifetime of materials), but offers long-term potential for sustainable hydrogen production with low environmental impact. [8]

(iii)High-temperature decomposition

High-temperature splitting of water occurs at about 3000 °C where 10% of the water is decomposed and the remaining 90% can be recycled. Efficiencies above 50% can be expected from this technology, which could lead to a substantial reduction in hydrogen production costs. The main technical issues concern materials development for corrosion resistance at high temperatures, high-temperature membrane, separation processes, heat exchangers, and heat storage media. And like all high-temperature processes, design aspects and safety are of crucial importance. [8]

Thermo-chemical water splitting is the conversion of water into hydrogen and oxygen by a series of thermally driven chemical reactions. These cycles were extensively studied in the late 1970's and 1980's [6], but there has been of little interest in the past 15 years. Although technically feasible and with a potential for high efficiency cycles with low cost, corrosion issues due to noxious fumes created during the reactions have hindered development of this technology. This technique would be particularly interesting if heat from solar concentrators was available as this could lead to a large-scale, emission-free hydrogen production. [8]

c. Hydrogen production from biomass

Because biomass resources consume CO_2 from the atmosphere as part of their natural growth process, producing hydrogen from biomass gasification is neutral in terms of greenhouse gas emissions. In order to convert biomass into hydrogen, a hydrogen-containing synthesis gas is normally produced following a similar processes to the gasification of coal such as steam gasification, entrained flow gasification and more advanced concepts such as gasification in supercritical water, application of thermo-chemical cycles, or the conversion of intermediates like ethanol [19]. Gasification and pyrolysis are the most promising medium-term technologies to reach commercialisation [20]. Biomass gasification is an R&D area shared between hydrogen production and biofuels production.

Other technologies using wet biomass are also being investigated because of the large energy requirements for the drying process. The production techniques vary according to available resources, location and climatic conditions but the major issues are the inconsistent quality and poor quality control of biomass feedstocks. It is therefore necessary to rationalise the preparation of fuel to produce more consistent, higher-quality fuels. Large-scale systems tend to be suitable for cheaper and lower quality fuels, while smaller plants require higher fuel quality and better fuel homogeneity. [19]

d. Centralised and distributed hydrogen production

(i) Centralised production

Large-scale industrial hydrogen production using fossil energy sources has the potential for relatively low cost units [21]. The major challenge is to decarbonise the hydrogen production process. The technology requires further development on hydrogen purification, gas separation, as well as acceptance for CO_2 capture and storage techniques which are not fully technically and commercially proven [22]. It is also essential to increase plant efficiency, reduce capital costs and improve reliability and operating flexibility. Figure 2 presents the principle of distribution network from a natural gas-based centralised hydrogen production plant.

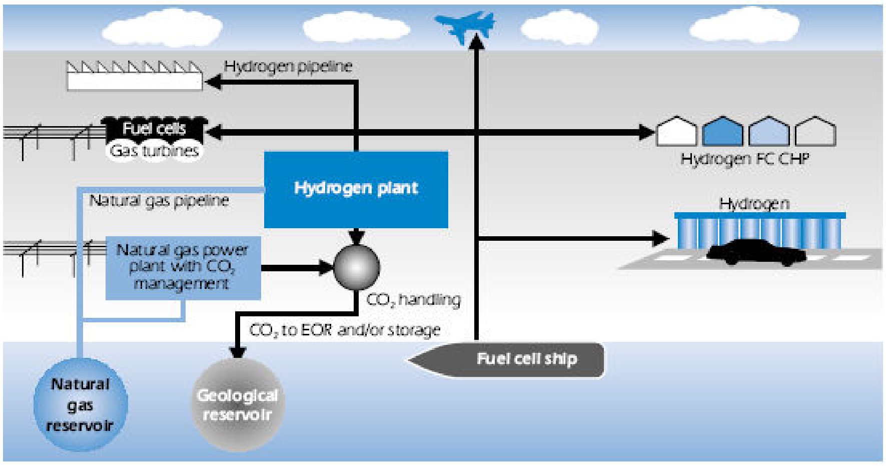


Figure 2: Large scale centralised hydrogen production with CO_2 capture [7]

An interesting option is to co-produce hydrogen and electricity in integrated gasification combined cycle plants. However, centralised hydrogen production requires large market demand, as well as the construction of a hydrogen transmission and distribution infrastructure and infrastructure for CO_2 storage if reforming hydrogen from fossil fuels [22]. In the future, centralised hydrogen production from high-temperature processes based on renewable energy and waste heat should be the best option to increase sustainability. Capture and storage of CO_2 would not be necessary anymore. [7]

(ii) Distributed production

Distributed hydrogen production can be based on both water electrolysis and natural gas processes. The main advantage of distributed production is a reduced need for the transportation of hydrogen, and therefore a reduced need for the construction of a new hydrogen infrastructure. Hydrogen transport is still expected to be mainly by truck, but distributed production could also use existing infrastructure such as natural gas or water pipelines, although some modifications would be necessary (e.g. wall thickness) to reduce gas losses [23].

On the other hand, production costs are commonly higher for small-capacity production units, whereas the efficiencies of production should be lower than in centralised plants [7]. In addition, it is unlikely that CO_2 will be captured in distributed fossil-fuelled plants (difficulty and cost).

Because distributed production systems could use the existing natural gas pipelines they represent a promising technology for the transition to a larger hydrogen supply. However, the availability of equipment for distributed production such as reformers is still low and further development is necessary to meet customer requirements (e.g. reliability, efficiency) despite the technology being significantly improved over the last few years, especially concerning compactness and lifetime. Standards for hydrogen production and storage (e.g. safety) will also need to be adapted to be used in enclosed spaces. [8]

e. Conclusions

This section has provided an overview of the existing and future techniques to produce hydrogen. For all these processes, which are at different stages of development, significant improvements are necessary in plant efficiencies, for capital costs and for reliability and operating flexibility.

Hydrogen production from natural gas and by electrolysis using grid electricity is expected to be the main source of hydrogen until 2020. Water electrolysis is notably a mature technology that can be used in the early phase of building a hydrogen infrastructure. [7]

During a transition period, hydrogen production based on centralised fossil-fuelled plants with CO_2 capture and storage should be the dominating technology even if the capture and sequestration of CO_2 needs to reach technical and economic maturity.

In the longer term, technologies based on renewable energy resources should become commercially competitive, gradually replacing fossil fuel-based equivalents. Hydrogen produced by electrolysis using electricity generated from renewable resources has the potential to be the clean energy carrier of the future, eventually eliminating greenhouse gas emissions from the energy sector.

Other methods for hydrogen production like production from biomass, photo-electrolysis, photo-biological and high-temperature processes are further away from commercialisation and need important development. They are considered as potential pathways for the long-term. A particular attention is placed on photo-induced water splitting that uses the energy of sunlight to separate water into hydrogen and oxygen.

Hydrogen is still about three times more expensive than petroleum to produce (when produced from its most affordable source, natural gas; Table 2). The major challenge is therefore cost reduction. For transportation, a key driver for the hydrogen economy, hydrogen must become cost-competitive with conventional fuels on a per-mile basis in order to gain a place in the commercial market. However, as hydrogen costs reduce with technology advancement and petroleum/diesel prices increase investment in the hydrogen infrastructure should increase. A major shift from fossil fuel-based production towards renewable sources is the only way to ensure that hydrogen production can be sustained, which is why only electrolysis-based approaches will be included in this project.

Method	Fuels	Overall efficiency (%)	H_2 cost (US$/GJ)
Steam reforming	Natural gas, oil	65-75	5-8
Gasification	Biomass, oil, coal	42-47	10-12
Pyrolysis	Biomass, coal	48	9-13
Electrolysis	Water	35-42	20-25

Table 2: Summary of the main hydrogen production methods [11]

2. Hydrogen storage

Hydrogen has a very high energy content by weight (about 3 times more than gasoline) but a very low energy content by volume (about 4 times less than petroleum), which makes hydrogen particularly difficult to store, especially within the size and weight constraints of a vehicle. [24]

The storage of hydrogen is a key element in any hydrogen energy system. Developing safe, reliable and cost-effective hydrogen storage technologies that meet performance and cost requirements is essential to achieve a future hydrogen economy. It is also the main barrier to the widespread use of hydrogen. It is necessary for both transport applications and other applications such as stationary power generation or refuelling infrastructure, which is why hydrogen storage represents a significant part of the current research activities [8]. A number of international collaborations focused on hydrogen storage exist, notably with the DOE (US Department Of Energy) [8] and the IEA (International Energy Agency) [7].

a. Gaseous hydrogen

The most common method to store gaseous hydrogen is to use steel tanks [25]. However, lightweight composite tanks designed to endure higher pressures are also becoming more common. Cryogas (gaseous hydrogen cooled to near cryogenic temperatures) is a third alternative that allows increasing the volumetric energy density of the gas. Glass microspheres, another promising storage technique, and composite tanks are discussed in the following section.

(i) Composite tanks

Composite tanks present many advantages: they are lighter than regular steel tanks and they are already commercially available, and safety-tested [24]. They can also withstand pressures between 350 and 700 bar. Composite tanks may also be used with cryogas to increase the storage capacities from their current levels. Their main disadvantages are the large physical volume required (which do not meet targets for light-duty vehicles for example [27]), their high cost and the energy required for compressing the gas to very high pressures. There are also some safety issues that still have to be resolved, such as the rapid loss of hydrogen in case of accident. The long-term effect of hydrogen on the materials under very cold conditions is also not perfectly understood yet and further research is therefore necessary.

(ii) Glass microspheres

The operation of glass microspheres in the storage of hydrogen can be described by three successive steps. First, miniature hollow glass spheres (about 50 micrometers in diameter) are filled with hydrogen at high pressure (350-700 bar) and high temperature (around 300°C) by permeation in a high-pressure vessel. The spheres are then cooled down to ambient temperature and transferred to the low-pressure vehicle tank. Finally, the microspheres are heated to 200-300°C in order to increase the glass permeability to hydrogen and start the release of gas to run the vehicle. [26]

The main drawbacks of this technology are the low volumetric density that can be achieved and the high pressure required for filling. The glass microspheres also slowly leak hydrogen at room temperatures and break easily during cycling. But the main operational challenge is the need to reach temperatures higher than the temperatures available from the PEM fuel cell of the vehicle (about 80°C). This could be resolved by transferring the spheres directly to the vehicle at high temperature. This would also increase the process efficiency.

Concerning their advantages, glass microspheres should be particularly safe as they store hydrogen at low pressure. R&D is still necessary to design stronger glasses, develop low-cost production techniques and reduce the hydrogen liberation temperature to less than 100°C. [26]

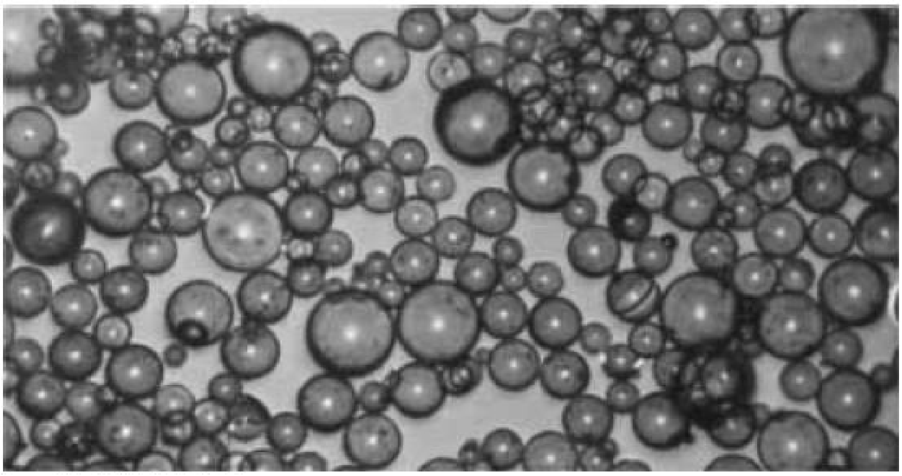


Figure 3: Glass microspheres for H_2 gas storage [26]

b. Liquid hydrogen

The conventional way to store hydrogen is as a liquid cooled down to cryogenic temperatures (below -253°C). Other options include storing hydrogen as a constituent in other liquids, such as $NaBH_4$ solutions, rechargeable organic liquids, or anhydrous ammonia NH_3. Cryogenic hydrogen, $NaBH_4$ solutions, and rechargeable organic liquids are the three promising methods. [8]

(i) Cryogenic liquid hydrogen (LH_2)

Cryogenic hydrogen, usually simply referred to as liquid hydrogen LH_2, has the advantage of an energy density much higher than gaseous hydrogen. High storage density can be reached at relatively low pressure. However, it is essential to note that about 30 to 40% of the energy is lost in the process of liquefaction. The other major disadvantage of LH_2 is the boil-off loss during storage, added to the fact that super-insulated cryogenic containers are needed [8]. It is also important to consider the general public's opinion seeing LH_2 as an unsafe and very high-tech system (e.g. leak, risk of explosion).

Hydrogen liquefaction is usually practiced only where achieving high storage density is absolutely essential, such as in aerospace applications (e.g. space rockets), but it has also been demonstrated in commercial vehicles and could be used as aircraft fuel in the future, since it provides the best weight advantage of any hydrogen storage. [24]

As mentioned above boil-off and energy requirements of the liquefaction process have a large impact on the energy efficiency of the cycle, which is why development of more efficient liquefaction processes, low-cost insulated containers and systems that automatically capture the boil-off and re-liquefy the fuel are the major research tasks for the future.

(ii) $NaBH_4$ solutions

Borohydride solutions are another possibility for the storage of hydrogen in a liquid form. More exactly, they can be used as a liquid storage medium for hydrogen. The catalytic hydrolysis reaction is:

$NaBH_4\ (l) + 2H_2O\ (l) = 4H_2\ (g) + NaBO_2\ (s)$ (ideal reaction) Equation 14

The main advantage of $NaBH_4$ solutions is that this technique allows controlling safely the generation of hydrogen onboard. The main drawback is that the reaction product $NaBO_2$ must be regenerated back to $NaBH_4$ off-board. On the financial aspect, using $NaBH_4$ solutions in vehicles may be prohibitively expensive (the cost of $NaBH_4$ regeneration should be reduced from present 50 US$/kg to less than 1 US$/kg). However, a few commercial companies already promote this technology and even if the needed cost reduction is unlikely, $NaBH_4$ solutions may be usable in high-value portable and stationary applications. [8]

(iii)Rechargeable organic liquids

Hydrogen can be indirectly stored in a liquid form using rechargeable organic liquids. Firstly an organic liquid is dehydrogenated to produce hydrogen gas onboard. Next, the dehydrogenated product is transported from the vehicle tank to a central processing plant while the vehicle tank is simultaneously refilled with H_2-rich liquid. Finally, the H_2-depleted liquid is re-hydrogenated and returned to the filling station. However, detailed safety and toxicity studies will have to be performed before considering any commercialisation.

However, handling liquid hydrogen may involve toxic chemical substances or high temperatures and will therefore require a safe infrastructure. A distributed production infrastructure will be necessary to minimise the transport cost to the refuelling stations. But building this infrastructure could be costly and should be combined with non-vehicular applications like stationary power production and aviation transport. [7]

c. Solid hydrogen

Hydrogen can be stored on the surface of solids (by adsorption) or within solids (by absorption). In adsorption, hydrogen attaches to the surfaces of a material either as hydrogen molecules or atoms. In absorption, hydrogen molecules split into atoms that are incorporated into the solid lattice framework, which would allow storing larger quantities of hydrogen in similar volumes at low pressure and room temperatures.

Storage of hydrogen in solid materials (hydrides) could therefore become a safe and efficient way to store energy, both for stationary and mobile applications. Indeed, a serious damage to a hydride tank (e.g. collision) would not cause danger, since hydrogen would remain in the metal structure.

Different options for solid storage include metal hydrides, nanotubes, fullerenes, activated charcoal, other forms of nanoporous carbon, porous semiconductors, and rechargeable organic or inorganic materials.

These suitable materials can be divided in four main groups: carbon and other high surface area materials, H_2O-reactive chemical hydrides, thermal chemical hydrides, and rechargeable hydrides. Materials within each of these groups are presented in Table 3:

Carbon and other high surface area materials - Activated charcoals - Nanotubes - Graphite nanofibers - MOFs, zeolites - Clathrate hydrates	**Chemical hydrides (H_2O-reactive)** - Encapsulated NaH - LiH and MgH_2 slurries - CaH_2, $LiAlH_4$
Rechargeable hydrides - Alloys and intermetallics - Nanocrystalline - Complex	**Chemical hydrides (thermal)** - Ammonia borozane - Aluminium hydride

Table 3: Overview of solid hydrogen storage options [7]

(i) Carbon and other high surface area materials

- **Carbon-based materials (nanotubes and graphite nanofibers)**

Hydrogen storage in any carbon-based material is attractive due to its low mass density. Carbon-based materials, like nanotubes and graphite nanofibers, have been intensively investigated over the last decade. It is now agreed that the exceptional hydrogen storage capacities (30-60 wt.%) in carbon nanotubes reported a few years ago are impossible and were measurement errors [7]. The properties needed to achieve practical room temperature storage are not clearly understood, and it is far from certain that useful carbon can be economically and consistently synthesised. A decisive issue is whether or not the hydrogen to carbon ratio can be increased and accessed reversibly both at ambient and cryogenic temperatures.

In conclusion, the potential for hydrogen storage in carbon-based materials is questionable, and some even suggest that all research work in the area should be stopped. [7]

- **Other high surface area materials**

Alternatives to carbon-based materials have been investigated for low-cost, safe hydrogen storage, particularly for large-scale stationary applications. The main examples of other high surface area materials are zeolites, metal oxide frameworks (MOFs), clathrate hydrates or other related microporous materials [8]. For stationary hydrogen stores, zeolites combine superior storage capacity per unit volume with a number of safety advantages over carbon-based materials. They can also store H_2 at cryogenic temperatures. However, the main question is whether they can be designed to reversibly store high levels of hydrogen at room temperature.

(ii) Rechargeable hydrides

No metal hydride system currently meets all the competing needs of an ideal hydrogen storage material (Table 5). Techniques to enhance the kinetics of hydrogen sorption/desorption in light metal hydrides are therefore essential.

Rechargeable hydrides have been at the centre of all R&D attentions for the last decade, which allowed building a large database with information about their properties for the IEA HIA Annex 17. Complex hydrides such as borohydrides, alanates and amides, provide high hopes for the future of energy storage. [24]

$NaAlH_4$ alanates have been studied intensively and their performance (Table 4) can be improved by catalyst mechanisms that are today well understood, but many issues still exist. Firstly cost remains too high to consider any commercialisation. Moreover, weight targets cannot be met by $NaAlH_4$ yet. Research on catalysed $Mg(AlH_4)$ showed that this type of alanate cannot equal the level of reversibility of $NaAlH_4$, which makes their near-term applicability unlikely. Extension of the catalyst concept to other alanates beyond $NaAlH_4$ is the main R&D subject in this area.

Type	Storage density (wt.% H_2)	Temperature (°C)
$LiAlH_4$	10.6	190
$NaAlH_4$	7.5	100
$Mg(AlH_4)$	9.3	140
$Ca(AlH_4)$	7.8	>230

Table 4: Properties of the most common alanates [7]

Despite having much higher potential capacities than alanates, borohydrides are much less studied than alanates. The reason is that they are in general too stable and not reversible enough. A positive aspect is that progress has been lately observed concerning the reversibility and destabilisation of $LiBH_4$. [24]

(iii)Chemical hydrides

Chemical hydrides are normally used in a semi-liquid form, enabling pumping and safe handling. Hydrogen is created by hydrolysis reactions triggered by the controlled injection of water. The liberation of hydrogen is exothermic and does not require any additional heat. MgH_2 probably offers the best combination of H_2 yield and affordability, but lowering the cost of processing the used hydroxide back into the starting hydride is necessary. Unfortunately, this is an energy-intensive process and it is unlikely that costs can be reduced to acceptable levels.

Ammonia borane is another type of chemical hydrides that could potentially be used to store hydrogen in a solid form. Preliminary results indicate that NH_4BH_4 can be thermally decomposed with very high hydrogen yields. However, the reaction is not reversible and off-board regeneration is required. Moreover, the question of the toxicity of gaseous boranes that could contaminate the fuel cell catalysts should be considered carefully. [28]

d. Conclusions

The main options for storage of hydrogen in gaseous, liquid, and solid form have been discussed. Table 5 summarises the main information concerning technology status, best options, and the main R&D issues that need to be addressed:

	Gaseous H_2 Storage	**Liquid H_2 Storage**	**Solid H_2 Storage**
Status	Commercially available, but costly	Commercially available, but costly	Very early development; many R&D questions
Best option	Carbon-fibre composite vessels (6-10 wt.% H_2 at 350-700 bar)	Cryogenic insulated dewars (ca. 20 wt.% H_2 at 1 bar and -250°C)	Too early to determine. Many potential options. Most-developed option: metal hydrides (potential for > 8 wt.% H_2 and > 90 kg/m3 H_2-storage capacities at 10-60 bar)
R&D issues	Fracture mechanics, safety, compression	High liquefaction energy requirement,	Weight, lower desorption

	energy, and reduction of volume	dormant boil off, and safety	temperatures, higher desorption kinetics, recharge time and pressure, heat management, cost, pyrophoricity, cyclic life, container compatibility and optimisation

Table 5: Characteristics of gaseous, liquid and solid H_2 storage options [7]

Comparison between the three storage options shows that solid H_2 storage offers great promises and presents many advantages compared to the other storage methods: lower volume, lower pressure, greater energy efficiency and higher purity of the hydrogen delivered. But compressed gas and liquid storage are the only commercially viable options today.

To conclude this technology review section, none of the hydrogen technology options are ideal solutions from both an engineering and economic perspective, and major developments are still required for hydrogen to be considered as a viable energy vector.

Today steam reforming and electrolysis powered by renewable sources are the most developed technologies. On the storage aspect compressed gas storage is the only viable option at the moment. These findings, combined with the review of hydrogen demonstration projects presented in the next section, were taken into account in the choice of the typical hydrogen energy systems and technologies to be modelled in this study.

II. Review and selection of hydrogen systems

A review of the different hydrogen systems existing around the world was carried out in order to identify a few generic energy systems representative of the current and prospective hydrogen market. These would then be developed as computer models. The hydrogen systems reviewed serve four main markets: [13]

- Transportation is slowly exhausting the world's oil resources. Most of today's demand is met by oil and the prospect of finding new major reserves becomes more and more unlikely. Many alternative fuels exist (e.g. bio-fuels, hydrogen). The market penetration of fuel cell vehicles has the potential to be high among the other competing technologies (conventional, hybrids) because of a high efficiency (fuel cells are much more efficient than internal combustion engines) that could compensate their higher capital cost.

- Industry: Already today there are many industrial users of hydrogen, mostly in relatively small quantities. The two major industrial markets for hydrogen are fertilizer production and steel. These two sectors could be suitable for large-scale hydrogen production plants.

- Electrical market: Hydrogen may be used for electrical production, particularly for production of peak electricity. Like the demand, the market price of electricity varies as a function of time and this variability creates the possibility for the genesis of a large hydrogen market, initially using hydrogen systems to produce electrical power when the price of electricity is at its maximum.

- Domestic market: The main targets for stand-alone power systems (SAPS) applications are remote regions relying on expensive diesel power, islands or northern communities. For example, diesel fuel is still the primary source of electricity in many remote communities. Europe has thousands of islands and Canada has over 300 northern communities [29]. Communities at the extreme edges of grids also represent potential users. These places do not favour large-scale hydrogen production techniques but may open a large market for small-scale stationary technologies if costs allow market entry.

