Modelling Green Energy Conversion Networks for Generating Hydrogen Electric Vehicle Fuel

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Abstract

Investigating the feasibility of using hydrogen as a fuel for electric vehicles requires a robust techno-economic comparison and feasibility analysis to determine its suitability as a competitor to pre-existing market alternatives. The relationships between two major abstractions in energy conversion networks—energy stores/resources and energy converters—were considered and explored, being modelled as a simple, directed, weakly-connected graph. This abstraction permits the formalisation of state-dependent operators that can be applied to numerically integrate the network state over time, hence permitting the utilisation of the dynamic programming methods to analyse and optimise potential systems subject to techno-economic constraints. As a rough prediction, in a simplified linear system transforming solar energy into hydrogen fuel, the total budget required is at minimum 70.8k€ per hydrogen electric vehicle, of which enough should be spent on photovoltaic cells to generate at least 4.6kW of PV capacity per HEV. This work is intentionally generalisable to a wide class of energy systems, and provides a stepping stone for future investigations modelling real-world systems in greater depth and complexity.

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1 Introduction

The global shift away from fossil fuels towards renewable energy sources necessitates highly efficient and effective energy conversion networks. Thus it is increasingly important to develop robust methods for modelling and analysing the behaviour of such networks in order to determine their feasibility and optimise their performance.