Table 6 presents a selection of hydrogen energy systems installed all around the world:

Project Name	**Location**	**Energy sources**	**H_2 production**	**H_2 Storage**	**End use**	**Time of operation**	**Description**
Transportation							
Clean Air Now (CAN)	US	PV	Electrolysis	Gas	Refuelling station, transportation	1994-1997	
Zero-emission buses in real-world use	US-Canada	Grid; Natural gas (NG)	Electrolysis; Reforming	Gas, Liquid	Refuelling station, transportation	1996-	FC buses
Palm Desert RE/H_2 transportation project	US	PV	Electrolysis	Gas	Refuelling station, transportation	1996-1999	FC cars

Munich Airport	Germany	Grid, PV; NG; Ext. supply	Electrolysis; Reforming	Liquid, Gas, Hydride	Refuelling station, transportation	1999-	FC buses and cars
Honda solar hydrogen refuelling station	US	PV, Grid	Electrolysis	Gas	Refuelling station, transportation	2001-	FC cars
CH2IP	Canada	Green	Electrolysis	Gas	Refuelling station, transportation	2001-2004	
ECTOS	Iceland	Grid, Hydro, Geotherm al	Electrolysis	Gas	Refuelling station, transportation	2001-2005	FC buses developed
Sunline Clean Fuels Mall	US	PV; NG	Electrolysis; Reforming	Gas	Refuelling station, transportation	N/A	
Las Vegas refuelling station	US	NG	Reforming	Gas	Refuelling station, transportation	2002-	H_2 not used for fuelling is directed to a PEMFC and the electricity is sent to the Las Vegas grid (enough for 30 homes)
H_2 from biomass for urban transportation	US	Biomass	Pyrolysis and Reforming	Gas	Refuelling station, transportation	2002-	Use of peanut shells, experimental phase
CUTE	Europe (8 sites), China, Australia	Grid, Green; NG; Ext. supply	Electrolysis; Reforming	Gas, Liquid	Refuelling station, transportation	2003-2005	Characteristics depending on site: refuelling station, FC buses
Malmö filling station	Sweden	Wind	Electrolysis	Gas	Refuelling station, transportation	2003-	Dispenser incorporates a H_2 and natural gas mixing system
Vancouver refuelling station	Canada	Steam-methane	Reforming	Liquid	Refuelling station, transportation	2005-	
Integrated RE/H2 power system							
Grimstad renewable energy park	Norway	PV	Electrolysis	Gas	Integrated RE/H_2 power system	N/A	FC, gas turbine, heat
Stand-alone RE system based on H_2 production	Canada	Wind, PV	Electrolysis	Battery, Gas	Integrated RE/H_2 power system	2001-	FC, H_2-fuelled generator
HARI	UK	PV, Wind, Hydro	Electrolysis	Gas	Integrated RE/H_2 power system	2001-	FC, heat
PURE	UK	Wind	Electrolysis	Gas	Integrated RE/H_2 power system	2002-	FC, FC cars, heat

Totara Valley	New-Zealand	Wind	Electrolysis	Pipeline	Integrated RE/H_2 power system	2002-2008	Both local heating and power generation via a FC or hydrogen ICE; 2km Hy-Link
Production of H_2 only							
Stuart renewable energy test site	Canada	PV	Electrolysis	Gas	Production of H_2 only	1991-1996	
Solar H_2 plant on the Markus Friedli residential house	Switzerland	PV, Grid	Electrolysis	Battery, Metal hydride	Production of H_2 only	N/A	Private installation
H_2 generation from stand-alone wind powered electrolysis systems	Italy	Wind	Electrolysis	Battery	Production of H_2 only	1994-1997	Only production of H_2
Hydrogen energy for the future of New-Zealand	New-Zealand	Coal	Coal gasifier	-	Production of H_2 only	2002-2008	Small scale distributed electricity production from FC or gas engines
Very small-scale H2 system							
INTA solar hydrogen facility	Spain	PV	Electrolysis	Gas, Metal hydride	FC only	1991-1996	The control selects the number of operating cells of the electrolyser as a function of the solar irradiation
PHOEBUS Jülich demonstration plant	US	PV	Electrolysis	Battery, Gas	FC only	1994-2003	
SAPHYS	Italy	PV	Electrolysis	Battery, Gas	FC only	1994-1998	
SCHATZ solar hydrogen project	US	PV	Electrolysis	Battery, Gas	FC only	1995-1998	
Windmill-electrolyser system for H_2 production at Stralsund	Germany	Wind, PV	Electrolysis	Gas	FC only	Around 1997	
Integrated H_2 energy system in Takasago	Japan	Grid	Electrolysis	Metal hydride	FC only	N/A	Conversion of excess electricity during night-time
SERC/Yurok	US	PV; External supply	-	Battery, Gas	Telecommunication station	1999-	
FIRST	Spain	PV	Electrolysis	Battery, Metal hydride	Telecommunication station	2000-2004	Two different projects with and without H2 production

Table 6: Overview of the main hydrogen projects by 2006 [30]

The hydrogen systems reviewed were sorted according to their end application and three categories were defined:

- Small-scale hydrogen applications
- Remote stand-alone power system
- Hydrogen filling station and transportation

A further category was identified during this research that, although not present in the current case studies, is often proposed as a use for hydrogen and is of increasing academic/ industrial interest and could present market opportunities for the future hydrogen industry: [29]

- Energy buffering for large grid-connected renewable systems

1. Low power applications

Remote telecommunication systems (from minimal installations of 1W to relay stations for mobile phones in the 10kW-range) present an interesting energy supply challenge, because they require reliable, unattended power system operation in locations where grid power is not available due to the remoteness, reliability or safety issues. Photovoltaic power systems are widely used in these conditions. However, the deployment of solar power systems depends largely on the amount of solar radiation available. The variability of the solar resource usually requires some form of energy back-up such as batteries or a diesel generator. Alternatively the use of fuel cells in combination with solar power could improve power availability and system reliability.

Effectively the fuel cell acts as an emergency system for powering the telecommunication equipment. The main advantage of the addition of the fuel cell is that power availability is increased. It is possible to ensure that the system will be properly powered with availability close to 100%.

Usually a relatively large PV array and batteries are required but if a fuel cell is added and operates for only a small percentage of the time (around 10%), the PV array size and batteries could be largely reduced with a significant reduction of visual impact.

Maintenance requirements compared with the alternative of a conventional diesel generator can be also reduced significantly (Yurok project [31]).

Examples of this type of system are the INTA solar hydrogen facility [32] and the FIRST (Fuel cell Innovative Remote energy System for Telecom) project in Spain [33].

2. Stand-alone power system

One third of the world's population doesn't have access to a reliable energy source. Stand-alone power systems (from a several kW to a few MW in size) could provide a option for remote applications such as remote monitoring stations, isolated houses or communities where grid power is not available (e.g. small islands or mountain regions). An increasing number of stand-alone power systems (SAPS) now include renewable technologies (e.g. wind or solar) in combination with diesel generators or batteries for back-up power, but the majority of large SAPS are still based on fossil fuel power. [6]

Such applications could represent an initial market niche for renewable-hydrogen technologies that could be competitive in the medium term. Indeed, replacing the conventional back-up systems by fuel cells would reduce fossil fuel dependence and associated emissions with low O&M costs. It is also interesting to note that implementing SAPS can be an opportunity to fight unemployment and depopulation in remote areas [6]. Table 7 presents a SWOT analysis for the introduction of hydrogen technologies into SAPS: [6]

Strengths	Weakness
- No need for fuel transport - Experience in handling compressed gases - Noise level lower than competing technologies - Potential for high density energy storage - Seasonal energy storage without energy losses - Able to handle power fluctuations; can be combined with intermittent renewable energy sources - Increased renewable energy integration to 100% - Low and predictable O&M costs - Reduced environmental impact - Safety of power and energy supply	- Codes and standards not defined (safety issues, technical specifications…) - Immature technology (fuel cells and PEM electrolysers) - Low availability and high cost of small electrolysers - Capital cost - Lack of life-time experience - Weak supply network (consultants, engineers…)
Opportunities	**Threats**
- Existing SAPS based on renewables in which hydrogen could be incorporated - Current national and EU financing schemes - New job opportunities - Increasing number of companies involved in the energy sector - Reduction of environmental impact	- No available market study in EU - Inadequate commercialisation plan - Limited practical experience - Hydrogen not known or accepted as an energy storage medium - Inadequate legislative framework (regulations, permissions of installation…) - Low interest and priority from SAPS suppliers

Table 7: SWOT analysis for Hydrogen-SAPS

Depending totally on the weather, the renewable resource available on site rarely matches the fluctuating electrical demand of the system and so some form of balancing mechanism is inevitably required, as well as some form of long term energy storage. Until the arrival of hydrogen energy systems, this would be carried out using a combination of batteries and diesel generators.

The three key elements that compose a hydrogen energy stand-alone power system are a mechanism for converting electrical energy from a combination of renewable sources (e.g. wind or solar) into hydrogen, a means of storing the hydrogen and a method for reconverting the chemical energy of hydrogen back into electricity. Batteries can still be used for short-term energy fluctuations but they become expensive, bulky and inefficient beyond a few days of storage, while hydrogen offers long-term and large-scale capacity storage achievable at a lower cost.

As illustrated in Figure 4 an electrolyser is used to store the excess electricity generated by renewables (electrolysis of water) while the fuel cell (or hydrogen engine) transforms the hydrogen back into electricity when the renewable energy available is not sufficient.

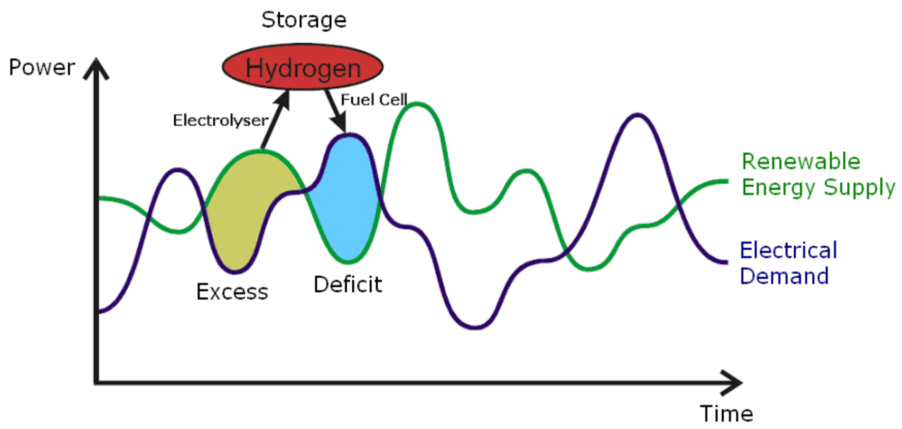


Figure 4: Hydrogen SAPS: a balancing mechanism [adapted from 29]

Numerous projects trying to demonstrate the feasibility of hydrogen stand-alone power systems are developed around the world; for example the HARI (Hydrogen and Renewables Integration) project in Leicestershire, the SAPHYS (Stand-Alone small size Photovoltaic Hydrogen energy System) project and the PURE (Promoting Unst Renewable Energy) project at the northern extremity of the Shetland Isles.

3. Energy buffering system

The intermittency of the wind presents problems in forecasting the energy output from a wind farm. This is a problem that is faced by the energy traders who are bidding into the energy market, and reduces the confidence and available financial yield of a wind farm. The intermittency and unpredictability of the wind also results in the requirement for spinning reserve capacity to be provided by other energy sources. These are drawbacks of wind energy and to various degrees most renewable energies technologies.

The concept of energy buffering for large wind farms could therefore represent an important market in the future. Although other technologies such as flow batteries are also investigated at the moment, using hydrogen to reduce the variability of the wind farms output might be an interesting alternative. Moreover the hydrogen stored could also be used as a fuel for transportation and non-stationary applications. [29]

4. Filling station with on-site hydrogen generation

Around the world, more and more concepts of hydrogen vehicles are being developed. City buses running on hydrogen are also introduced and tested in urban areas. To support this deployment, a large infrastructure is necessary. This infrastructure includes sites for centralised or decentralised hydrogen production, and a transportation and distribution network.

At the moment, there are no installations for centralised hydrogen production. Another source of hydrogen must be found. The most cost-effective options are to use the power from the grid or the waste hydrogen from petroleum refineries. But a more sustainable choice is to produce hydrogen on-site using renewable energies. This last option was the one investigated and modelled in this project.

For periods when the renewable resource is insufficient to satisfy the hydrogen demand, a back-up system is required to produce the electricity necessary. This back-up can be provided by a set of diesel generators.

A few examples of hydrogen filling stations around the world are the stations of Vancouver (Canada) [34], Reykjavik (Iceland) [35], and Hamburg (Germany) [36]. Several stations are also in operation in California [37].

The Munich airport is an interesting case. Indeed, up to 50% of emissions at airports are caused by ground vehicles. The introduction of hydrogen vehicle fleets with a limited range refuelled at a central depot thus presents a very sensible option. [38]

5. Conclusions

The market analysis has identified four main markets for hydrogen applications: transportation, SAPS, electrical and industrial markets. These are represented in Figure 5. Additionally, a review of existing demonstration projects (e.g. California, EU, UK [39]) has been carried out and helped to identify the hydrogen systems most likely to meet the needs of the target markets: low power applications and stand-alone power systems for isolated areas (SAPS market), large-scale energy buffering systems (electrical/industrial market) and filling stations (transport market). The development of these systems as computer models is described in the following sections.

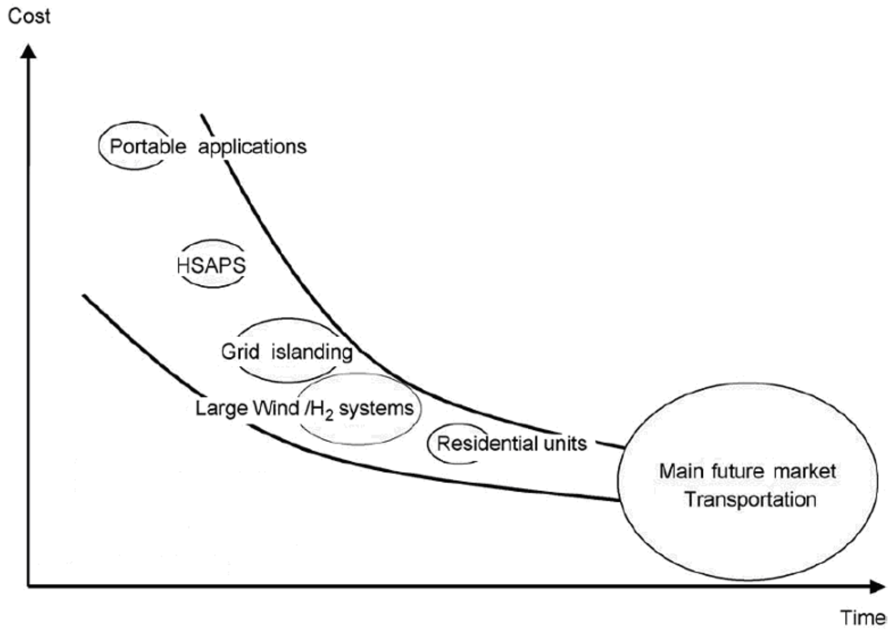


Figure 5: The route to market for hydrogen applications [6]

C. Modelling activities

The literature review presented in the previous part of this report identified the four typical hydrogen systems to be modelled as part of this project. In this section the following are described:

- the modelling software used and the systems models developed,
- the component models used to build the generic systems,
- the cost-benefit calculations and their implementation in TRNSYS,
- the design of the user-friendly interface,
- the optimisation process for use with the systems models,
- the results analysis tool,
- the methodology for the use of the models in sizing and optimisation.

I. Modelling tools

The TRNSYS simulation tool was used to construct the model; TRNSYS was chosen because it already included hydrogen component models (HYDROGEMS [15]) that could be adapted to the needs of the project.

TRNSYS is a TRaNsient SYstems Simulation program with a modular structure developed by the University of Wisconsin [1]. TRNSYS allows the user to specify the components that constitute a system and the manner in which they are connected. The program can recognise the system organisation and simulate its operation. The TRNSYS library includes many of the components (called “types”) commonly used in thermal and electrical energy systems, as well as component routines to manage the integration of weather data or other time-dependent forcing functions and output of simulation results. The modular nature of TRNSYS gives the program a large flexibility, and makes it possible to add mathematical models not included in the standard TRNSYS library.

TRNSYS (originally developed in 1975) is a reference program for researchers and engineers around the world thanks to its capacities in the analysis of systems whose behaviour is dependent on time. TRNSYS is particularly suited for the analysis of solar systems (solar thermal and PV systems), low energy buildings and HVAC systems, renewable energy systems, cogeneration or fuel cells.

HydroGems is a series of HYDROGen Energy ModelS designed for the simulation of integrated renewable and hydrogen energy systems. The HydroGems library includes component subroutines for PV arrays, wind turbines, generator systems, advanced alkaline water electrolysers, high-pressure hydrogen gas storage, metal hydride storage, proton exchange membrane fuel cells, alkaline fuel cells, compressors, power conditioning equipment, and logical control functions. All the models have been tested against different renewable and hydrogen installations around the world.

The compatibility between HydroGems and TRNSYS makes it possible to integrate the HydroGems component models within the standard library of TRNSYS. This characteristic makes HydroGems particularly useful for system design or redesign and the optimisation of control strategies for integrated renewable and hydrogen energy systems. [15]

The HydroGems components underpin the generic systems models developed in this project and so a brief description of the mathematical models for the different elements of the HydroGems library can be found later in this report. More comprehensive details are available in the HydroGems User Guide where the parameters, inputs and outputs are described for each "type" [1].

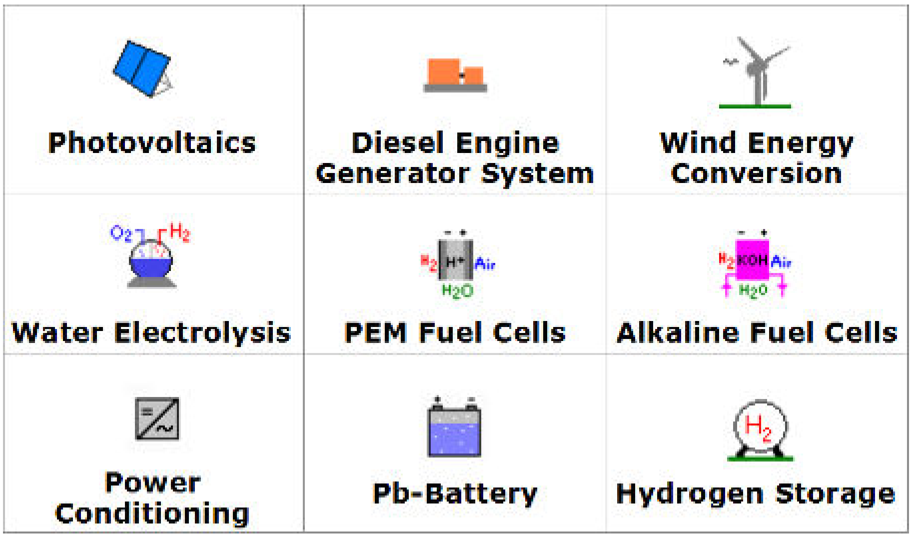


Figure 6: HydroGems components [15]

II. Description of the models and the main components

This section describes the models developed on the TRNSYS platform and the components included in the models.

1. Structure of the generic systems models

Following a review of hydrogen energy projects (see section B.II) it was determined that the majority of systems are typically composed of four main elements:

- Renewable energy technologies (e.g. PV, wind turbines) are used as primary source of energy. Weather data are of course required here.
- An electrolyser is used to produce hydrogen using the excess energy generated by renewables.
- The hydrogen produced by the electrolyser is stored in pressurized gas tanks. A compressor can also be included.
- A fuel cell transforms the stored hydrogen back to electricity when the renewable resource is not sufficient. Occasionally, the fuel cell can be replaced by a hydrogen engine or a diesel back-up generator.

Power conditioning components are also necessary to connect the electrolyser and the fuel cell to the system controller.

With regards to the development of TRNSYS models of the 4 generic systems (Figure 8 to Figure 11) some additional specialist "components" are required:

- Data I/O components are required to provide boundary conditions (i.e. climate data) to the model and extract results. The extracted data is used in both the economic analysis of each system and in the optimisation process.
- Systems control algorithms.

Figure 7 presents the general structure of a hydrogen energy system modelled in TRNSYS. The main parameters, inputs and outputs of the system are summarised, as well as the way the components are linked:

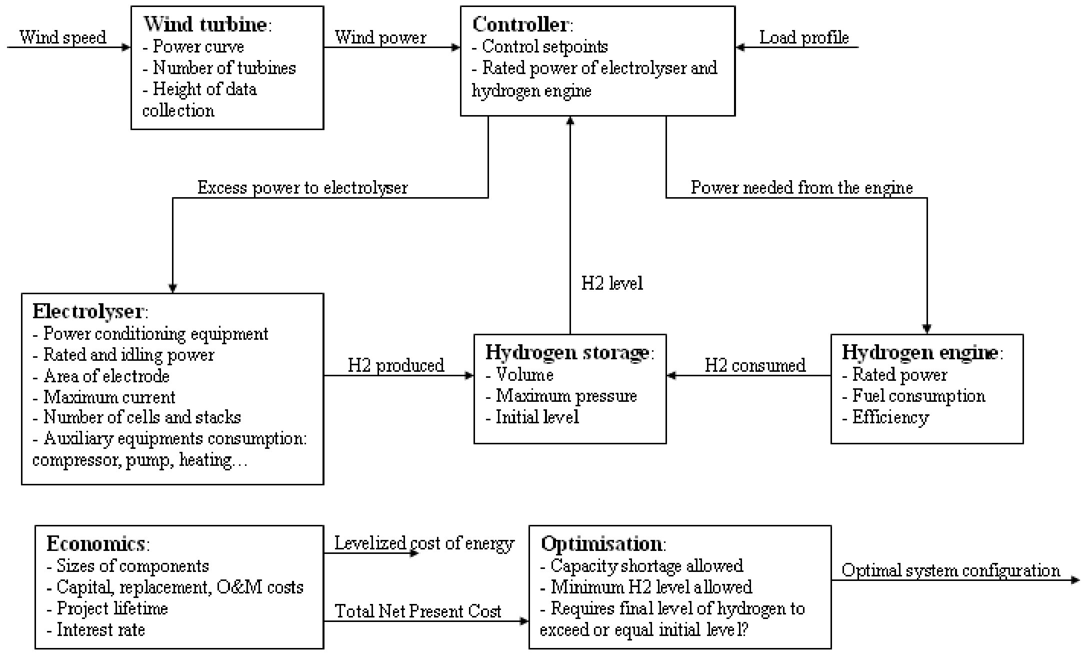


Figure 7: Block diagram of a wind/hydrogen system modelled in TRNSYS

Figure 8 to Figure 11 show the four generic hydrogen systems that have been developed on the TRNSYS platform. One can see that all four models present a common structure:

- A power generation part that includes input files (electrical load, wind speed, solar irradiation) and power production technologies (PV modules, wind turbines, diesel).
- A controller controlling the operation of the system.
- A hydrogen part that includes electrolyser, compressor, hydrogen storage, fuel cell and power conditioning equipments.
- An economic part to calculate the economic performance of the system.
- A series of input and equation blocks used to describe, control and optimise the system.
- A series of outputs blocks (printers, plotters) used to view and analyse the simulation results.

The next section describes the components underpinning these models and their implementation in TRNSYS.

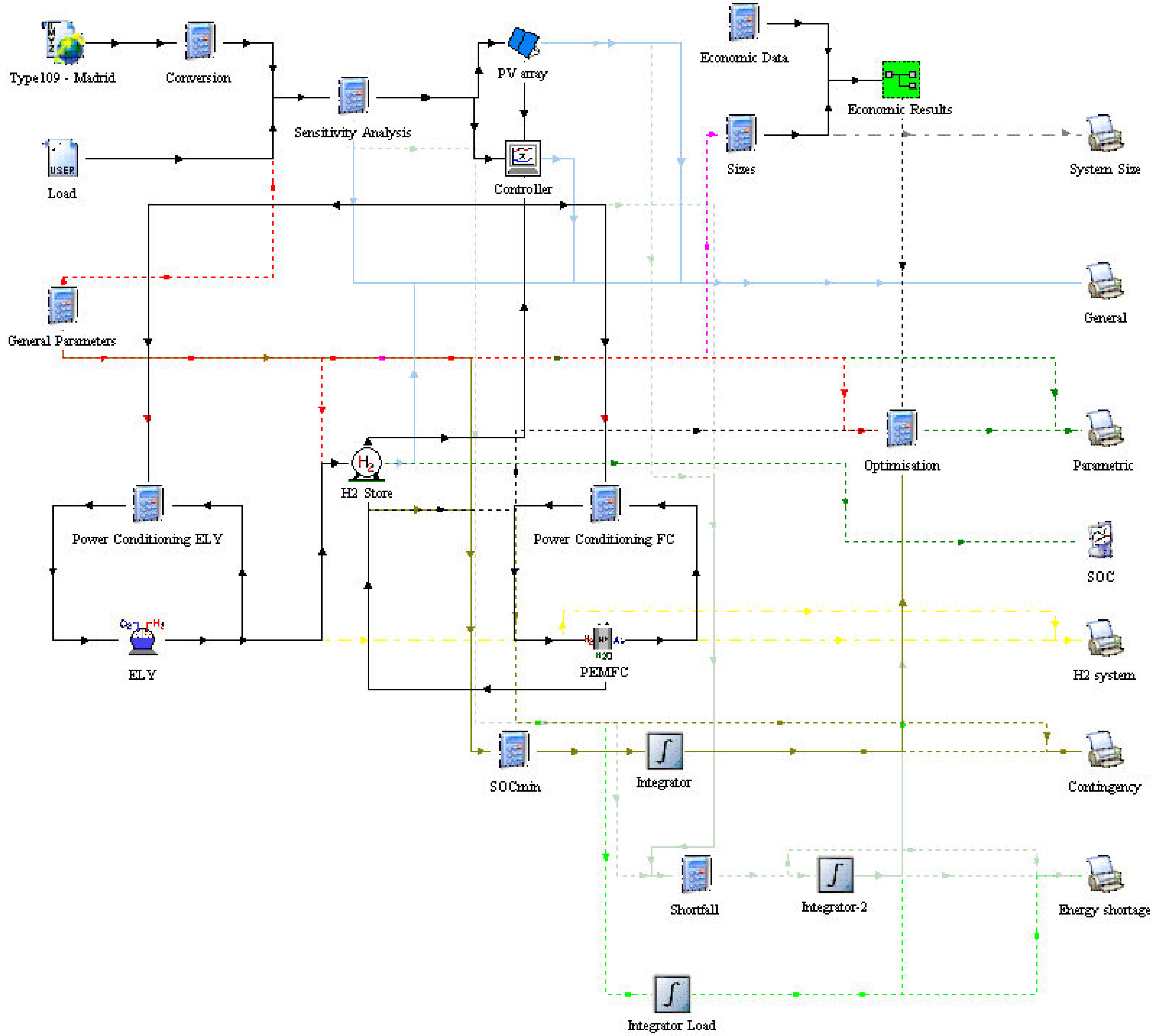


Figure 8: Small scale system model developed with TRNSED

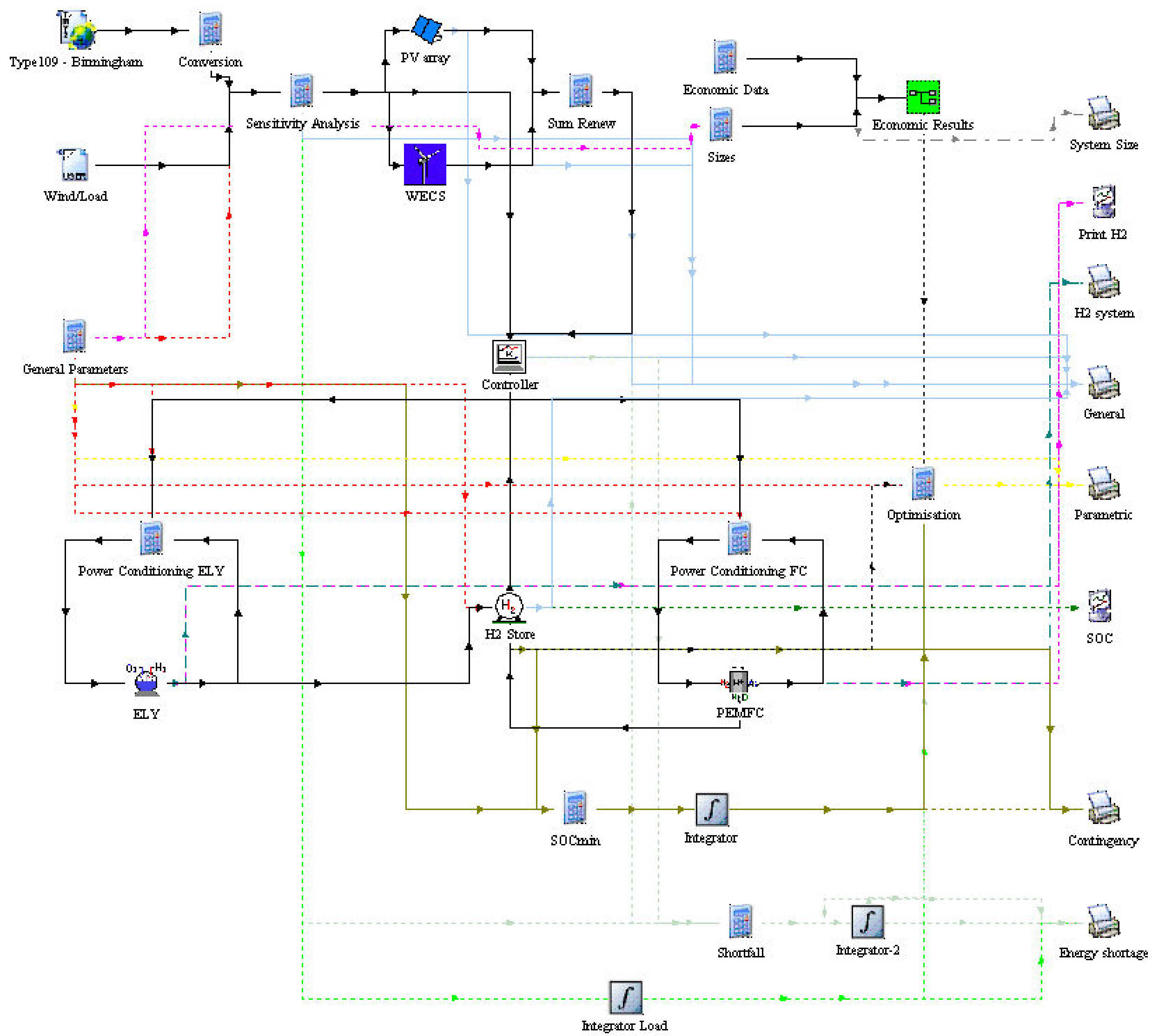


Figure 9: Stand alone power system model developed with TRNSED

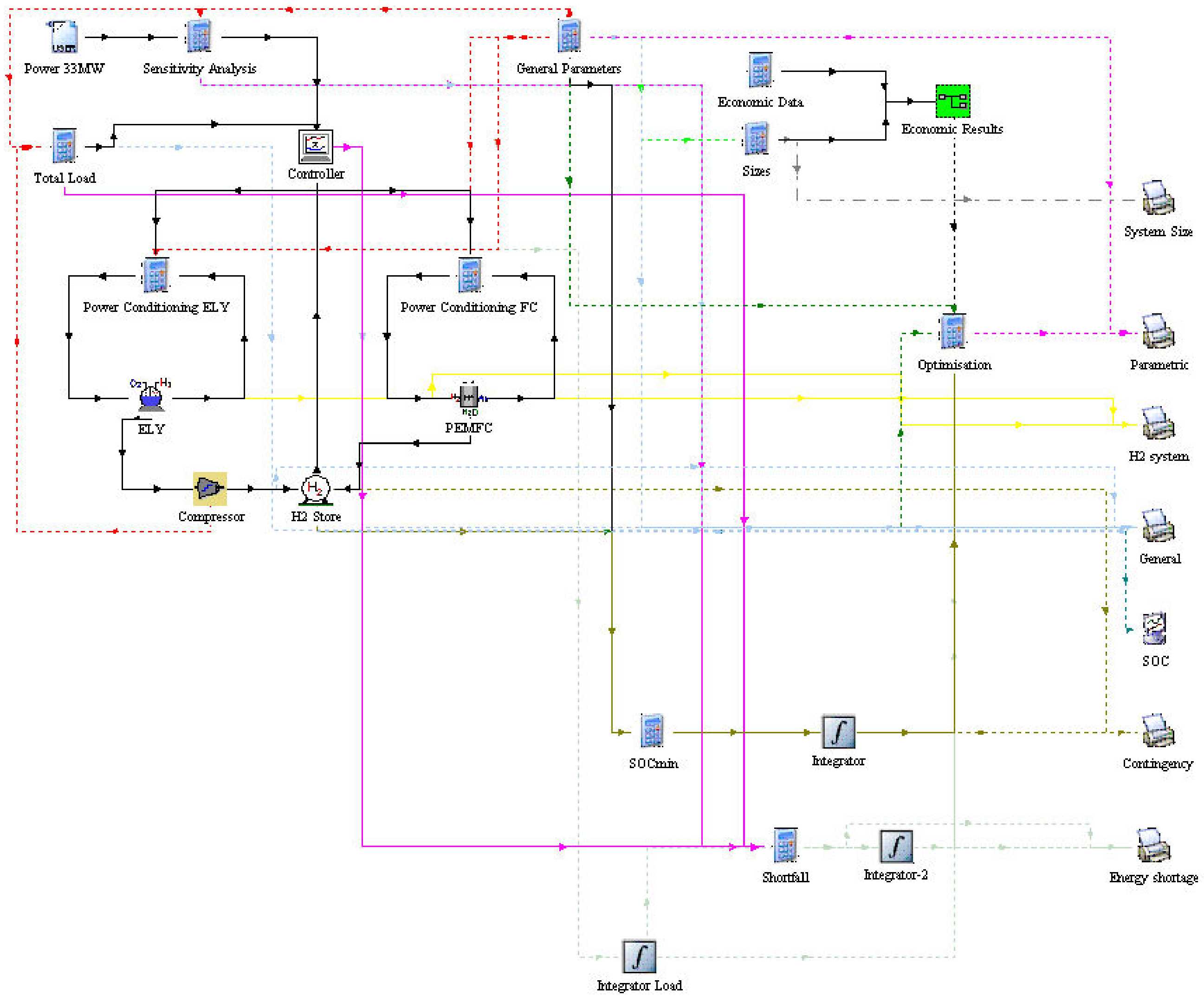


Figure 10: Energy buffering system model developed with TRNSED

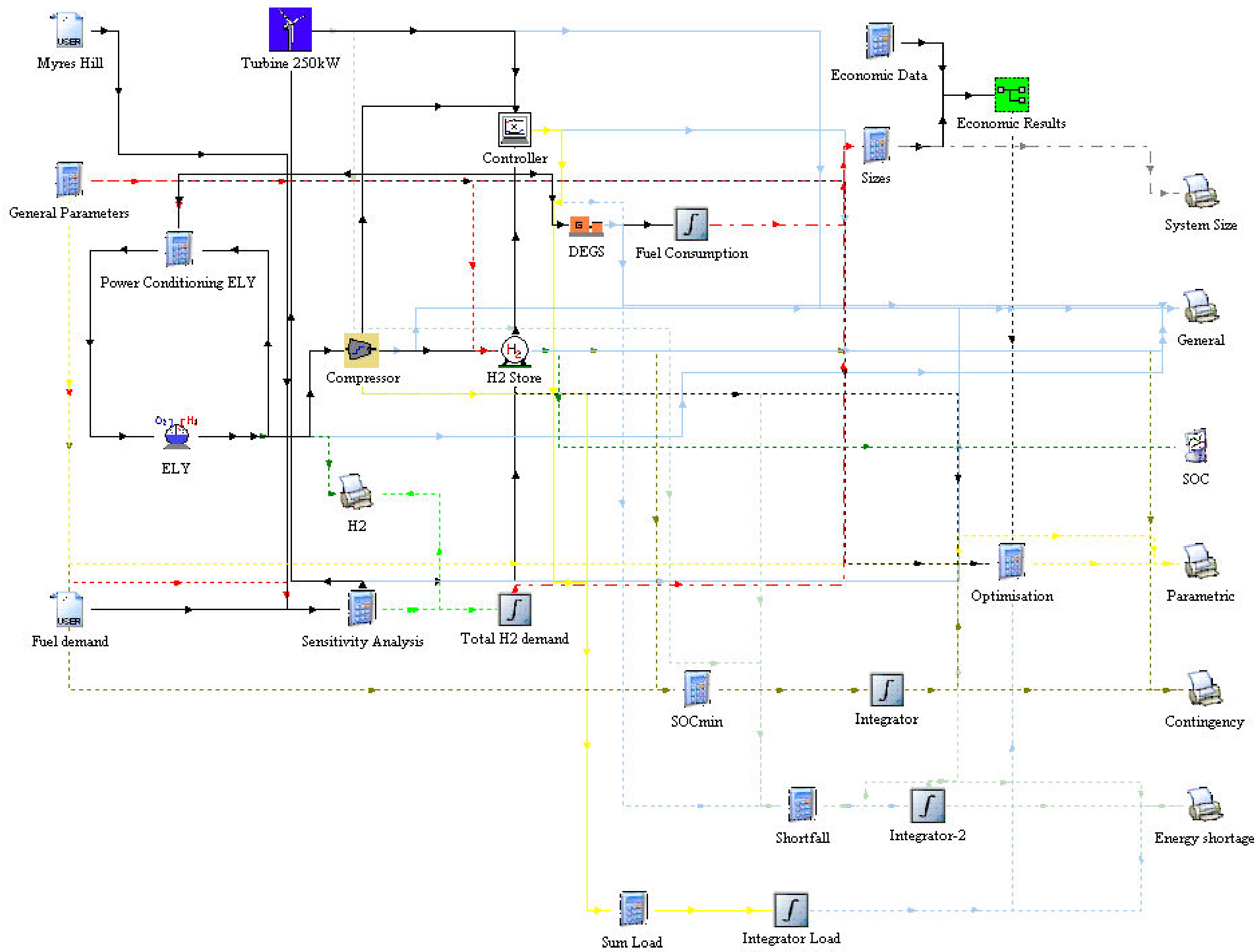


Figure 11: Hydrogen filling station model developed with TRNSED

2. Mathematical models

The components used to create the generic systems models were adapted from those developed by Ulleberg [15]. The advanced alkaline electrolyser, compressed gas storage, a multistage compressor, a power conditioning equipment, a proton-exchange membrane fuel and the model of photovoltaic module are briefly presented here. For more comprehensive descriptions refer to Ulleberg [15].

a. Advanced Alkaline Electrolyser

This model is based on a combination of thermodynamics, heat transfer and empirical electrochemical equations. The electrochemical model is based on a temperature dependent I-U curve for a given pressure and a Faraday efficiency curve independent of temperature and pressure.

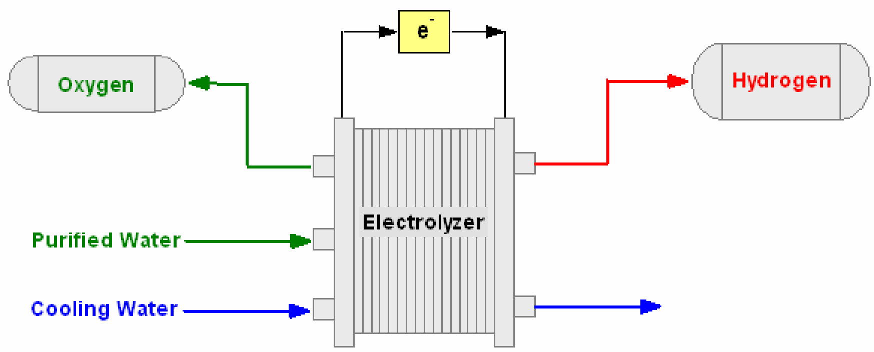


Figure 12: Electrolyser principle [15]

The splitting of water into hydrogen and oxygen can be achieved by passing a direct electric current between two electrodes separated by an aqueous electrolyte with good ionic conductivity. The electrolyte is usually aqueous potassium hydroxide where the potassium ion K^+ and hydroxide ion OH^- take care of the ionic transport.

The anodic and cathodic reactions are:

Anode: $2OH^-(aq) \Rightarrow \frac{1}{2}O_2(g) + H_2O(l) + 2e^-$ Equation 15

Cathode: $2H_2O(l) + 2e^- \Rightarrow H_2(g) + 2OH^-(aq)$ Equation 16

The total reaction for splitting water is:

$H_2O(l) + electricity \Rightarrow H_2(g) + \frac{1}{2}O_2(g)$ Equation 17

Electrochemical model

- **Current-voltage characteristic (per cell)**

The electrode kinetics of an electrolyser cell is modelled using empirical I-U relationships. Overvoltages and ohmic resistance play an important role in the modelling of the I-U curve:

$$U = U_{rev} + \frac{r'}{A} I + s' . \log\left(\frac{t'}{A} I + 1\right) \qquad \text{Equation 18}$$

with U the operation cell voltage, I the current through the cell, U_{rev} the reversible voltage (U_{rev} = 1.229V at standard conditions but changes with temperature and pressure), A the electrode area and:

$$r' = r_1 + r_2 \times T \text{ (Resistance of electrolyte)} \qquad \text{Equation 19}$$

$$\left.\begin{aligned} s' &= s_1 + s_2 \times T + s_3 \times T^2 \\ t' &= t_1 + t_2 / T + t_3 / T^2 \end{aligned}\right| \text{(Overvoltages on electrodes)} \qquad \text{Equation 20}$$

being T the temperature of the electrolyte (K).

- **Faraday efficiency**

The Faraday efficiency η_f is the ratio between the real and theoretical maximum amount of hydrogen produced by the electrolyser. An increase in temperature leads to a lower electrical resistance, more parasitic current losses and lower Faraday efficiencies. The following empirical expression describes these phenomena for a given temperature:

$$\eta_f = \left(\frac{I_{density}{}^2}{a_1 + I_{density}{}^2}\right) \times a_2 \qquad \text{Equation 21}$$

where $I_{density}$ is the current density, a_1 and a_2 are empirical parameters.

- **Hydrogen production**

According to Faraday's law, the production rate of hydrogen in an electrolyser cell is proportional to the electrical current. The total hydrogen production rate $\dot{n}_{H_2}$ (mol.s^{-1}) in an electrolyser is:

$$\dot{n}_{H_2} = \eta_f \times N_{cells} \times \frac{I}{n \times F} \qquad \text{Equation 22}$$

with η_f the Faraday efficiency, I the current through the cell, N_{cells} the number of cells, n and F (Faraday's constant) are constant respectively equal to 2 and 96485.

- **Energy efficiency**

The generation of heat in an electrolyser is mainly due to electrical inefficiencies. The energy efficiency η_e can be calculated from the thermoneutral voltage U_{tn} (U_{tn} = 1.482V at standard conditions but changes with temperature and pressure) and the cell voltage U_{cell}:

$$\eta_e = \frac{U_{tn}}{U_{cell}}$$ Equation 23

As shown in Figure 13, for a given temperature an increase in hydrogen production (i.e. in current density I_{ely}) increases the cell voltage U_{cell} and therefore reduces the energy efficiency. For a given current density, the energy efficiency increases with increasing cell temperature T_{ely}:

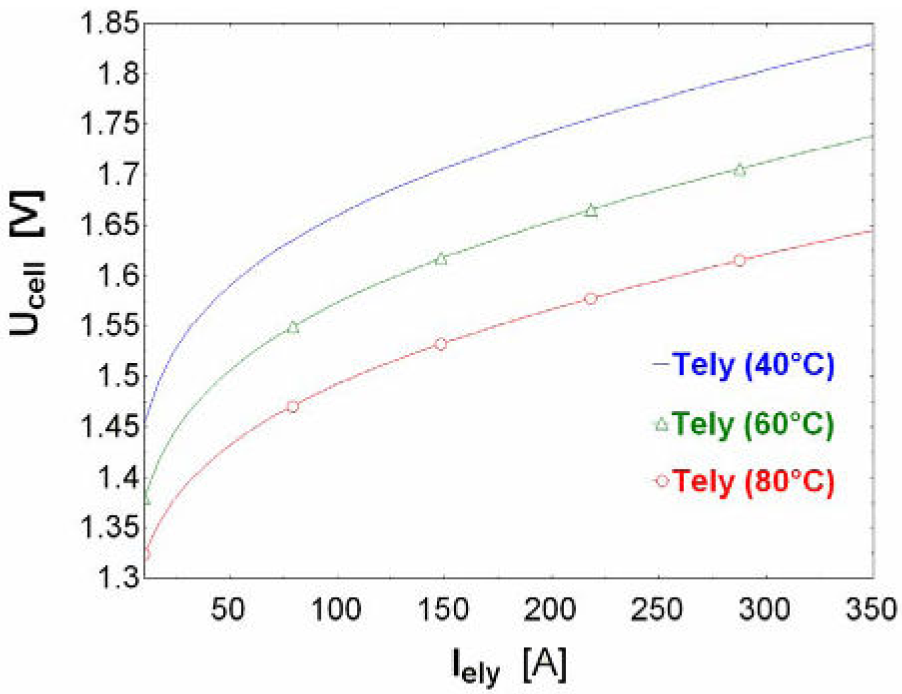


Figure 13: Cell voltage-current curves for different temperatures [15]

- **Overall efficiency**

The overall efficiency η_{tot} of the electrolyser is simply the product of the Faraday and energy efficiencies:

$$\eta_{tot} = \eta_f \times \eta_e$$ Equation 24

b. Compressed gas storage

This model calculates the pressure in the storage based on either the ideal gas law or van der Waals equation of state for real gases.

According to the ideal gas law, the pressure p of a gas storage tank is given by:

$$p = \frac{n \cdot R \cdot T_{gas}}{V_{gas}}$$ Equation 25

with the gas constant R = 8.314 J.K^{-1}.mol^{-1}.

According to the Van der Waals equation of state, the pressure of a real gas stored in a tank is:

$$p = \frac{n \cdot R \cdot T_{gas}}{V_{gas} - n \cdot b} - a \cdot \frac{n^2}{V_{gas}{}^2}$$ Equation 26

with $a = \frac{27 \cdot R^2 \cdot T_{cr}^2}{64 \cdot p_{cr}}$ and $b = \frac{R \cdot T_{cr}}{8 \cdot p_{cr}}$ Equation 27

where T_{cr} is the critical temperature (K) and p_{cr} the critical pressure (Pa) of the gas.

The model simply performs a mass balance of gas entering and leaving the storage and calculates the pressure corresponding to the mass of hydrogen in the tank. If the pressure rises beyond a certain level, the excess of hydrogen is dumped.

c. Multistage compressor

This model is a multi-stage polytropic compressor (1 to 5 stages). The work and cooling need for the compressor are calculated. A 2-stage compressor is presented here as an example.

Thermodynamic model

This model is based on an ideal gas in a quasi-equilibrium compression process (i.e. a process in which all states through which the system passes can be considered as equilibrium states). A polytropic process is a quasi-equilibrium process which describes the relationship between pressure and volume during a compression. It can be expressed as:

$(pV)^N = constant$, where p and V are the pressure and volume of the ideal gas, and N is a constant for a particular process.

- **Polytropic work (ideal gas)**

1st compression stage:

$$W_1 = \frac{N \cdot R \cdot T_{low}}{N-1}\left[1 - \left(\frac{p_x}{p_1}\right)^{\left(\frac{N-1}{N}\right)}\right]$$ Equation 28

2nd compression stage:

$$W_2 = \frac{N \cdot R \cdot T_{low}}{N-1}\left[1 - \left(\frac{p_2}{p_x}\right)^{\left(\frac{N-1}{N}\right)}\right]$$ Equation 29

where $N = 1.4$ is the polytropic compression factor, R the universal gas constant (8.314 $J.K^{-1}.mol^{-1}$), T_{low} is the initial temperature and p_x is the intermediate pressure.

Overall compression work:

$$W_{comp} = \dot{m}_{in} \times (W_1 + W_2) \qquad \text{Equation 30}$$

where $\dot{m}_{in}$ is the mass flow rate (kg.s^{-1}).

- **Isothermic work**

$$W_{iso} = \left| -R \times T_{low} \times \ln\left(\frac{p_2}{p_1}\right) \right| \qquad \text{Equation 31}$$

$$P_{iso} = \dot{m}_{in} \times W_{iso} \qquad \text{Equation 32}$$

- **Isentropic efficiency**

$$\eta_{isen} = \frac{P_{iso}}{P_{comp}} \qquad \text{Equation 33}$$

The isentropic efficiency actually compares the actual performance of the compressor and an idealised performance which neglects the change in entropy.

d. Power conditioning unit

This model is based on empirical efficiency curves for electrical converters (DC/DC) or inverters (DC/AC or AC/DC).

Power conditioners are devices that can invert DC power to AC power (and vice versa) and function as DC/DC converters, needed to transfer DC power from one voltage to another.

The power loss P_{loss} for a power conditioner is mainly dependent on the electrical current running through it. The power loss for a power conditioner can be described as:

$$P_{loss} = P_{in} - P_{out} = P_0 + (U_S / U_{out}) P_{out} + \left(R_{ipn} / U_{out}^{\;2}\right) P_{out}^{\;2} \qquad \text{Equation 34}$$

with P_0 the power loss, U_s the set point voltage, R_{ipn} the internal resistance, P_{in} and P_{out} the power input and output, U_{out} the voltage output.

With respect to the nominal (maximum) power P_{nom} of the power conditioner, the equation becomes:

$$\frac{P_{in}}{P_{nom}} = \frac{P_0}{P_{nom}} + \left(1 + \frac{U_S}{U_{out}}\right) \cdot \frac{P_{out}}{P_{nom}} + \frac{R_{ipn}}{U_{out}^{\;2}} \cdot P_{nom} \cdot \left(\frac{P_{out}}{P_{nom}}\right)^2 \qquad \text{Equation 35}$$

Either the input power P_{in} or the output power P_{out} can be specified as inputs.

The efficiency of the power conditioner η is:

$$\eta = \frac{P_{out}}{P_{in}} \qquad \text{Equation 36}$$

The current output is:

$$I_{out} = \frac{P_{out}}{U_{out}}$$ Equation 37

e. Proton-Exchange Membrane fuel cell (PEMFC)

This model is based on a combination of theoretical and empirical results.

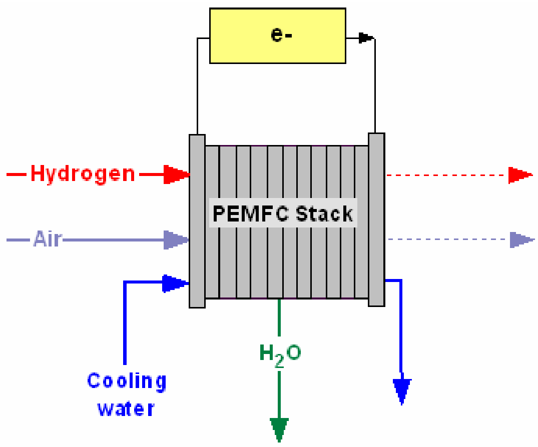


Figure 14: PEMFC principle [15]

A fuel cell converts the chemical energy of a fuel and an oxidant (pure oxygen or air) to direct electrical current. The two following equations show the anodic and cathodic reactions taking place in a PEMFC.

Anode: $H_2(g) \Rightarrow 2H^+(aq) + 2e^-$ Equation 38

Cathode: $2H^+(aq) + 2e^- + \frac{1}{2}O_2(g) \Rightarrow H_2O(l)$ Equation 39

The total fuel cell reaction is: $H_2(g) + \frac{1}{2}O_2(g) \Rightarrow H_2O(l)$ Equation 40

The process produces electricity, water and heat.

Electrochemical model

The performance of a fuel cell is represented by its output voltage. The basic expression for the voltage of the single cell U_{cell} is:

$$U_{cell} = E + \eta_{act} + \eta_{ohmic}$$ Equation 41

where E is the thermodynamic potential, η_{act} is the anode and cathode activation overvoltage (the voltage loss associated with the anode and cathode), and η_{ohmic} is the ohmic overvoltage (the losses associated with the proton conductivity of the solid polymer electrolyte and electronic internal resistances).

The thermodynamic potential is defined through the Nernst equation:

$$E = 1.23 - 0.00085 \cdot (T - 298) + 0.0000431 \cdot T \cdot \ln\left(p_{H_2} \cdot p_{O_2}^{\ 0.5}\right) \qquad \text{Equation 42}$$

being T the temperature (K), p_{H2} and p_{O2} respectively the pressure of hydrogen and oxygen (bar).

The activation voltage is based on theoretical equations from kinetic, thermodynamic and electrochemistry fundamentals while temperature and current experimental data were used to calculate the ohmic overvoltage.

f. Photovoltaic array

This model is based on an equivalent circuit of a one-diode model, also known as the 5-parameter model (see Figure 15). The model can be used for modules made of silicon cells or other types of materials. A maximum power point tracker (MPPT) algorithm which finds the maximum power point automatically is also included the model.

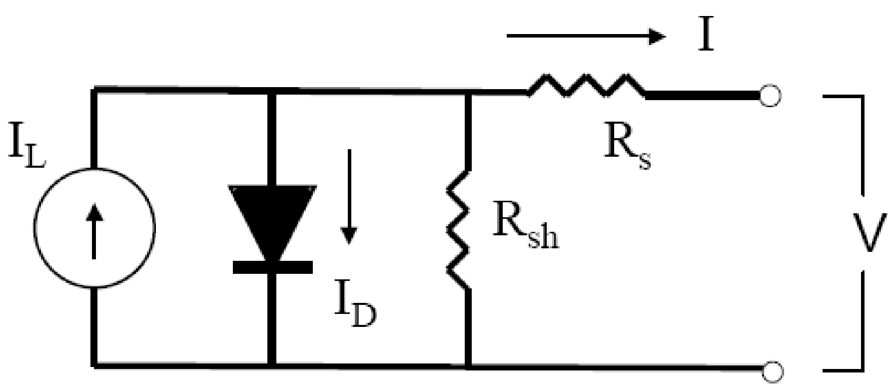


Figure 15: The equivalent circuit for the PV generator model [15]

Electrical model

- **Current-voltage characteristic**

Using the previous equivalent circuit the relationship between the operation current I and the operation voltage U of the equivalent circuit is described by:

$$I = I_L - I_D - I_{sh} = I_L - I_0\left\{\exp\left(\frac{U + IR_S}{a}\right) - 1\right\} - \frac{U + IR_S}{R_{sh}} \qquad \text{Equation 43}$$

with I_L the light current, I_D the diode current, I_{sh} the shunt current, I_0 the diode reverse current, R_s and R_{sh} the series and shunt resistance, a the curve fitting parameter.

- **Open circuit voltage**

$$U_{OC} = a \cdot \ln\left(\frac{I_L}{I_0}\right) \qquad \text{Equation 44}$$

- **Cell and array power**

$$P_{cell} = U_{cell} \cdot I_{cell}$$
$$P_{tot} = N_s \cdot P_{cell} \qquad \text{Equation 45}$$

where N_S is the number of cells in series, U_{cell} and I_{cell} are the cell voltage and current.

- **Cell efficiency**

$$\eta = \frac{P_{cell}}{A_{cell} \cdot G_T} \qquad \text{Equation 46}$$

The cell efficiency is defined as the ratio of the energy produced over the incident of solar energy, G_T being the incident solar radiation ($W.m^{-2}$) and A_{cell} the cell area (m^2). It is a good measure of performance of the PV cell.

g. Master level controller for SAPS

The master level controller component available in the TRNSYS library is designed to control a stand-alone power system including wind turbines (or another source of renewable power like PV, or a combination of renewables), an electrolyser, a fuel cell, a hydrogen storage tank and a set diesel engine generator.

The control strategy is based on the state-of-charge (SOC) of hydrogen in the tank and on different set points defined on the following graph:

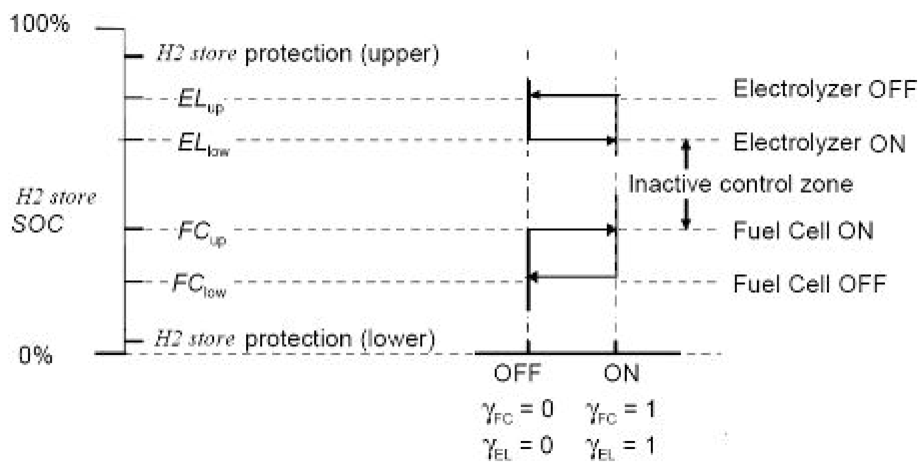


Figure 16: Control strategy based on the SOC of the hydrogen storage

The decisions of the controller are based on the mini-grid busbar power balance according to the following algorithm:

$$P_{busbar} = P_{WECS} + N_{DEGS,min}\, P_{DEGS,max} + P_{FC,min} - P_{Load} - P_{Ely,min}$$

EXCESS POWER ($P_{BUSBAR} > 0$)

1. Electrolyser status

• If the electrolyser is currently OFF (Idling):

- If SOC < EL_{low}, switch ON:
- Operate with $P_{ely,set} = P_{WECS} + N_{DEGS,min}\, P_{DEGS,max} + P_{FC,min} - P_{Load}$
- Else, remain OFF (Idling)

• Else (electrolyser is currently ON):

- If SOC > EL_{up}, switch OFF (Idling)
- Else, keep operating and $P_{ely,set} = P_{WECS} + N_{DEGS,min}\, P_{DEGS,max} + P_{FC,min} - P_{Load}$

• Constraints on $P_{Ely,set}$: If $P_{Ely,set} > P_{Ely,max}$ then $P_{Ely,set} = P_{Ely,max}$

2. Dump

• If PEly,max was reached: $P_{dump} = P_{WECS} + N_{DEGS,min}\, P_{DEGS,max} + P_{FC,min} - P_{Load} – P_{Ely,set}$

POWER DEFICIT ($P_{BUSBAR} < 0$)

1. Switch off fuel cell if necessary, based on the H2 storage tank level

• Switch Fuel cell to idling mode if the fuel cell is currently ON and SOC < FC_{low}

• Keep idling if the fuel cell is currently OFF and SOC ≤ FC_{up}

2. DEGS, Electrolyser and Dump

• If the fuel cell is currently OFF (idling):

- Find NDEGS, the minimum number of operating DEGS that generates a power excess, assuming the electrolyser is idling. N_{DEGS} is the minimum value for which ($P_{WECS} + N\, P_{DEGS,max} + P_{FC,min} - P_{Load} – P_{Ely,min}$) ≥ 0
- Electrolyser operates at $P_{Ely,set} = P_{WECS} + N\, P_{DEGS,max} + P_{FC,min} - P_{Load}$
- No dumped power: $P_{dump} = 0$

• Else (the fuel cell is currently ON):

- Find N_{DEGS}, the minimum number of operating DEGS that generates a power excess, assuming the electrolyser is idling and the fuel cell is at maximum power. N_{DEGS} is the minimum value for which ($P_{WECS} + N\, P_{DEGS,max} + P_{FC,max} - P_{Load} – P_{Ely,min}$) ≥ 0
- Assume electrolyser is idling
- Set Fuel cell power: $P_{FC,set} = P_{Load} + P_{Ely,min} - P_{WECS} - N\ _{PDEGS,max}$

- If $P_{FC,set} < P_{FC,min}$ then impose $P_{FC,set} = P_{FC,min}$
- Set Electrolyser power to use all power that would be dumped:

$$P_{Ely,set} = P_{WECS} + N\ P_{DEGS,max} + P_{FC,max} - P_{Load}$$

With:

- PWECS (W): Power generated by the wind turbines
- PDEGS,max (W): Rated power generated by one diesel generator (DEGS)
- PDEGS,set (W): Power setpoint for each DEGS
- NDEGS: Number of DEGS operating at fixed power
- NDEGS,min: Minimum number of DEGS operating at any time
- NDEGS,max: Maximum number of DEGS operating at any time
- PFC,min (W): Minimum (idling) power of the fuel cell
- PFC,max (W): Rated power of the fuel cell
- PFC,set (W): Power setpoint for the fuel cell
- PEly,min (W): Minimum (idling) power of the electrolyzer
- PEly,max (W): Rated power of the electrolyzer
- PEly,set (W): Power setpoint for the electrolyzer
- PLoad (W): Power to the load
- Pdump (W): Dumped power
- Pbusbar (W): Power balance on the mini-grid bus bar
- SOC: State of charge of the energy storage
- ELlow: State of charge for which the electrolyzer is switched ON
- ELup: State of charge for which the electrolyzer is switched OFF
- FClow: State of charge for which the fuel cell is switched OFF
- FCup: State of charge for which the fuel cell is switched ON

3. Cost-benefit analysis

TRNSYS does not have readily available cost models in its standard libraries. To enable the user to undertake technical AND financial analysis of hydrogen systems it was necessary to develop cost-benefit functions for use with the generic TRNSYS systems models developed for this project. The equations used in the analysis are derived from standard economics [40].

Renewable and non-renewable energy sources typically have dramatically different cost characteristics. Renewable sources tend to have high initial capital costs and low operating costs, whereas conventional non-renewable sources tend to have low capital and high operating costs. For that reason the economic model must take into account both capital and operating costs. [41]

The aim of the analysis is to derive two key economic indicators: the total net present cost and the levelized cost of energy. The total net present cost condenses all the costs and revenues that occur within the project lifetime and is therefore used to rank all the system configurations in the optimisation process. The levelized cost of energy also gives an interesting indication of the economic performance of the system.

For each component of the system, the user specifies the initial capital cost, which occurs in year zero, the replacement cost, which occurs each time the component reaches the end of its lifetime, and the O&M cost, which occurs each year of the project lifetime. The discount rate and the project lifetime are also specified by the user.

a. Initial capital cost

The initial capital cost of a component is the total installed cost of that component at the beginning of the project.

b. Annualised capital cost

The annualised capital cost of each component is calculated using the following equation [42]:

$$C_{acap} = C_{cap} \times CRF\left(i, R_{proj}\right) \qquad \text{Equation 47}$$

where:

C_{cap} = initial capital cost of the component
CRF() = capital recovery factor
i = interest rate
R_{proj} = project lifetime in years

- The **capital recovery factor** is used to calculate the present value of an annuity (a series of equal annual cash flows). It is calculated with the following equation:

$$CRF(i, N) = \frac{i(1+i)^N}{(1+i)^N - 1} \qquad \text{Equation 48}$$

where *N* is the number of years.

- The **annual real interest rate** (or just ***interest rate***) is the discount rate used to convert between one-time costs and annualised costs. The annual real interest rate is related to the nominal interest rate by the equation:

$$i = \frac{i' - f}{1 + f} \qquad \text{Equation 49}$$

where:

i' = nominal interest rate (the rate at which a loan can be obtained)
f = annual inflation rate

- The **project lifetime** is the length of time over which the costs of the system occur. It is used to calculate the annualised replacement cost and annualised capital cost of each component, and the total net present cost of the system.

c. Annualised replacement cost

The annualised replacement cost of a system component is the annualised value of all the replacement costs occurring throughout the lifetime of the project, minus the salvage value at the end of the project.

Each component's annualized replacement cost is calculated using this equation:

$$C_{arep} = C_{rep} \times f_{rep} \times SFF\left(i, R_{comp}\right) - S \times SFF\left(i, R_{proj}\right) \qquad \text{Equation 50}$$

where:

C_{rep} = cost of replacement of the component at the end of its lifetime (may be different from the initial capital cost)

R_{comp} = lifetime of the component

- f_{rep} has to be introduced because the component lifetime can be different from the project lifetime, is given by:

$$\begin{cases} f_{rep} = CRF\left(i, R_{proj}\right) / CRF\left(i, R_{rep}\right), R_{rep} > 0 \\ f_{rep} = 0, R_{rep} = 0 \end{cases} \qquad \text{Equation 51}$$

- R_{rep}, the replacement cost duration, is given by:

$$R_{rep} = R_{comp} \times INT\left(\frac{R_{proj}}{R_{comp}}\right) \qquad \text{Equation 52}$$

where INT() is the integer function, returning the integer portion of a real value.

- The **salvage value** is the value remaining in a component at the end of the project. A linear depreciation of components is assumed, meaning that the salvage value of a component is directly proportional to its remaining life. The salvage value S is given by:

$$S = C_{rep} \times \frac{R_{rem}}{R_{comp}} \qquad \text{Equation 53}$$

- R_{rem}, the remaining life of the component at the end of the project lifetime, is given by:

$$R_{rem} = R_{comp} - \left(R_{proj} - R_{rep}\right) \qquad \text{Equation 54}$$

- The **sinking fund factor** is used to calculate the future value of a series of equal annual cash flows. The equation to use is:

$$SFF\left(i, N\right) = \frac{i}{\left(1+i\right)^{N} - 1} \qquad \text{Equation 55}$$

d. O&M (operation and maintenance) cost

The O&M cost of a component is the annual cost of operating and maintaining that component.

e. Annualised cost

For each component the capital, replacement and maintenance costs along with the salvage value and any other costs are used to find the component's annualised cost. The annualised cost of each component is equal to the sum of its:

- annualised capital cost
- annualised replacement cost
- annual O&M cost
- annual fuel cost if applicable

The annualised cost can be used to compare the costs of different components because it measures their relative contribution to the total net present cost.

f. Total net present cost

The total net present cost is the main economic output of this analysis. It is used to assess the economic performance of the system over its entire lifetime. All systems are ranked according to net present cost, and all other economic outputs are calculated for the purpose of finding the net present cost. The net present cost is calculated according to the following equation:

$$C_{NPC} = \frac{C_{ann,tot}}{CRF\left(i, R_{proj}\right)} \qquad \text{Equation 56}$$

where:

$C_{ann,tot}$ = total annualized cost [$/yr]
CRF() = capital recovery factor
i = interest rate [%]
R_{proj} = project lifetime [yr]

g. Levelized cost of energy

The levelized cost of energy (COE) is defined as the average cost per kWh of useful electrical energy produced by the system. To calculate the COE, the annualised cost of producing electricity is divided by the total useful electric energy production. The equation for the COE is:

$$COE = \frac{C_{ann,tot}}{E_{load,served} + E_{grid,sales}} \qquad \text{Equation 57}$$

where:

$C_{ann,tot}$= total annualized cost of the system [$/yr]
$E_{load,served}$= Load served [kWh/yr]
$E_{grid,sales}$= total grid sales [kWh/yr]

The COE is a convenient metric with which to compare systems but it is not used to rank systems in this model. Indeed, the total NPC is better than the COE as an economic metric because it is a more trustworthy number, for the following reasons:

The COE is simply the average cost per kWh of electricity. But in developing a precise mathematical definition of the COE, some questions arise. For example, in calculating the total amount of useful electricity produced by the system, the amount of electricity the system actually serves is used rather than the total electric demand. The two are not equal if some unmet load is allowed. The result is that the value of COE is also somewhat disputable, which is not the case for the total NPC. It doesn't require any judgment, which is why it is chosen as the main economic criterion. [41]

h. Implementing cost-benefit analysis in TRNSYS

The economic equations described in the previous section have been integrated into the TRNSYS models by creating some additional equation-blocs (Figure 17). A few precautions had to be taken, for example to avoid divisions by 0. The structure is presented in Figure 18.

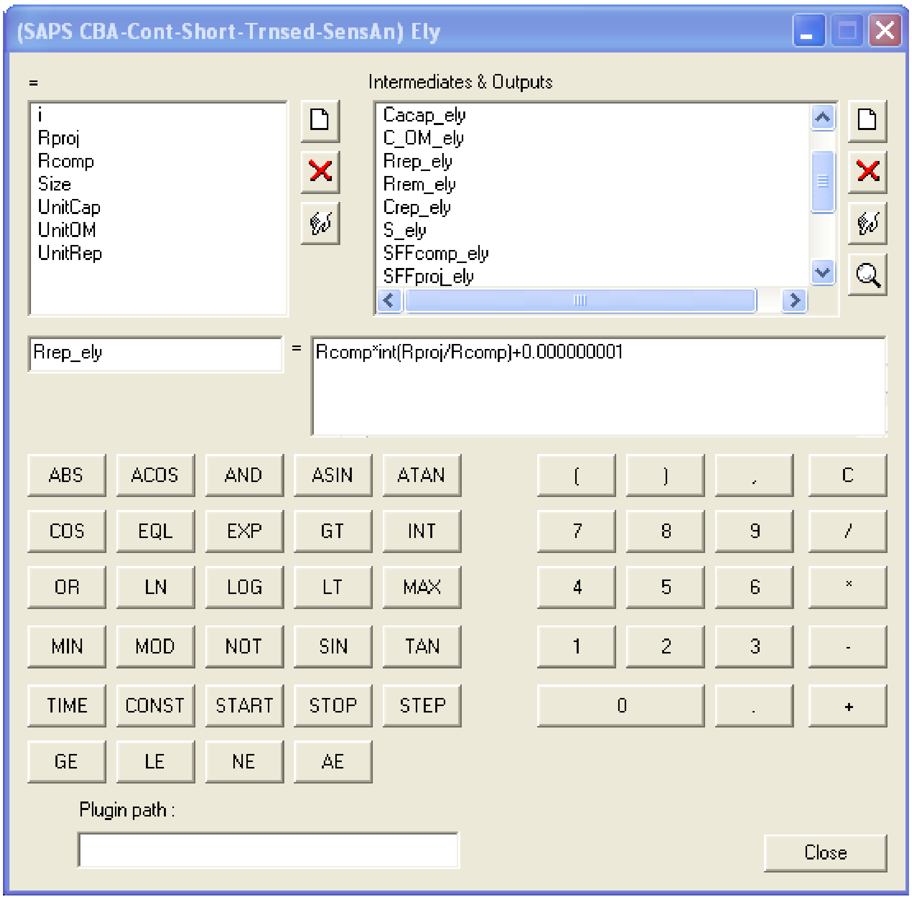


Figure 17: Equation-bloc in TRNSYS

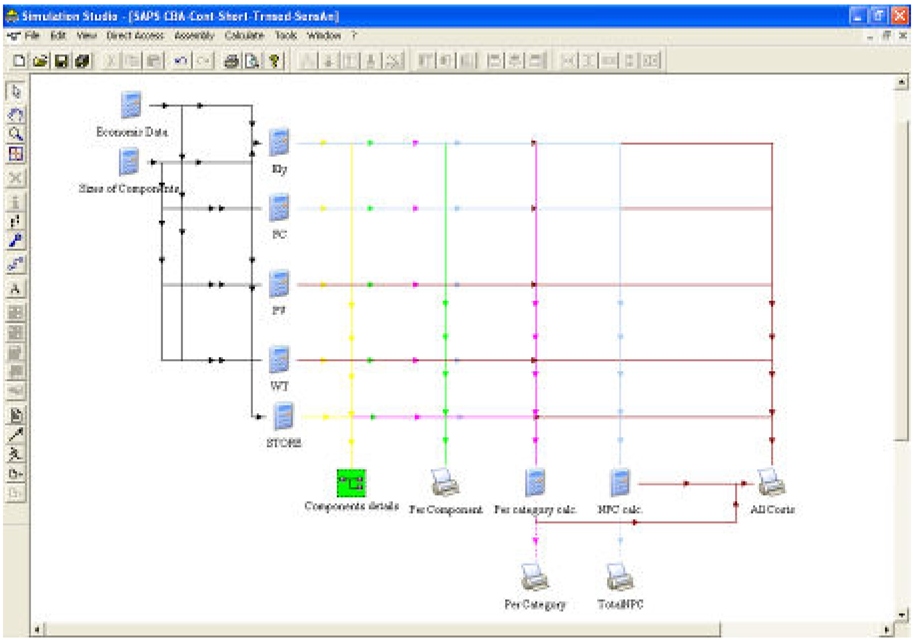


Figure 18: Implementation of the cost-benefit model in TRNSYS

4. Analysis of the results

Different output "devices" can be used in TRNSYS to extract data from the simulations. The most common one is the printer that generates text files to output selected system variables at specified intervals of time. However these results given as time-series are not convenient to use if a concise analysis of the performance of the system is to be done.

To aid in the analysis of the generic systems performance it was therefore necessary to produce an Excel-based analysis tool to process and display the TRNSYS outputs in a user-friendly manner.

The tool presents the technical and economic performance of the system modelled; this is composed of four parts: technical performance, monthly graphs, components operation and cost-benefit analysis.

a. Technical performance

This part of the tool summarises the configuration of the system with the exact size of each component, the average load and the peak load over the year of simulation.

The page also presents the detailed performance of the system:

- the energy production of the wind turbines, the PV array and the fuel cell,
- the total load and the energy consumption of the electrolyser,
- the unmet electric load,
- the year-end, average and minimum states-of-charge of hydrogen in the tank.

In addition, the page contains three graphs representing the contribution of each component in the energy production and consumption, as well as a graph showing the hydrogen state-of-charge over the year.

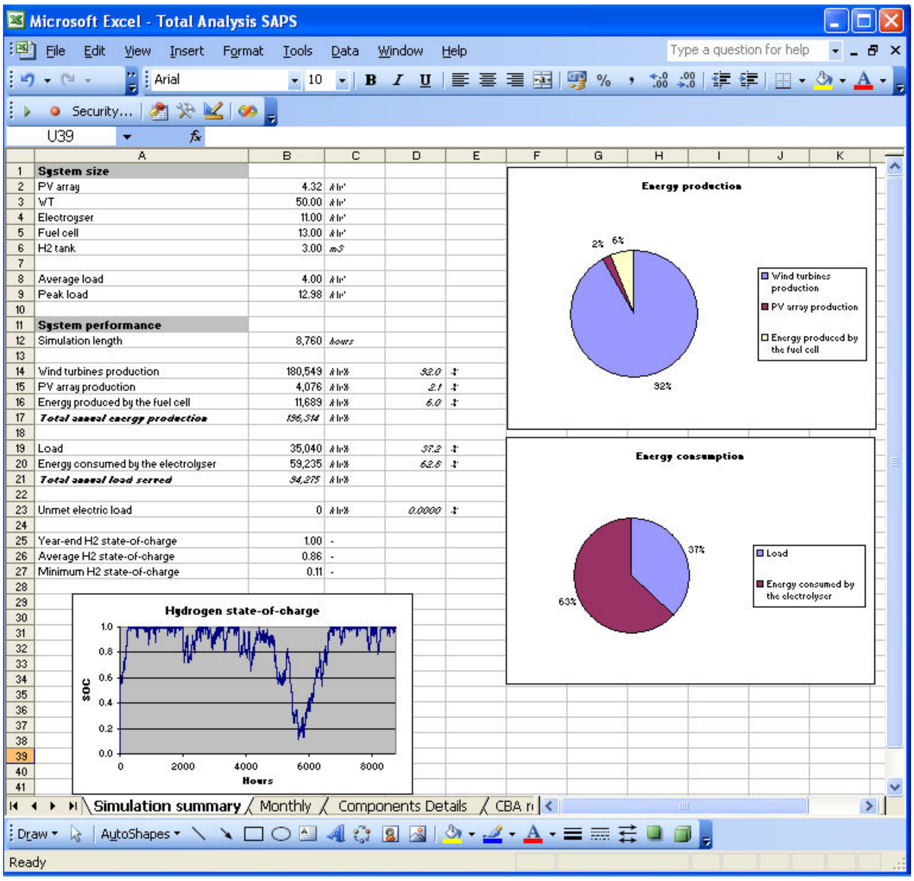


Figure 19: System summary and performance

b. Monthly graphs

This second part presents the total energy production and consumption of each component of the system per month. It also presents the monthly average state-of-charge of stored hydrogen. Additionally, the information described above is shown on three separate graphs.

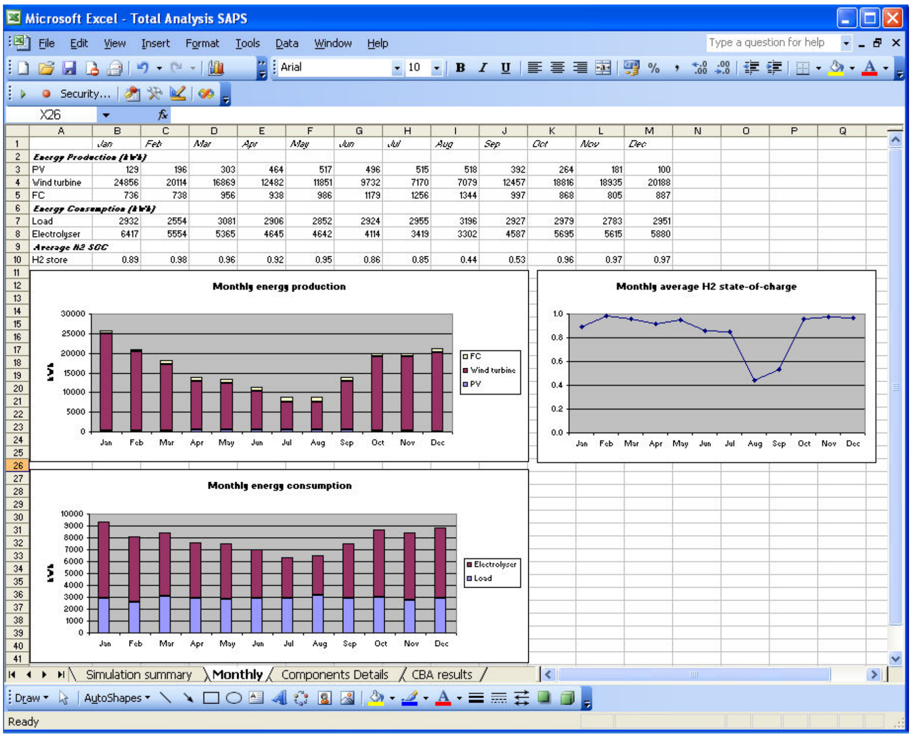
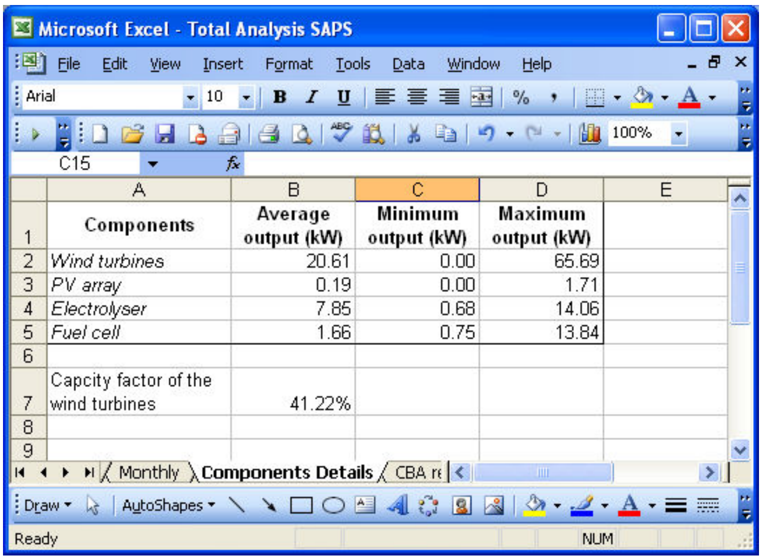


Figure 20: Monthly graphs

c. Components operation

This third part gives the average, minimum and maximum output powers of the wind turbines, the PV array, the electrolyser and the fuel cell (and the compressor if applicable).



Components	Average output (kW)	Minimum output (kW)	Maximum output (kW)
Wind turbines	20.61	0.00	65.69
PV array	0.19	0.00	1.71
Electrolyser	7.85	0.68	14.06
Fuel cell	1.66	0.75	13.84
Capcity factor of the wind turbines	41.22%		

Figure 21: Components operation

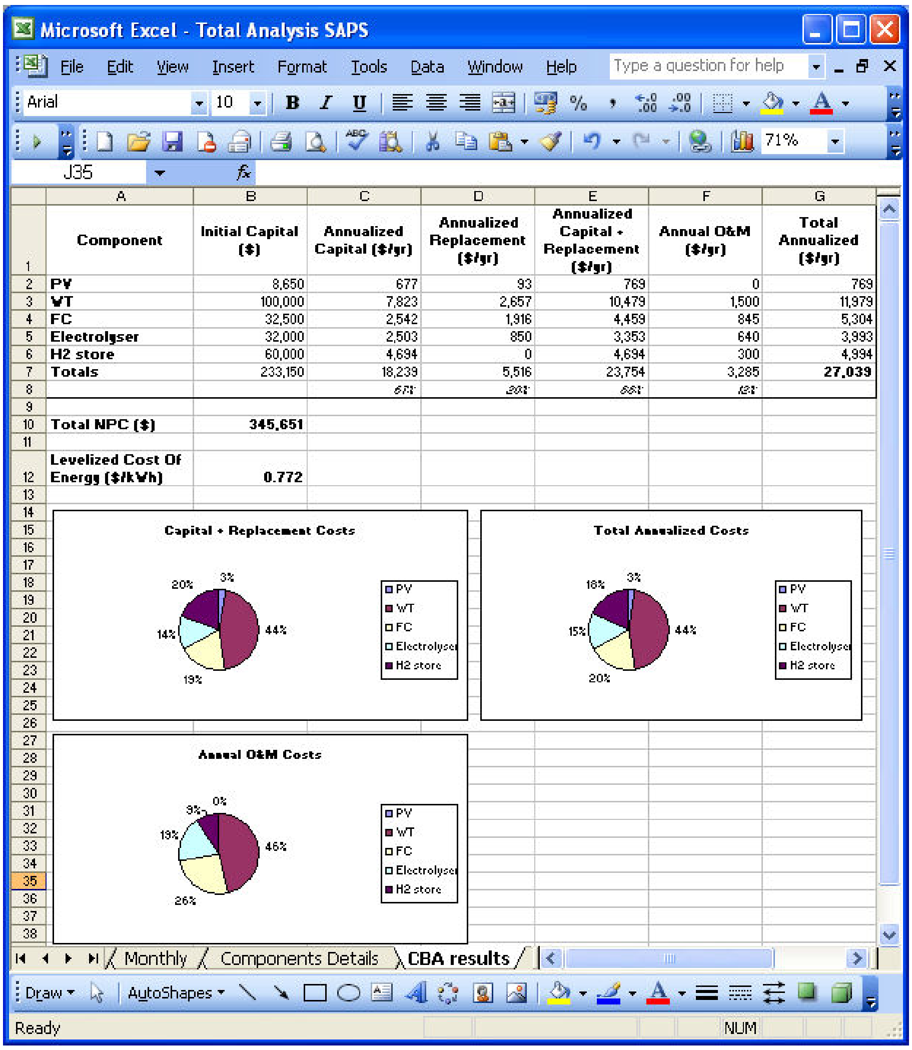
d. Cost-benefit analysis

Finally the last part of the tool deals with the economic results of the analysis; this shows a detailed breakdown of the system costs. Each row corresponds to a component of the system, and the final row shows the totals for each column. The different costs calculated are:

- initial capital cost
- annualised capital cost
- annualised replacement cost
- O&M cost
- fuel cost (if applicable)
- total annualised cost

The two most important cost outputs, the total net present cost and the levelized cost of energy are also presented here.

The pie charts on the CBA sheet break down the costs of the system by component. The first graph shows the annualised capital plus replacement costs, and the second shows annual O&M costs (plus fuel costs if relevant). The third chart shows the total annualised cost, which is the sum of the first two.



Component	Initial Capital ($)	Annualized Capital ($/yr)	Annualized Replacement ($/yr)	Annualized Capital + Replacement ($/yr)	Annual O&M ($/yr)	Total Annualized ($/yr)
PV	8,650	677	93	769	0	769
WT	100,000	7,823	2,657	10,479	1,500	11,979
FC	32,500	2,542	1,916	4,459	845	5,304
Electrolyser	32,000	2,503	850	3,353	640	3,993
H2 store	60,000	4,694	0	4,694	300	4,994
Totals	233,150	18,239	5,516	23,754	3,285	27,039
Total NPC ($)	345,651					
Levelized Cost Of Energy ($/kWh)	0.772					

Figure 22: Cost-benefit analysis and economic performance

5. TRNEdit: creating distributable stand-alone TRNSED applications

a. Advantages

Communicating results is of course an essential part of a modelling study. Normally, results are submitted in a report to the client. If the client wants to modify something in the analysis, he has to go back to the simulator to have the new cases rerun.

A very useful feature in TRNSYS is a method called TRNSED. It allows TRNSYS users to share simulation work with non-technical users. For the TRNSYS programmer, reading and editing the TRNSYS input file is relatively easy, but for those not familiar with TRNSYS manipulating the file might be much more confusing.

In this project, TRNEdit was used to design a user-friendly interface for the TRNSYS models of the generic systems, allowing inexperienced TRNSYS user to apply them.

By using a specialised TRNSYS editor called TRNEdit the programmer can add commands to transform the TRNSYS input file into a TRNSED file: TRNSED eliminates unwanted details and generates a customised interface with only selected parameters and inputs. It presents a simplified view of the TRNSYS file with only a few parameters available to users; selected inputs can be viewed, changed before running the simulations. Parametric simulations (for optimisation) and post-simulation plots are also accessible. Additional help can be included by the programmer if necessary.

Customised TRNSED interfaces for each of the generic systems models have been developed as part of this project. To illustrate the graphical and practical advantages of TRNSED the TRNSYS and TRNSED graphical representations of a stand alone power system for the hydrogen stand-alone power system model are compared on Figure 23 and Figure 24:

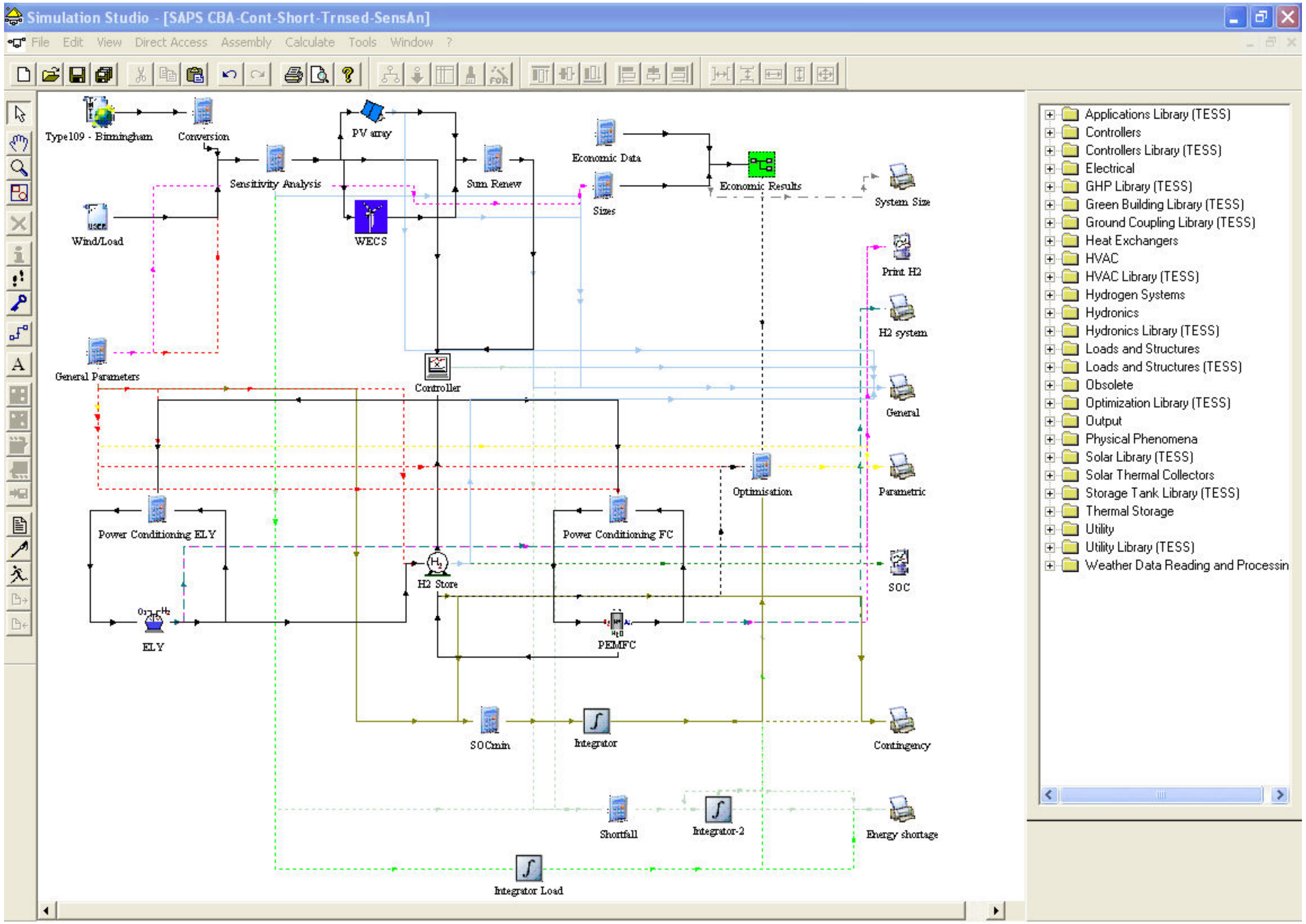


Figure 23: TRNSYS simulation studio. Representation of a SAPS

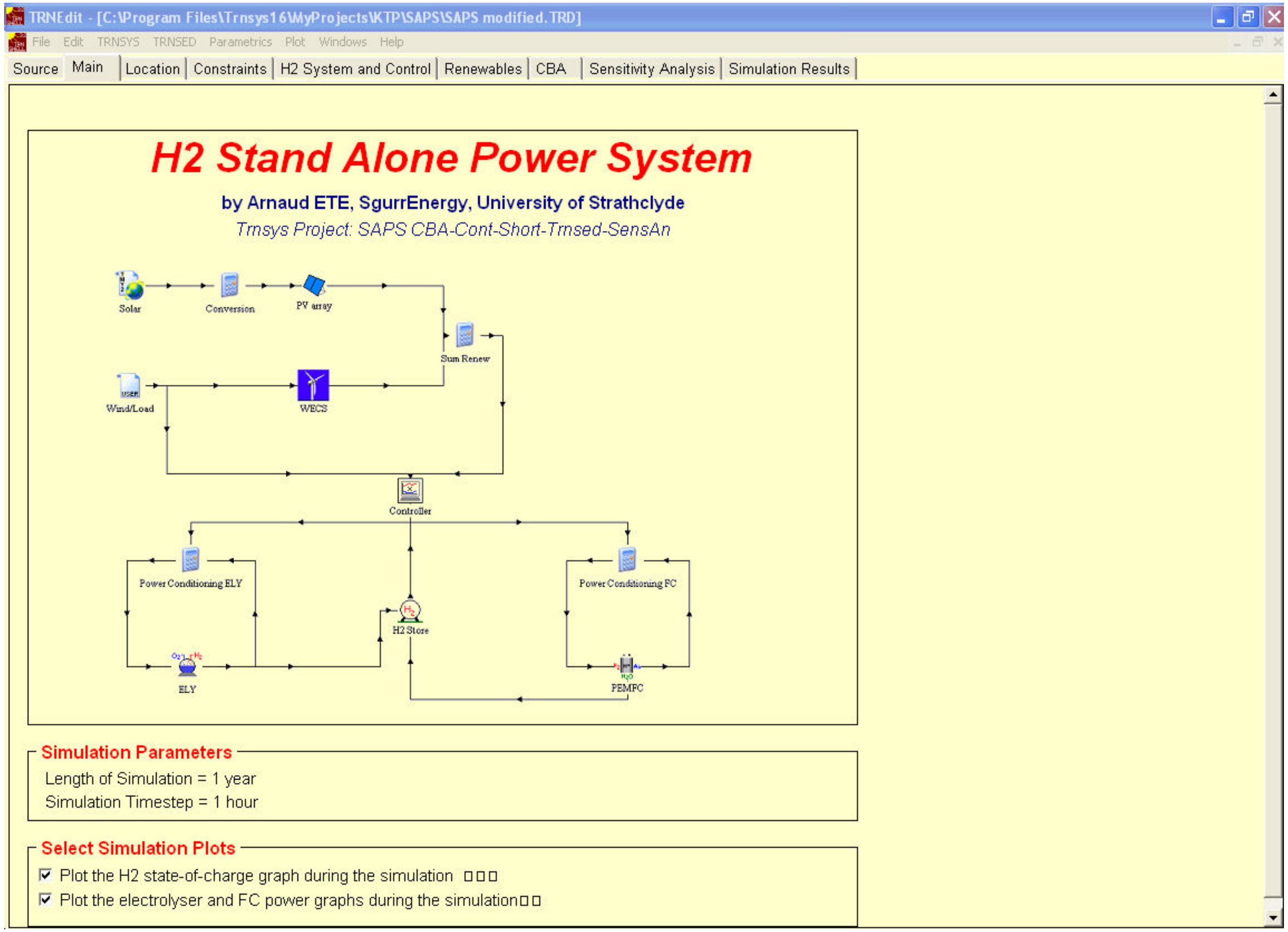


Figure 24: User-friendly TRNSED interface of a SAPS model

The TRNSED model is much easier to use with its different tabs on top of the window (which will be described in the next chapter) whereas the raw TRNSYS file is complicated and can only be used by experienced TRNSYS users. Most of the icons on the TRNSYS window are actually useless for the user. Using TRNSED allows a faster access to the essential parameters of the simulation and reduces the possibility to make mistakes.

TRNSED also gives direct access to the parametric runs. This option makes the optimisation of system performance much more straightforward than with TRNSYS.

Moreover, TRNSED executables are stand-alone applications that can be distributed to a wide user community.

b. TRNSED features

For this report only the hydrogen stand-alone power system (HSAPS) model is presented in order to avoid any redundancy in presenting the four models in detail. The other models all have the same general structure.

The TRNEdit interface designed for this project has been divided into 9 tabs that follow the methodology used to simulate and optimize a hydrogen energy system: source, main, location, constraints, H_2 system and control, renewables, cost-benefit analysis, sensitivity analysis and simulation results.

- The “source” tab is where all the code for the application lies. It is possible to navigate between the “source” tab and the other tabs to see the results of changes in the code on the interface (the application is updated every time).
- The “main” tab (Figure 25) is principally a presentation tab. It includes a simplified graphical representation of the TRNSYS model, a help-file describing the system, and check-boxes to choose whether or not to plot the hydrogen state-of-charge and the electrolyser and fuel cell power graphs during the simulation.

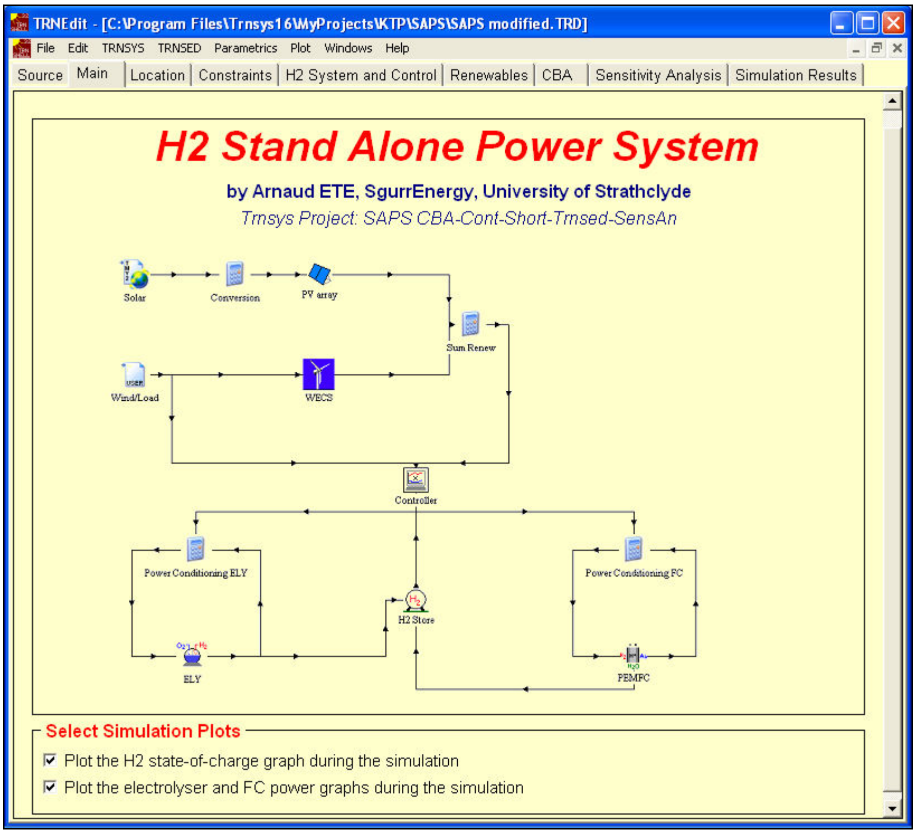


Figure 25: Home page

- The “location” tab (Figure 26) allows the user to describe the wind and solar resources of the site, as well as the load profile (electrical demand).

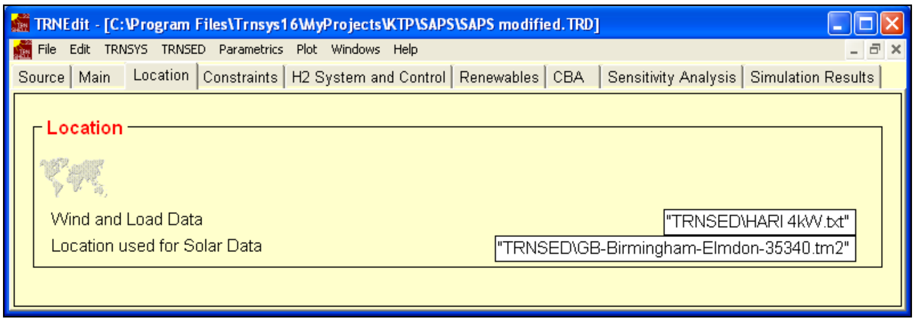


Figure 26: Location page

- The “constraints” tab (Figure 27) allows the user to define different constraints on the operation of the system. These three constraints have been described before in this report:
    - The minimum allowed hydrogen level in the tank.
    - The maximum allowed capacity shortage.
    - Whether or not the year-end hydrogen level must equal or exceed the initial level in the tank.

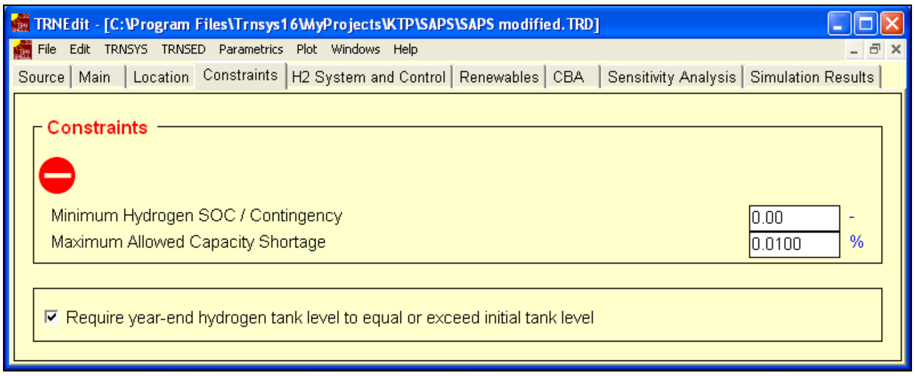


Figure 27: Constraints page

- In the "H_2 system and control" tab (Figure 28) the user can change essential parameters concerning the hydrogen components of the system and the way the system is controlled. Here are the parameters that can be changed:
    - the electrolyser rated power
    - the fuel cell rated power
    - the hydrogen tank volume
    - the maximum tank pressure
    - the initial hydrogen level in the tank
    - the four set-points defining the operation of the electrolyser and the fuel cell (switching on/off)

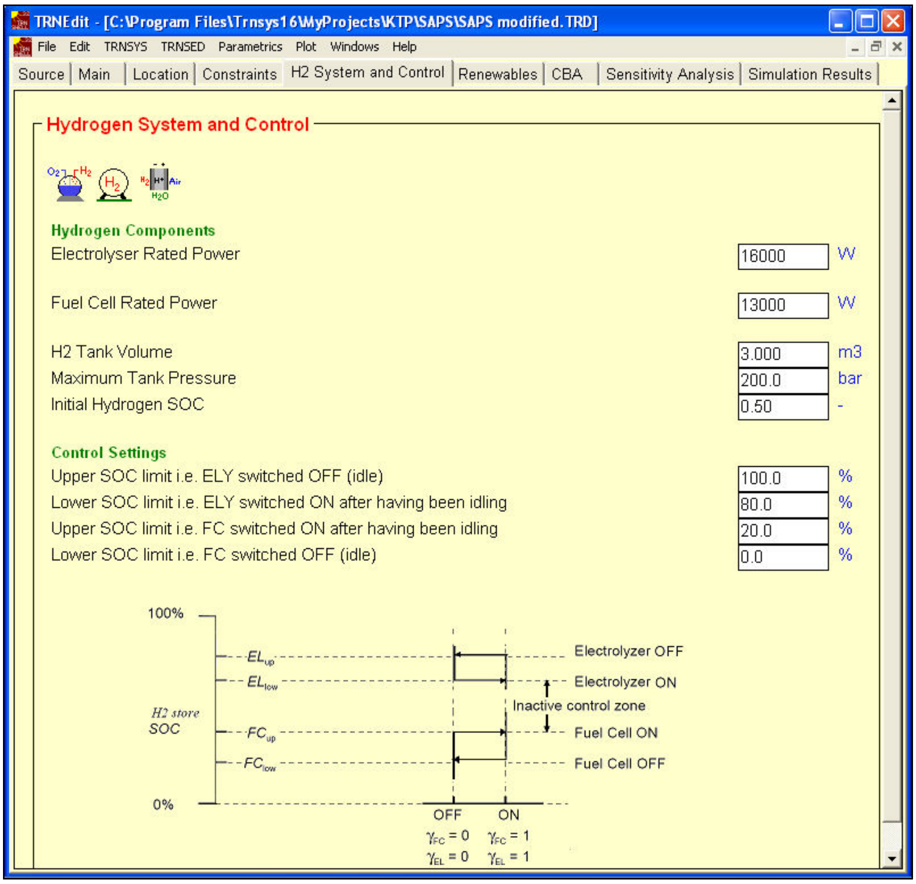


Figure 28: Hydrogen and system control page

- The “renewables” tab (Figure 29) gives access to parameters concerning the solar and wind installations. The parameters that can be changed are:

  - the slope of the surface of the PV panel
  - the azimuth angle of the PV panel
  - the peak power of a single PV module at Standard Test Conditions
  - the number of PV modules connected in parallel
  - the site elevation (m)
  - the data collection height (m)
  - the hub height (m)
  - the number of wind turbines
  - the wind turbine model (from a pull-down menu) and its power

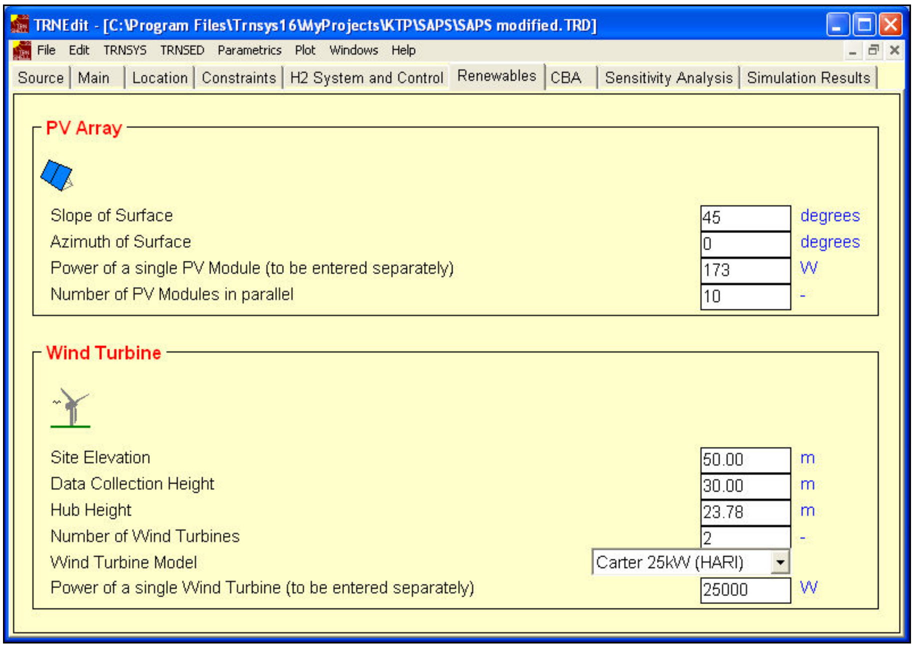


Figure 29: Renewables page

- The “CBA” tab (Figure 30) concerns the economic aspect of the simulation and integrates the cost benefit models developed in this project. The user specifies the capital, replacement, O&M costs and the lifetime of each component of the system. The interest rate and the project lifetime can also be modified. The user also has the possibility to use the defaults values entered in the model if such information is not available.

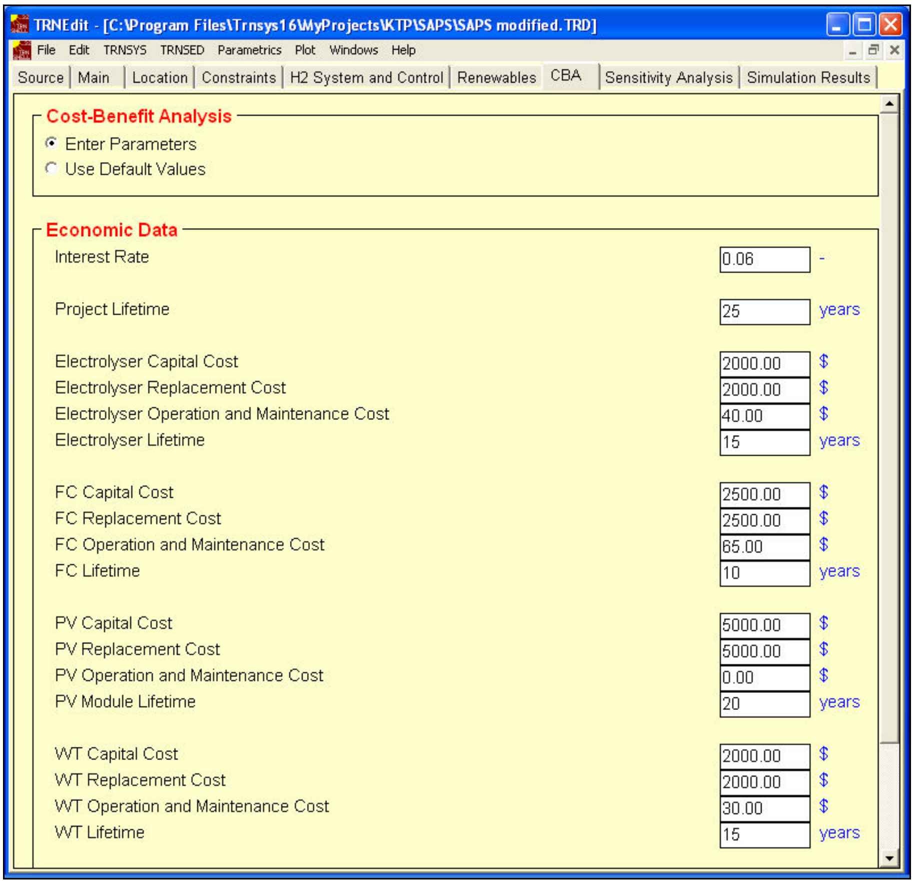


Figure 30: Economic page

- The "sensitivity analysis" tab (Figure 31) allows the user to modify (by a multiplication factor) the renewable resource and the load to see the impact these changes have on the performance of the system.

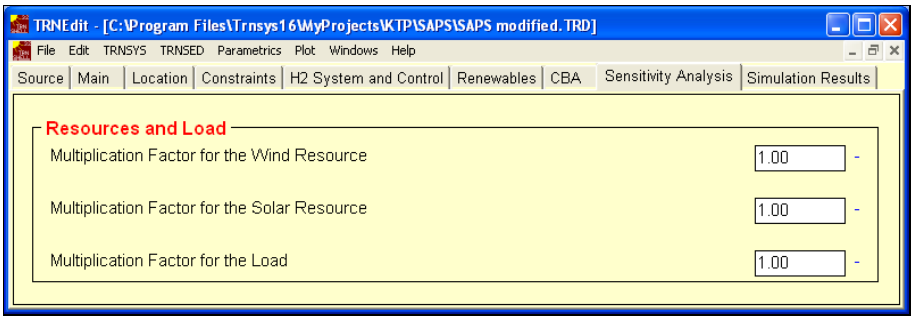


Figure 31: Sensitivity analysis page

- Finally the last tab "simulation results" (Figure 32) gives direct access to a help file describing the optimisation process step-by-step, as well as links to the Excel-based analysis tool developed during this project. These give concise results for:
  - the results of the parametric runs (described in the next section)
  - the results of the simulation given as time-series (hourly data)
  - the detailed technical and economic analysis of the simulation

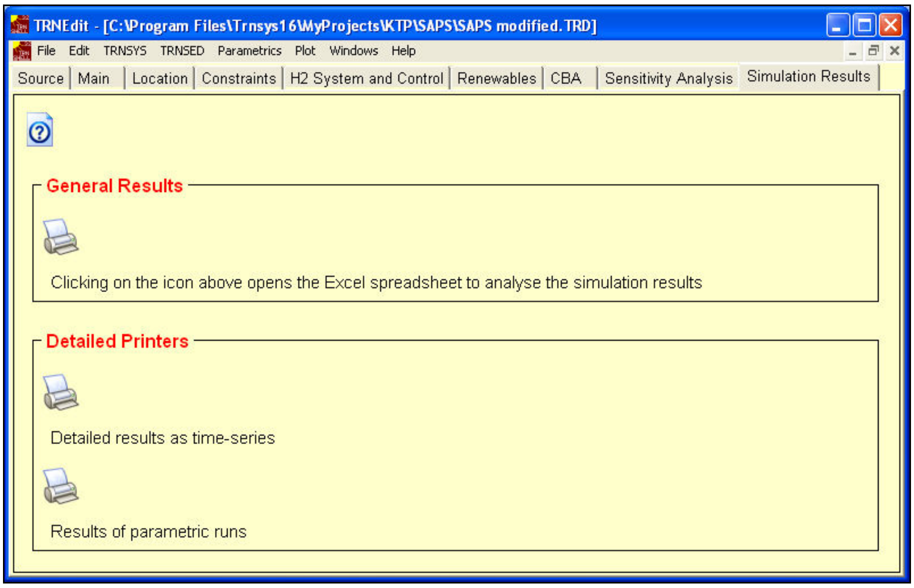


Figure 32: Simulation results page

The TRNSED interface also provides a direct access to the parametric runs set-up which can used to optimise the performance of the hydrogen system being analysed.

6. Conclusions

A library of four generic hydrogen energy systems has been developed on the TRNSYS platform. These have been augmented with user-friendly interfaces and the ability to perform parametric runs.

A methodology has been developed, utilising the elements above, to optimise the performance of these hydrogen systems. To assist in the assessment of performance an Excel-based results analysis tool has been developed, which produced concise and clear results from each performance simulation, enabling the user to readily identify the system characteristics which give optimum performance.

III. Using the Modelling to Optimise Performance

One of the benefits cited previously regarding the development of hydrogen systems models was their use in design optimisation. This section describes how the models and tools described previously can be used to optimise performance.

1. Optimisation Process

a. Options and constraints

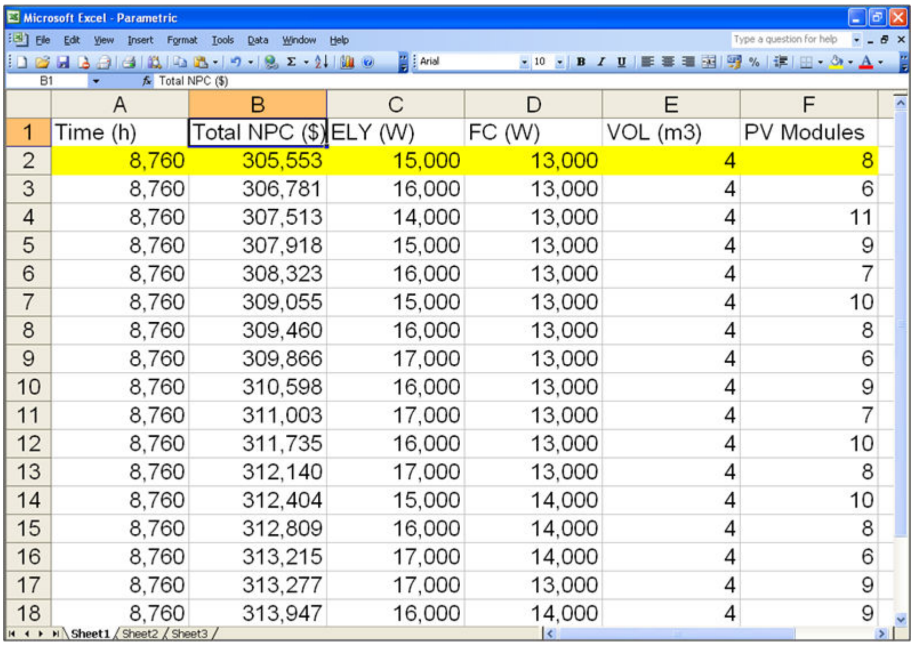
The optimisation process is based on the cost of the system. In addition to the costs of the different components (c.f. cost-benefit analysis), other factors can have an influence on the total cost calculated by TRNSYS. Indeed, the user has the possibility to impose three constraints on the operation of the system:

- The minimum hydrogen level in the tank: when the H_2 level in the tank goes below this limit, an arbitrary penalty (with a factor of 10^9) is added to the total cost of the project (because of this penalty the configuration will be ranked at the bottom of the optimisation list). This is done to ensure that the operation of the system will be sustained over the year if the weather conditions differ from the ones assumed in the model.
- The maximum allowed capacity shortage: if the total annual capacity shortage exceeds this level, an arbitrary penalty (with a factor of 10^9) is added to the total cost of the system.
- The user can choose whether or not the level of hydrogen at the end of the year of simulation must equal or exceed the initial level in the tank. This is done to ensure a sustainable operation over the year. Once more, an arbitrary penalty (with a factor of 10^9) is included here.

b. The iterative process

The procedure followed to optimise a system using the TRNSED models is as follows:

- Create a parametric table containing all the system configurations to be simulated from the TRNEdit window. The parameters to be optimised must be selected here. It is convenient to create this table with Excel. Running the table will simulate all the configurations one by one.
- Once all the simulations have been completed, it is possible to access the "results of parametric runs" from the "Simulation Results" tab of the TRNSED application. For each feasible configuration, TRNSYS has created a line in the Excel file with the sizes of the components and the corresponding total NPC of the system. The non-feasible configurations have been ignored. The feasible configurations can then be ranked according to their total NPC to find the cheapest one, as shown on Figure 33.



	A	B	C	D	E	F
1	Time (h)	Total NPC ($)	ELY (W)	FC (W)	VOL (m3)	PV Modules
2	8,760	305,553	15,000	13,000	4	8
3	8,760	306,781	16,000	13,000	4	6
4	8,760	307,513	14,000	13,000	4	11
5	8,760	307,918	15,000	13,000	4	9
6	8,760	308,323	16,000	13,000	4	7
7	8,760	309,055	15,000	13,000	4	10
8	8,760	309,460	16,000	13,000	4	8
9	8,760	309,866	17,000	13,000	4	6
10	8,760	310,598	16,000	13,000	4	9
11	8,760	311,003	17,000	13,000	4	7
12	8,760	311,735	16,000	13,000	4	10
13	8,760	312,140	17,000	13,000	4	8
14	8,760	312,404	15,000	14,000	4	10
15	8,760	312,809	16,000	14,000	4	8
16	8,760	313,215	17,000	14,000	4	6
17	8,760	313,277	17,000	13,000	4	9
18	8,760	313,947	16,000	14,000	4	9

Figure 33: Results of the iterative process in Excel

- The optimal system can then be simulated. Once the simulation is completed, the "simulations results" Excel spreadsheet presents the detailed analysis of the system technical and economic performance (Chapter II.4).

This process can be repeated several times to optimise the system more accurately. Indeed it is better to refine the optimum research step by step in order to create parametric tables of reasonable size (the simulation time can be long).

This procedure is summarised on this flow chart:

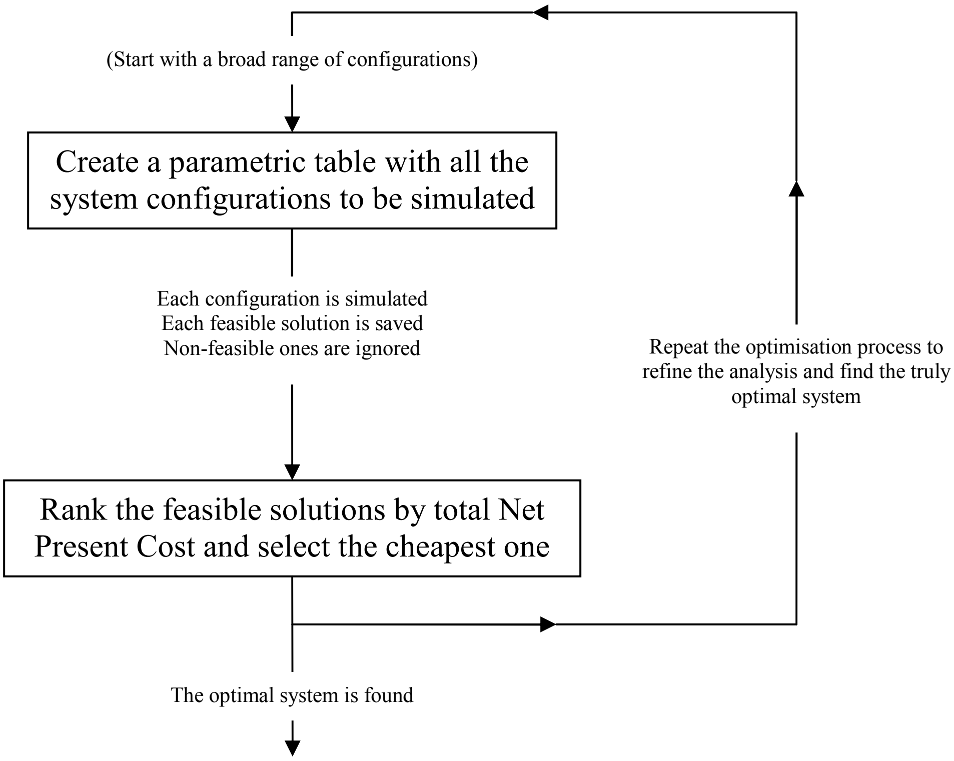


Figure 34: Flow chart of the optimisation process

2. Methodology

In order to analyse the performance of the hydrogen energy systems a general methodology has been developed which uses the TRNSYS application augmented with the cost-benefit model and the optimisation procedure. The following flowchart presents this methodology and explains how to model a hydrogen energy system, from the building of the TRNSYS model to the analysis of the simulation final results:

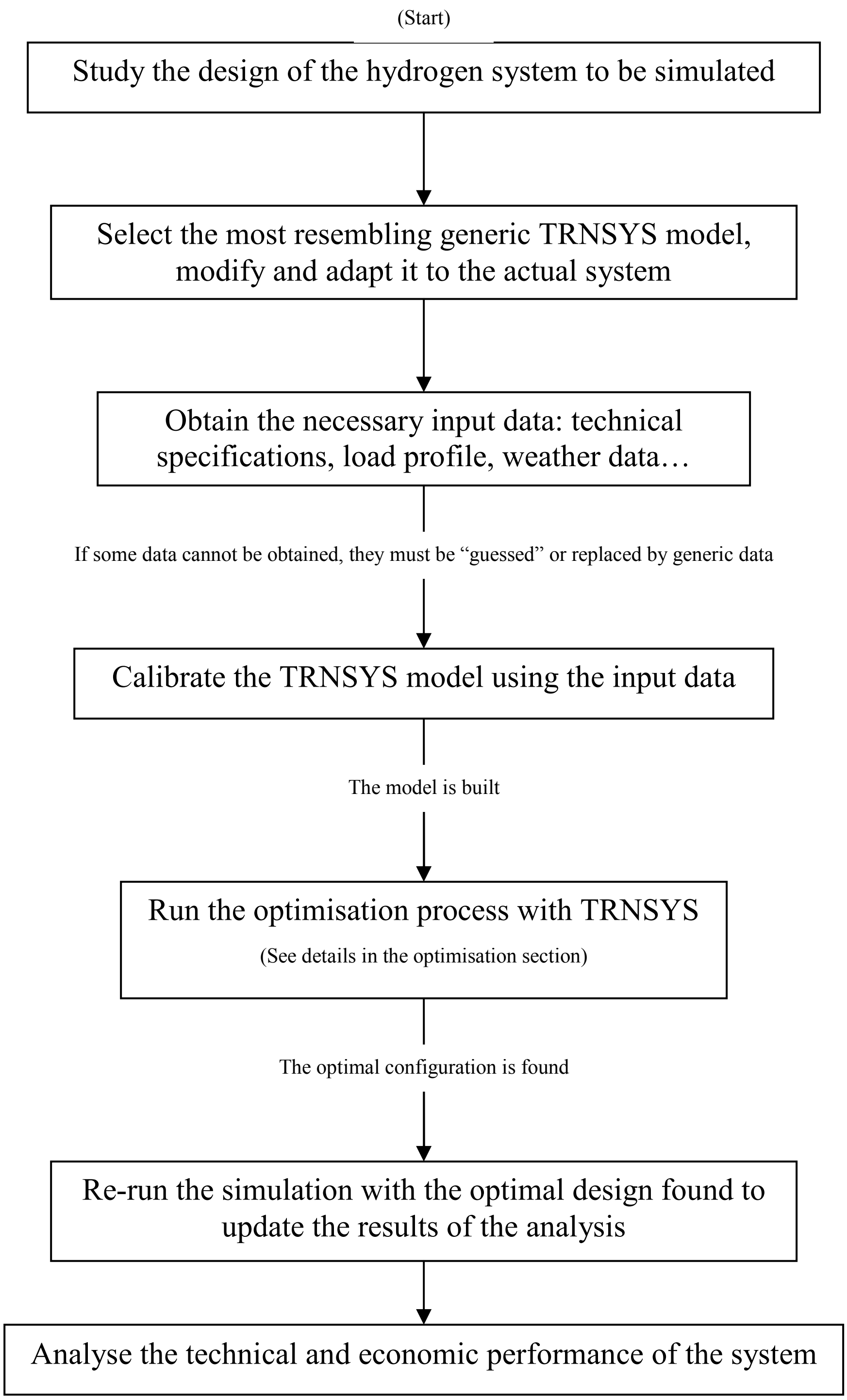


Figure 35: Flow chart of the general methodology to use the models

The methodology is based upon a technical and economic analysis of the hydrogen system annual performance. The TRNSYS model takes into account the technical specifications of the system as well as the weather data and energy requirements of the site to calculate the annual performance of the system. This includes the energy production and consumption for each component, and the level of stored hydrogen on an hourly basis.

The optimisation process, described in the previous section is an iterative process based on the cost-benefit calculations described in Chapter II.3. Within the process, key system parameters (e.g. storage capacity) are varied in an attempt to determine the optimal system configuration able to satisfy the energy requirements. The technical and cost-benefit models are therefore combined to search for the system configuration with the lowest total cost. The optimal system is then determined and its technical and economic performance can be analysed.

The validation of the models developed is described in Chapter IV and the models with the optimisation process are finally applied to a case study in Chapter V.

IV. Validation of the models

Validating and testing the TRNSYS models is indispensable before considering any commercial application in order to make sure that they give accurate and reliable results. This section gives some examples of validation applied to component individual component models.

1. Techniques of validation

Depending on the component, three different techniques have been considered to validate the models:

- Use of other modelling tools. The results of simulations in TRNSYS can be compared with the results of simulation under identical conditions using other modelling tools (e.g. HOMER). This technique has been used for the PV generator and the wind turbine models.

- Use of the literature. Results and curves obtained with TRNSYS can be compared against other results and typical curves found in the literature. For example, a paper presenting the development of a Matlab-Simulink model for stand-alone power systems has been used [43]. The results presented in this paper were compared with the results of the TRNSYS models. Equations can also be compared between the models. This technique was used for the validation of the PV generator, the electrolyser, the PEM fuel cell, the compressor and the gas storage models.

- Use of real operational data. Simulation outputs can be compared with operational data from real-life projects. This technique can provide very interesting results but it present the drawback to require a lot of details about the project (technical specifications, weather conditions and detailed operational data) to perform an accurate comparison. It is generally difficult to obtain such information, as it will be explained in the next chapter of this report.

2. Validation examples

Each component of the systems has been tested individually (PV, wind turbine, electrolyser, fuel cell, power conditioning, hydrogen tank, control strategy). The following examples give an indication of the validation work undertaken for the project.

a. PV generator

Static testing

To test the static performance of the TRNSYS PV model, its results were compared to manufacturer's data and results from an equivalent Matlab-Simulink model. Both models use the equivalent circuit for PV generator model presented in Figure 15.

The curves in Figure 36 were obtained from TRNSYS for the Flagsol (KFA) 150 cell module. The curve extremities and the maximum power point match the technical published characteristics of the module:

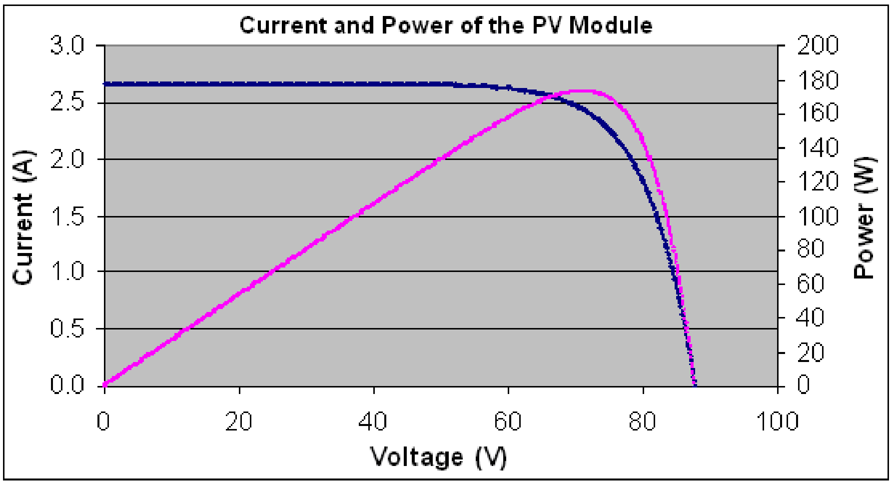


Figure 36: Typical I-U and P-U characteristics for a PV generator (Simulation in TRNSYS)

Short circuit current at reference (I_{sc})	2.664 A
Open circuit voltage at reference (V_{oc})	87.720 V
Reference cell temperature	25°C
Reference solar radiation	1000 W/m^2
Maximum current at reference	2.448 A
Maximum voltage at reference	70.731 V

Table 8: Characteristics of the Flagsol (KFA) solar module

The same simulation has been run with the Solarex MX-64 module (Figure 37). Again the results match the published data. Additionally a Matlab-Simulink model gave identical results [43].

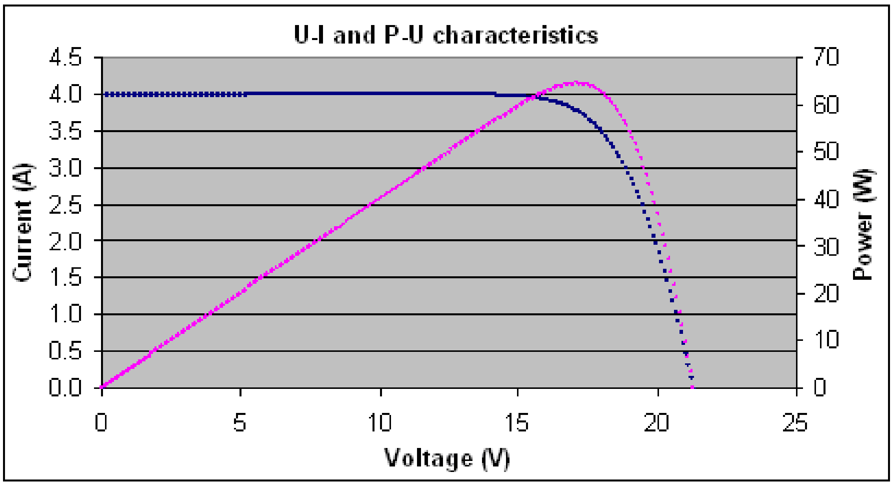


Figure 37: Current-voltage and power curves for the Solarex MX-64 module (Simulation in TRNSYS)

b. Wind turbine

Again this is an inter-model comparison between HOMER and TRNSYS and comparison to the manufacturer's published characteristics. Figure 38 compares the results for the wind turbine model (type Carter 25kW). The three curves (the power curve from the manufacturer, HOMER and TRNSYS) match well; the only slight difference is for wind speeds over 25 m/s where the models differ in the treatment of safety shut-downs of the turbine.

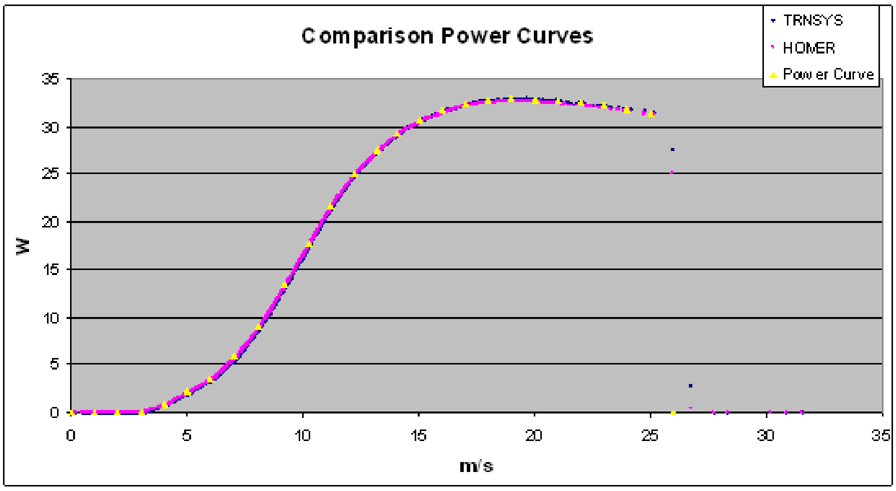


Figure 38: Comparison between the wind turbine models in HOMER and TRNSYS

Temporal precision

Work was also done to compare the energy production of wind turbine model in TRNSYS using 10 minute- and 1 hour-average wind speed data for the same period. This is done in order to determine if the use of hourly data is accurate enough. As can be seen on Figure 39, the results follow the same curve, especially for wind speeds between 5 and 20 m/s. The differences beyond these limits can be explained by two reasons:

- Cut-in and cut-off wind speeds: some information is lost in the hourly average as the wind speed can go temporarily beyond these limits within such a long interval without being taken into account.
- Sudden variations of wind speeds during a 1hour-period: the power curve is not linear so sudden variations affect the average calculations (the average of the power delivered every 10 minutes is not equal to the power corresponding to the hourly average).

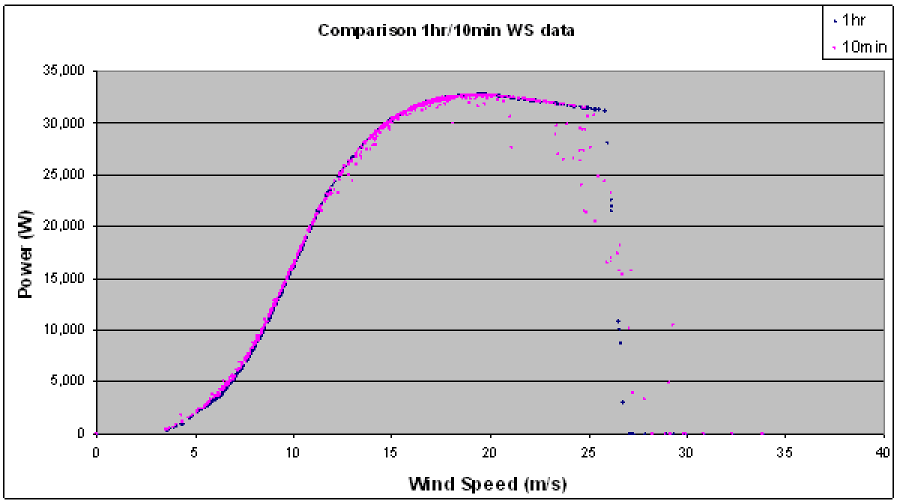


Figure 39: TRNSYS simulation using 10 minute- and 1 hour-average wind speed data

However, the total difference is minimal between the two simulations (only 0.5% in the total energy production over a one month-period). The conclusion is that both types of data can therefore be used for the TRNSYS simulations.

c. Fuel cell

Figure 40 represents the relationship because the power supplied by the fuel cell and the volume of hydrogen consumed. As one can see, the relationship is not linear. The power delivered increases with the volume of gas consumed until a saturation point (around 12.5Nm^3 here). From this point the power delivered by the fuel cell decreases.

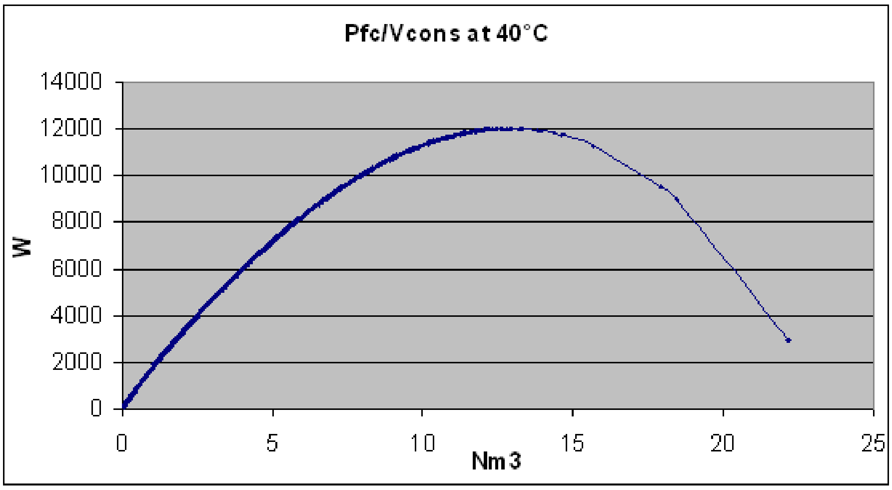


Figure 40: Relationship between the power delivered by the FC and the volume of H_2 consumed

(Simulation in TRNSYS)

The temperature dependence of the PEM fuel cell model in TRNSYS has also been observed. Figure 41 and Figure 42 show the effect of temperature on the cell voltage and power of the fuel cell.

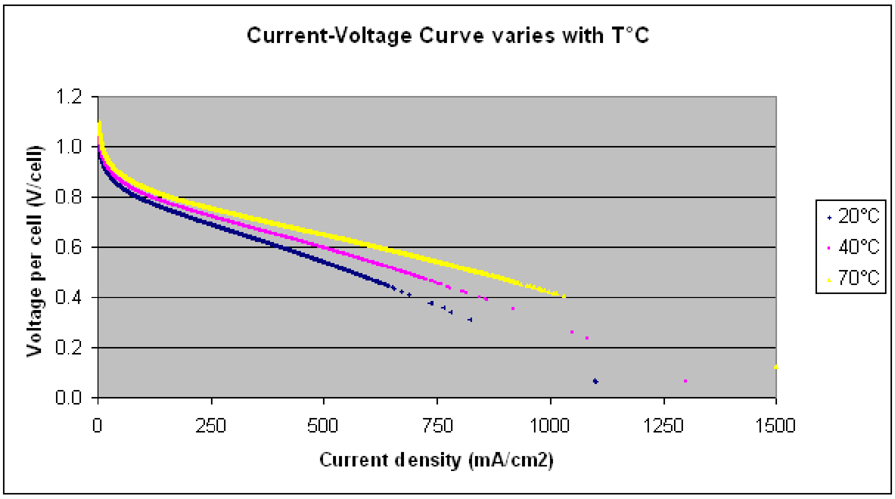


Figure 41: PEM fuel cell voltage at different temperatures

(Simulation in TRNSYS)

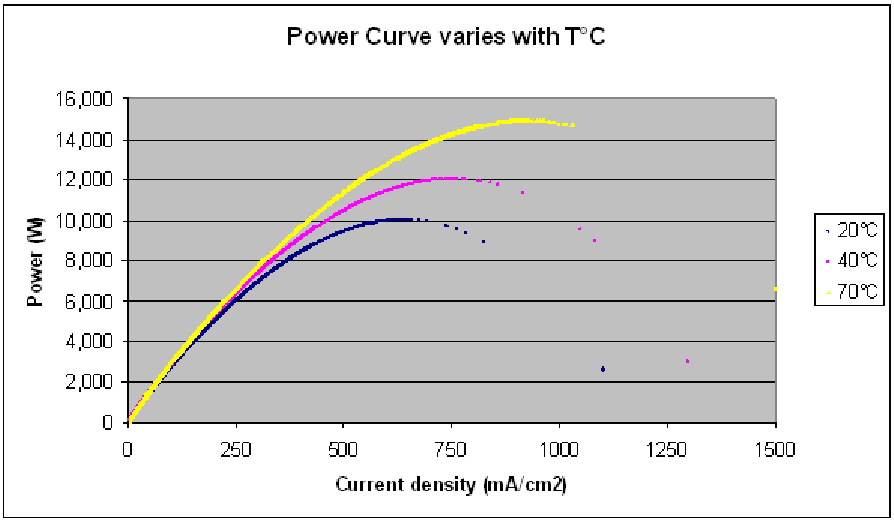


Figure 42: PEMFC power at different temperatures (Simulation in TRNSYS)

d. Control strategy

Finally, the operation of the system controller (Master Controller) in TRNSYS has also been tested. Once the simulation is run, the hourly data have been compared to calculations performed with Excel and using the theoretical equations used by the controller (see Section II.2). The results obtained were absolutely identical, which confirms that the controller operates correctly.

e. Convergence tolerance

One of the main issues faced during the building of the models concerned the convergence of the calculations in TRNSYS. The convergence tolerance, defined in the general parameters of TRNSYS, is used in the tolerances statement to specify the error tolerance controlling the convergence of input and output variables to be used during a simulation.

The default value is 0.001, which appeared to be too high for some of the models like the Hydrogen SAPS. As shown in Figure 43 a tolerance too high generated some inaccuracies in the calculations when compared to the theoretical results (obtained from the equations). These inaccuracies had serious consequences on the simulation results, particularly the energy balance of the system.

The solution was therefore to decrease this convergence tolerance (10^{-7} gave satisfactory results for all the models). Even if it increases slightly the simulation time (more iterations are needed), reducing this parameter improved the accuracy of the calculations.

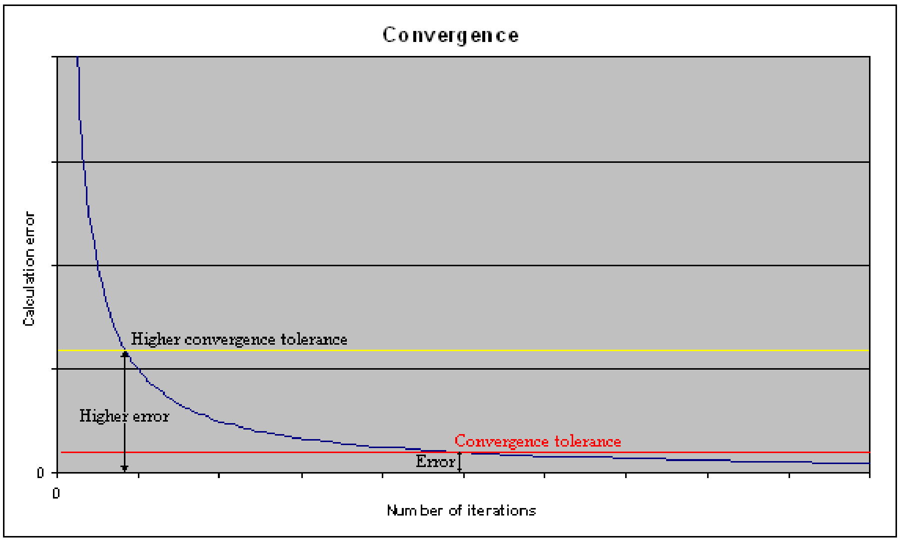


Figure 43: Convergence tolerance and calculation error

f. Conclusions

This chapter presented the process of validation of the HydroGems models. The components have been tested individually and the operation of the entire system has also been verified to ensure the control strategy was operating correctly. Two techniques have been used: comparison with other modelling tools (HOMER and Matlab-Simulink) and comparison with typical results (and graphs) from manufacturers.

The results presented here have been satisfactory. The results found in TRNSYS compared very well against results from other tools and manufacturers data and as far as it is possible within the time and resource constraints of the project these validation studies indicate that the component models in TRNSYS are sufficiently accurate to perform reliable simulation studies.

V. Case study: the Utsira Project in Norway

Although the validation process described in the previous paragraph indicated that the models produced realistic results, the process only assessed individual component performance. However to assess the performance of the system model as a whole it was necessary to apply it to a real project: the Utsira Project in Norway [44].

The modelling of the Utsira project was undertaken in collaboration with IFE in Norway and Statoil Hydro. Some of the useful outputs of this work were the validation of the TRNSYS systems models using real data and the opportunity to show that the models can be successfully applied to a working system. The results have been published in two academic papers. [45] [46]

Utsira is a small island community with 235 inhabitants, located approximately 18 kilometres off the west coast of Norway.

Figure 44: View of the Utsira Island (Google Earth)

Figure 45: Norway's Utsira Island [44]

1. Overview of the Utsira system

A wind/hydrogen demonstration project was officially launched at Utsira by Hydro (now StatoilHydro) and Enercon in July 2004. The realisation of the project came after several years of concept development, system design and project planning (2000-2004) to create the world's first full-scale stand-alone renewable energy system where the energy input is provided by wind and stored hydrogen.

The objective of the project is to demonstrate how renewable energy can provide a safe and efficient energy supply to remote areas where there is sufficient resource and/or insufficient infrastructure.

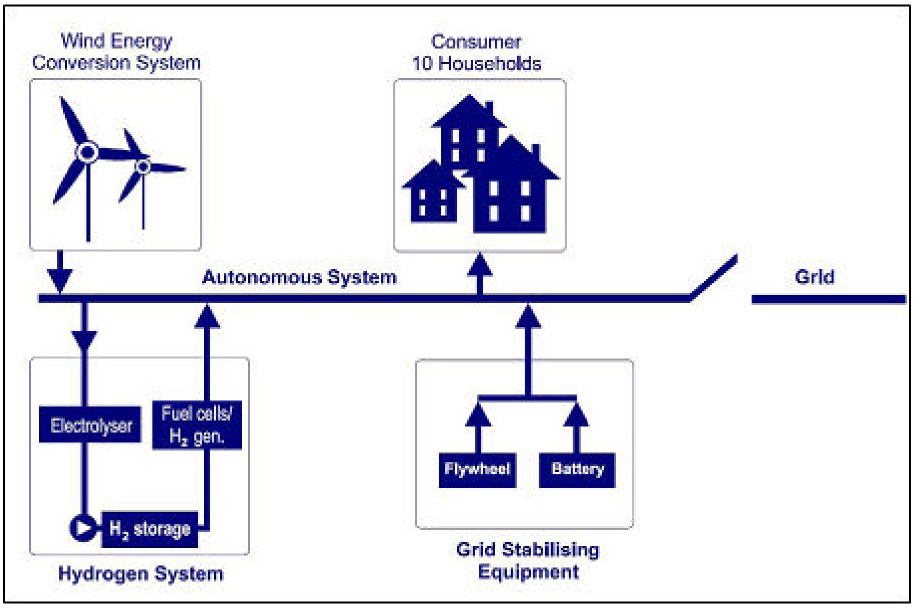


Figure 46: Representation of the wind-hydrogen system at Utsira [44]

As shown in Figure 46 the system serves 10 households, whose energy demand is exclusively provided by renewable sources (wind energy, either directly or indirectly via hydrogen). Wind power and hydrogen combine to provide an autonomous and continuous and supply of energy to the community. Indeed, wind power alone cannot supply all the energy necessary because of its intermittency but Utsira has enough wind power to be self sufficient. Hydrogen can be used to provide energy storage to ensure a sustainable energy system. The system, which has been in operation since winter 04/05, is shown in Figure 47 and includes:

Figure 47: The hydrogen energy system on Utsira Island [44]

- Wind turbine 600 kW
- Hydrogen engine 55kW
- Fuel cell 10 kW (not in use)
- Alkaline electrolyser 10 Nm^3/h, 48 kW
- Compressor 5.5kW (2-stage)
- Hydrogen storage 2400 Nm^3 at 200 bar
- Battery 35 kWh
- Flywheel 200 kW_{max}, 5 kWh
- Master synchronous machine 100 kVA

2. Analysis of operational data

Over the past 2 years a significant amount of data from stand-alone operation has been collected from the Utsira system. The work described here used operational data (10-minute averages) measured at Utsira during the period 1-30 March 2007 (Figure 48). The data was provided by the system operators StatoilHydro. The top plots show the wind power production and load power demand, while the bottom plots show the power produced by the H_2 engine and power consumed by electrolyser (including auxiliaries and compressor) as well as the pressure in the gas storage.

A decrease in the hydrogen pressure from 145 bar to 33 bar can be observed over the entire period. The data shows that stand-alone operation is only achieved about 65% of the time. A closer look at the data (hour 420-720) shows that the electrolyser frequently needed to operate on grid-electricity in order to produce extra hydrogen and level out the storage pressure, which otherwise would have decreased very rapidly. This indicates that the plant is not producing enough hydrogen.

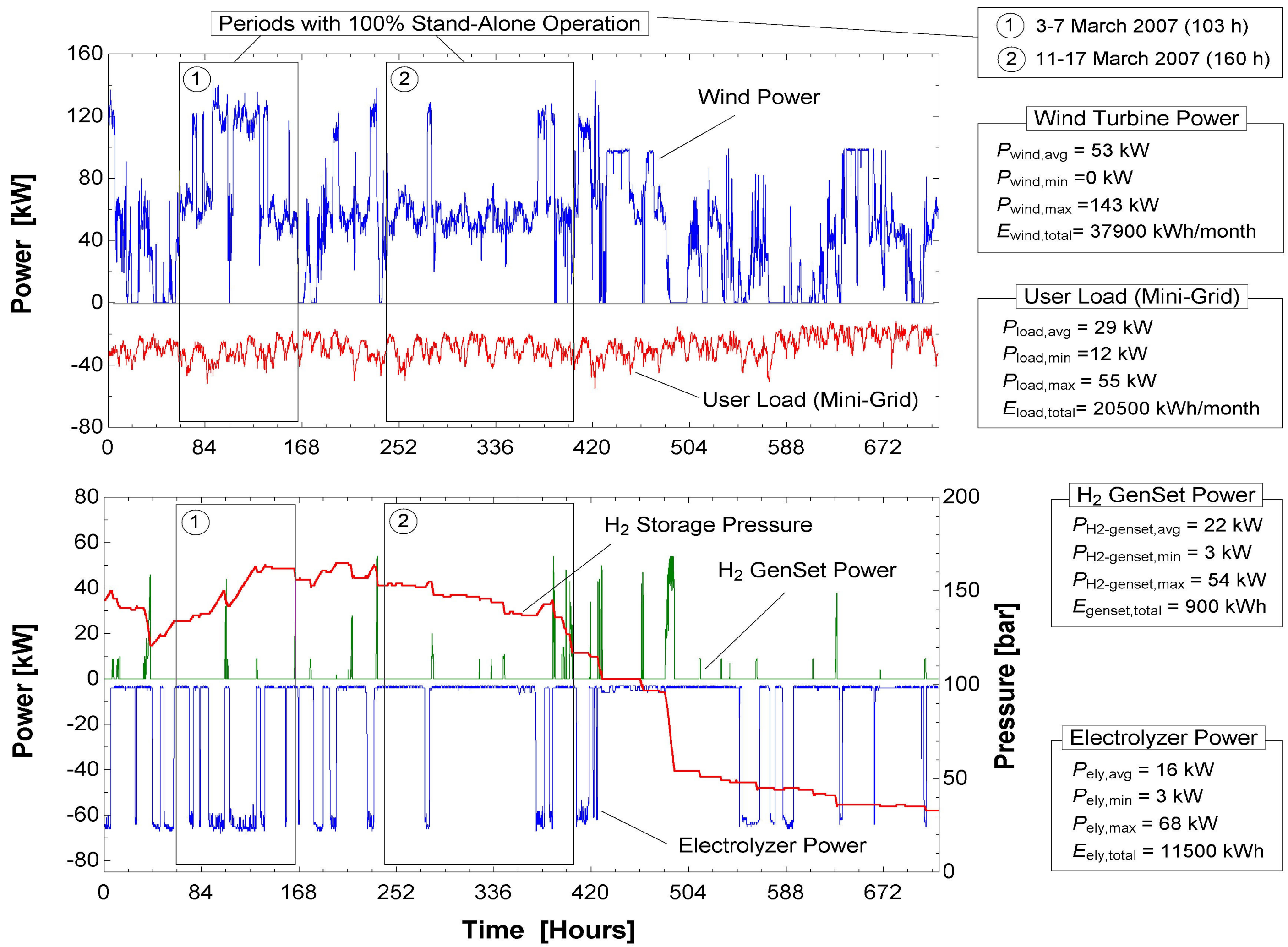


Figure 48: Operational data (10-minute averages) from Utsira, 1-30 March 2007

An important part of the design work at Utsira has been dedicated to the development of the power conditioning system. The system has been working properly for the past 24 months, except the DC/AC inverter for the fuel cell that encountered some severe technical difficulties.

A battery, a synchronous generator and a flywheel ensure that the voltage and frequency on the local mini-grid is kept within standard tolerances. To study the performance of the power system it is better to focus on a shorter time period (5 March) as illustrated on Figure 49. It shows the on/off-switching of the electrolyser and hydrogen engine as a function of the net available power (wind power minus user load). In the power conditioning system the flywheel is constantly being charged and discharged, which explains the fluctuating behavior of the power (hour 101-107).

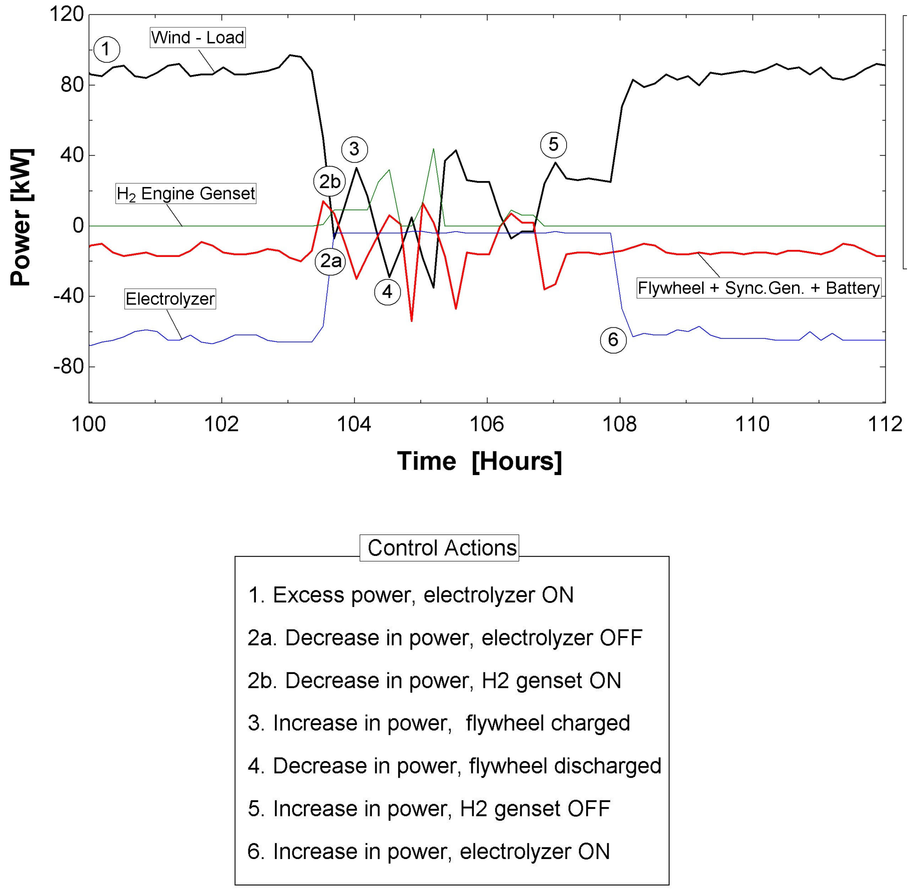


Figure 49: Operational data (10-minute averages) measured at Utsira on 5 March 2007

3. Calibrating of the system components in TRNSYS

A model of the Utsira system was developed using the generic SAPS system model described in Section B.II. The model has been calibrated using field data (described in the next section) and was then applied in an optimisation study of the Utsira system (Section V.5).

In the stand-alone operation of the Utsira system, only one of the two 600W wind turbines installed on the island is used (the second one directly exports the power produced), and has been mechanically rated at 140kW. As mentioned before, the fuel cell is not in operation.

The first objective of the modelling study was to calibrate the electrolyser and the hydrogen engine models with real data (fuel consumption and efficiency curve; Figure 50) and manufacturer specifications.

To validate the operation of the engine model, the longest period of uninterrupted engine operation (hours 484-492) was selected in the operational data and the results of the simulation were compared to the operational data. The results of the comparison presented in Figure 51 are satisfactory.

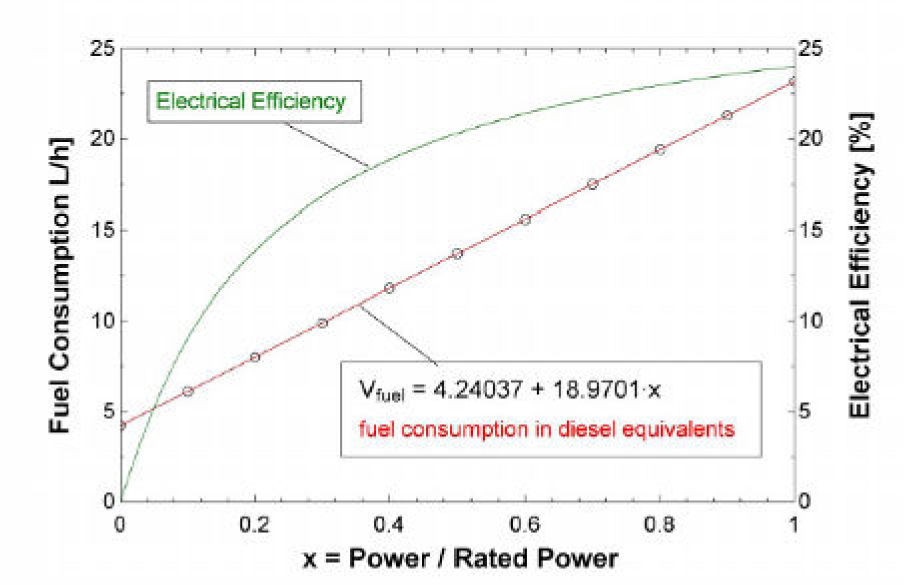


Figure 50: Performance of the hydrogen engine at Utsira

As shown in Figure 50 the maximum hydrogen engine efficiency is around 25%, but in practice the engine often operates at part load at a much lower efficiency.

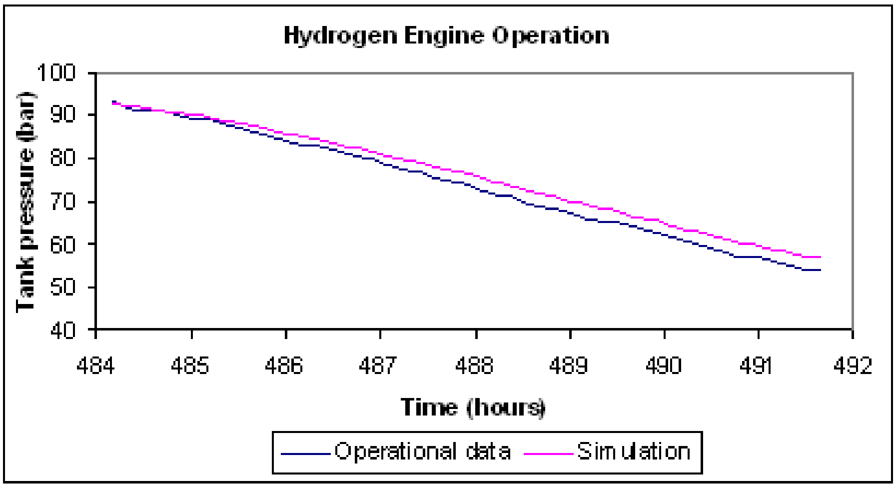


Figure 51: Validation of the operation of the hydrogen engine at Utsira

An EES (Engineering Equation Solver) model [1] was used to calibrate the electrolyser model in TRNSYS (Figure 52). To verify that the model was operating correctly the same method was used and the longest period of uninterrupted electrolyser operation (hours 108-131) was selected in the operational data. The results of the simulation were then compared to the operational data, as shown in Figure 54 that represents the pressure in the hydrogen tank. Again, the results are very satisfactory.

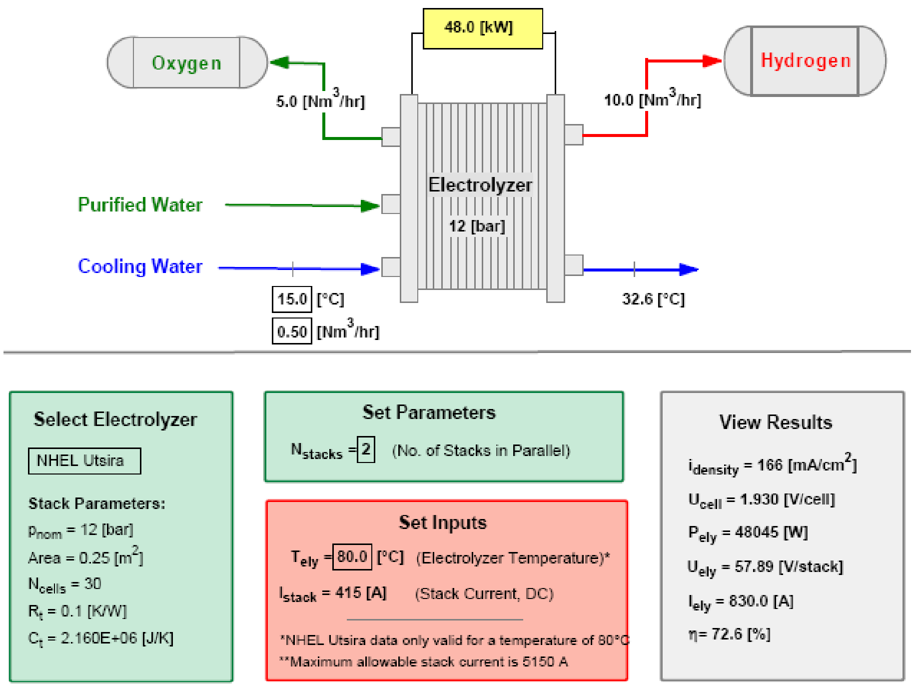


Figure 52: Calibration of the Utsira electrolyser model

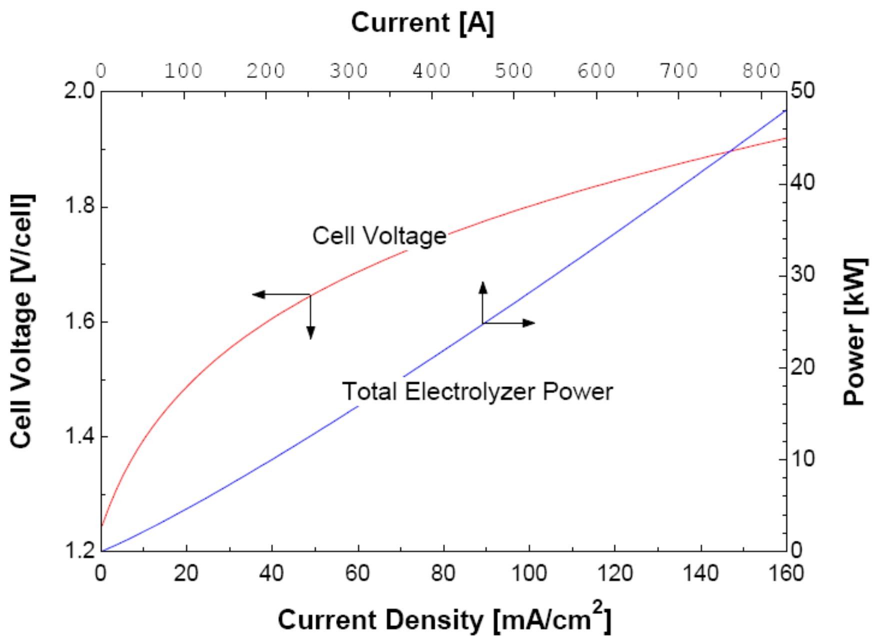


Figure 53: Current and power curves for the Utsira electrolyser

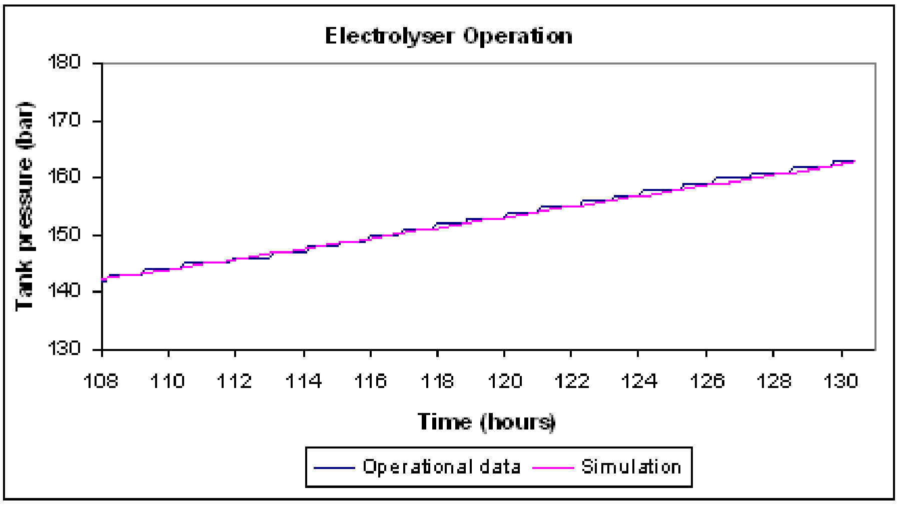


Figure 54: Operation of the electrolyser at Utsira, real and simulated

Finally, an important part of the modelling concerned the auxiliary power equipment for the electrolyser. These include the compressor, feed water pump, drier, deoxidiser, instrument air compressor, cooling water compressor and pump, ventilation fans, heating, lights and power electronics (transformer/rectifier). As the operational data provided was not sufficiently detailed, additional equations based on previous experience had to be included in the model.

As shown in Figure 55, the electrolyzer at Utsira only produces hydrogen when it operates between 50 and 100% of its full capacity; the electrolyser model and the control strategy in TRNSYS were modified to take into account this characteristic. When the excess power from the wind turbine corresponds to less than 50% of the electrolyser rated capacity, only a few auxiliary equipment are working (e.g. pump) and no hydrogen is produced; when the excess power from the wind turbine corresponds to more than 50% of the electrolyser rated capacity the power conditioning equipment and the compressor start operating and the electrolyser produces hydrogen up to 10 Nm^3/h at full capacity. Figure 55 also shows that the hydrogen engine consumes much more fuel (up to 80 Nm^3/h) than what is produced by the electrolyser (10 Nm^3/h). This causes problems in the long term operation of the system, as explained in the next sections.

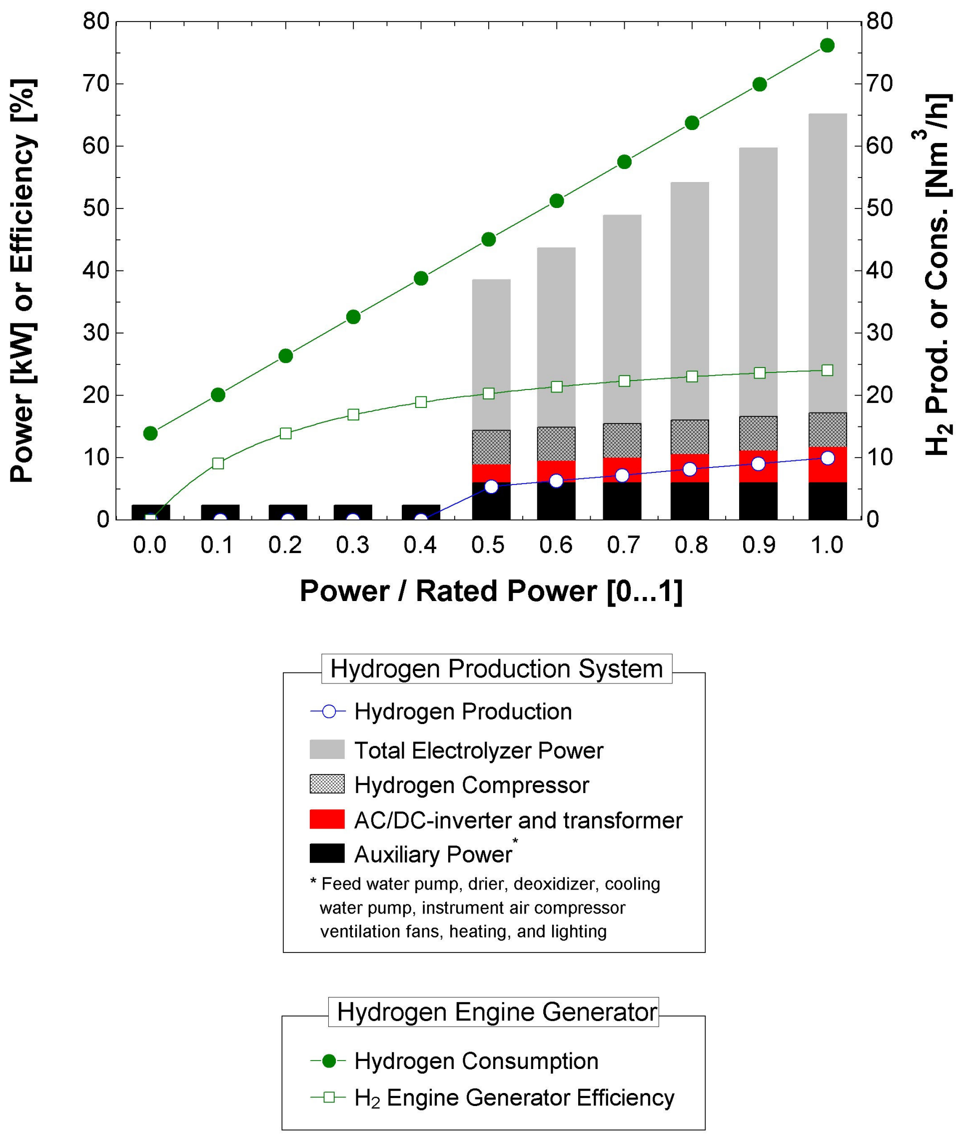


Figure 55: Modelled operation of the electrolyser and the hydrogen engine at Utsira

4. Simulation of the current system

In order to assess the performance of the Utsira system and improve its design a set of simulations were performed using the calibrated models for the wind turbine, electrolyser system, and hydrogen engine. The performance of the existing system configuration and three alternative system designs were simulated using the measured wind speed and user load data described in the previous chapter. The results are presented in Figure 56:

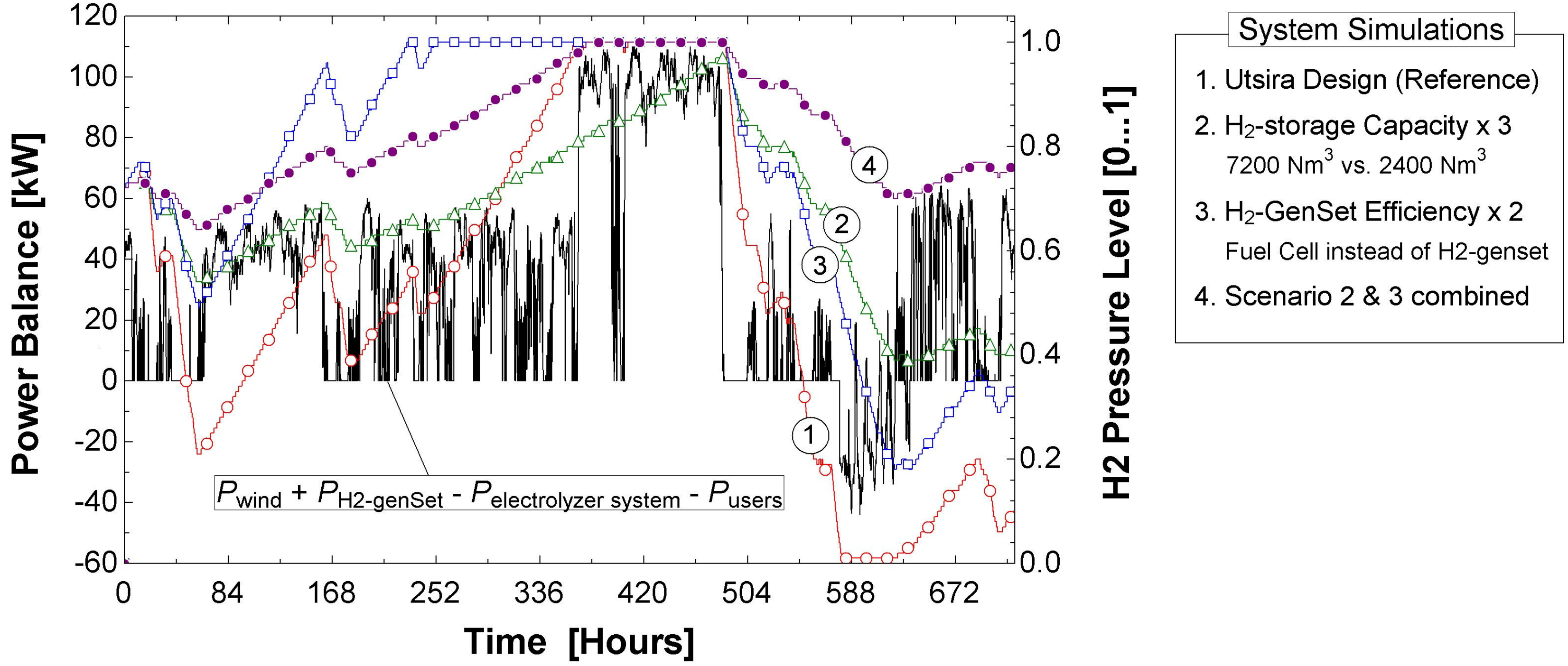


Figure 56: Improvement of the system design at Utsira (input data March 2007)

The black curve in Figure 56 represents the power balance (power inputs minus power outputs) in the system. A negative power balance means that the system is not able to satisfy the power requirements. Curve no1 (red) corresponds to the level of stored hydrogen for the Utsira system as it exists (used as reference). It shows that around hour 588, when the power balance in the system is negative, all the hydrogen in the tank has been consumed by the engine and the tank is empty, which causes the simulation to crash. A second simulation where the hydrogen storage capacity has been tripled is represented by curve no2 (blue). It shows that the tank never gets empty and the simulation can complete. However, the final hydrogen level in the tank is inferior to the initial level, which is an issue for long term operation. Similar results are obtained when the hydrogen engine is replaced by a fuel cell twice more efficient (curve no3, green). Finally when both options are combined (curve no4, purple), the simulation completes with a final hydrogen level superior to the initial level, which was the objective.

These results show that it is very difficult to achieve 100% stand-alone operation for longer periods of time with the actual Utsira system design. Full autonomy can only be achieved by improving the overall efficiency of the hydrogen production system (electrolyser) and by increasing the hydrogen storage size and/or by increasing the power generating efficiency of the unit. Additional simulations have therefore been undertaken to improve/optimise the Utsira system's performance.

5. Optimisation of the system

As indicated in the previous part, 100% stand-alone operation cannot be achieved in the long term with the existing system configuration. The Utsira system therefore provided the ideal opportunity to apply the optimisation process developed during the project and to demonstrate how the tool can be used to improve the design of a real hydrogen energy system.

To perform this optimisation one entire year of wind and load data was used for the year 2005.

Component	Lifetime (years)	Capital costs	O&M costs (% of capital costs)
Wind turbine	20	800 €/kW	1.5
Electrolyser	20	2000 €/kW	2.0
Compressor	12	5000 €/kW	1.5
H2 storage	20	4500 €/m³	2.5
H2 engine	10	1000 €/kW	2.0
Fuel cell	10	2500 €/kW	2.0

Table 9: Economic parameters used for the optimisation process

The economic parameters in Table 9 were used and two scenarios were investigated:

- In the first scenario, the existing hydrogen engine was kept and an optimal design was found.
- In the second scenario the inefficient hydrogen engine was replaced by a fuel cell (2 x more efficient) and a new optimal design was proposed.

For both scenarios the minimum state of charge in the tank was kept at 10% where the engine (or fuel cell) was switched off. For similar safety reasons, the electrolyser was switched off when the hydrogen level reached 95%.

In the first scenario where the inefficient hydrogen engine is kept unchanged, the optimal hydrogen system that ensures a 100% stand-alone operation includes:

- A 100 kW electrolyser
- A 50 kW hydrogen engine
- 11,100 Nm^3 of stored hydrogen (70 m^3 at 200bar)

The operation of this system is shown on Figure 57. This shows that the existing system at Utsira is too small to guarantee a total stand-alone operation over the year; the size of the electrolyser needed to be doubled and the hydrogen tank should be almost five times bigger.

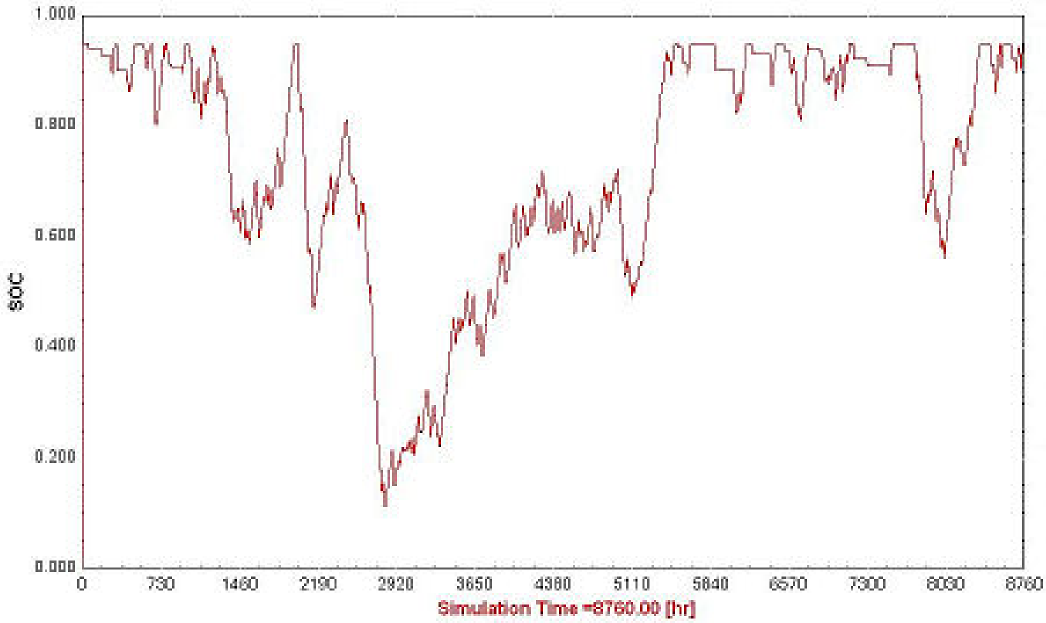


Figure 57: Level of stored hydrogen for the optimal system (Scenario 1)

In the second scenario, the inefficient hydrogen engine is replaced by a more efficient fuel cell that consumes half the hydrogen fuel. The optimal system that ensures a 100% stand-alone operation is:

- A 48 kW electrolyser
- A 50 kW fuel cell

- 4800 Nm^3 of stored hydrogen (30 m^3 at 200bar)

The operation of this system is shown on Figure 58. Replacing the engine by a fuel cell allows a substantial reduction of the size of the electrolyser and the storage tank. This corresponds to a reduction of about 20% in the total cost of the project. Compared to the system existing at the moment, only the size of the hydrogen tank should be doubled.

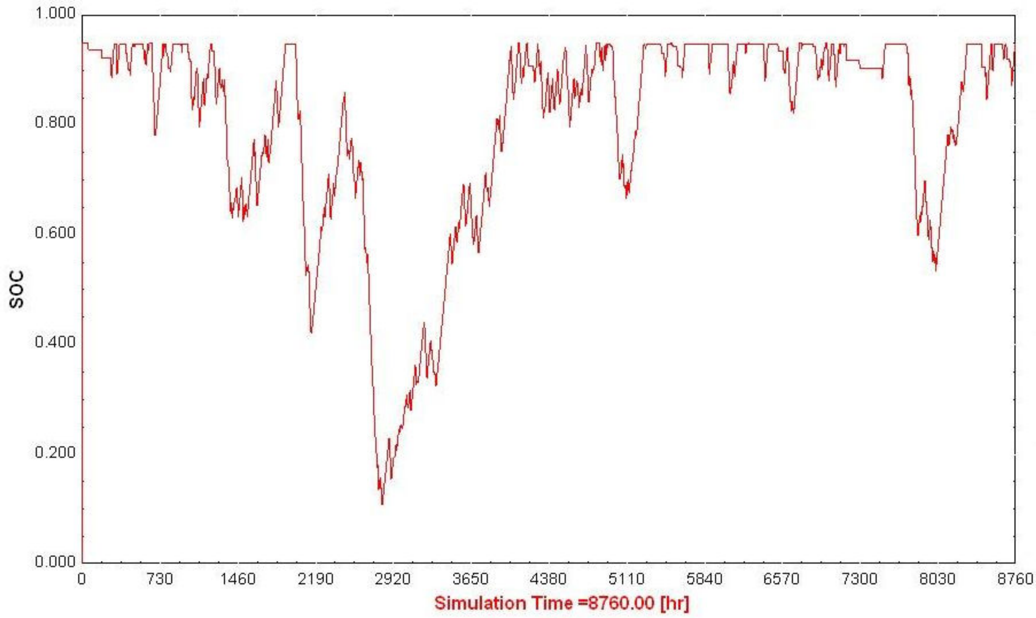


Figure 58: Level of stored hydrogen for the optimal system (Scenario 2)

In conclusion, this work has demonstrated the application of the toolkit developed for this project. Running the optimisation confirmed that the existing system is too small and cannot guarantee a 100% stand-alone operation for long periods of time. Full autonomy is only possible if the efficiency of the power generating system is increased (for example by replacing the hydrogen engine by a more efficient fuel cell) and by significantly increasing the size of the hydrogen storage. Replacing the existing engine by fuel cell technology also allows a substantial reduction in the cost of the optimal system. Figure 59 confirms that a system including a fuel cell would have better performance (higher level of hydrogen in the tank).

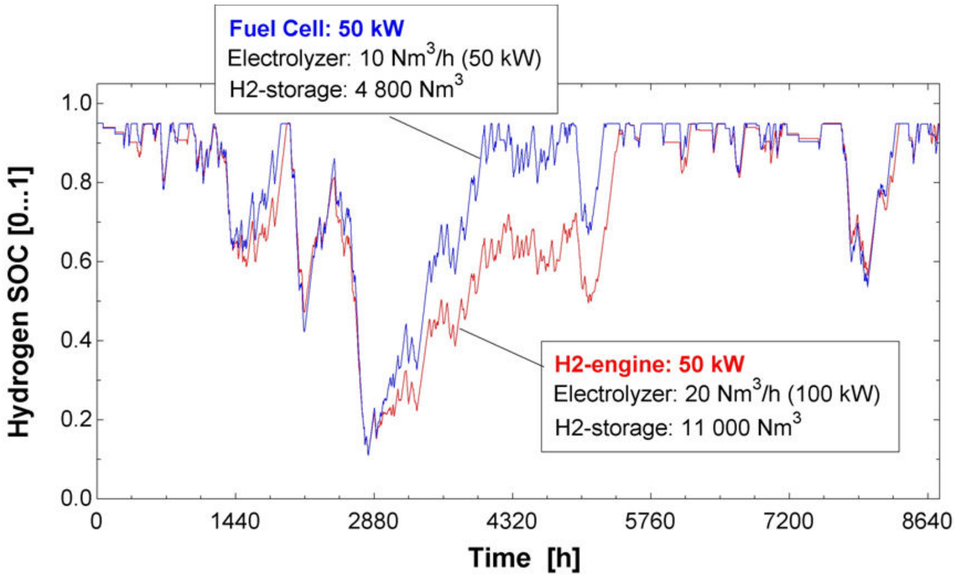


Figure 59: Compared operation of the optimal system with a fuel cell and a hydrogen engine

Conclusions

Most of the technologies that are essential to the implementation of sustainable energy systems based on hydrogen are either in their development or demonstration phase, and they have not reached commercialisation yet. More research is necessary to address the most critical issues, which are to increase the efficiency and reduce the cost of technologies. It is also crucial to ensure that all the relevant safety issues have been adequately addressed. Computer modelling has an important role to play to help achieving these objectives.

As part of this study, a library of four generic hydrogen system models were created on the TRNSYS platform:

- Low power application
- Stand-alone power system
- Hydrogen filling station
- Energy buffering systems for large wind farm

These systems were selected following a review of hydrogen projects because they are representative of the majority of the systems being developed in the world.

A cost-benefit model has been developed and linked to the technical models to analyse the economic viability of the systems. The model includes capital, replacement and O&M costs. The total net present cost and the levelized cost of energy are calculated to assess the economic performance of the project.

To allow inexperienced TRNSYS users to use the model, a user-friendly interface that presents a simplified view of the TRNSYS models has been developed. Only a few selected inputs can be viewed and changed before running the simulation.

A post-processing Excel-based tool for use in the analysis of the technical and economic performance of the systems has been created.

Finally, a cost-based optimisation methodology employing the elements above has been created to aid in the design and optimisation of hydrogen systems. This process is used to determine the optimal size of the main components of the system.

The stand-alone power system model was described in details in this thesis; the three other models have a similar structure and were built following the same methodology.

The models of the main components included in the four generic system models (PV module, wind turbine, electrolyser and fuel cell) have all been validated individually and the results were very satisfactory.

The system models and optimisation methodology have also been successfully applied on a real project: the Utsira project in Norway. The Utsira project is the world's first full-scale stand-alone renewable energy system where the energy input is provided by wind and stored hydrogen. The analysis of the system indicated that full energy autonomy was not possible at the moment over long periods of time. The analysis concluded that a few modifications to the system design were necessary: 100% stand-alone operation can only be achieved by increasing the size of the hydrogen storage and by increasing the efficiency of the hydrogen engine (e.g. by switching to a fuel cell technology).

This case study illustrates how computer modelling, used early in the design phase prior to the construction of the project, can help improving the design of hydrogen systems and therefore increase their performance. This is likely to result in substantial project costs reduction.

The results of this study have been published and presented at different international conferences specialised in renewable energy and hydrogen technologies. [45][46]

Further work could be done to improve the TRNSYS models. Different strategies to control the operation of the systems could for example be developed. At the moment only one control strategy, based on the state of charge of the hydrogen tank, is available in the TRNSYS library. Choosing the most suitable strategy to control the system should become part of the optimisation methodology. Other techniques of storage such as batteries, flywheels and metal hydrides could also be integrated to the models. Regarding validation, the models should be applied to other types of hydrogen energy systems than stand-alone power systems. The filling station and energy buffering models were not tested on existing projects as part as this study. This would demonstrate how the models can be used for the design of larger scale systems.

Acknowledgments

I would like to thank Richard Boddington, Geoff Hoffheinz (SgurrEnergy) and Doctor Nick Kelly (University of Strathclyde) for their role in the project. My KTP advisor, Doctor Gerry Black, and the rest of the KTP team also played an important role in this project. I would also like to thank Torgeir Nakken (StatoilHydro) for his help and time for providing some very useful information and operational data for the Utsira project. Michael Kummert (Mechanical Engineering Department, University of Strathclyde) gave me some precious advice in TRNSYS modelling. Last but not least, I would like to thank Øystein Ulleberg (Institute for Energy Technology in Norway; he is also the developer of the HydroGems models in TRNSYS and the hydrogen modelling expert leading the IEA Annex 18) for his crucial contribution to the project (TRNSYS workshop, collaboration on the Utsira project modelling).

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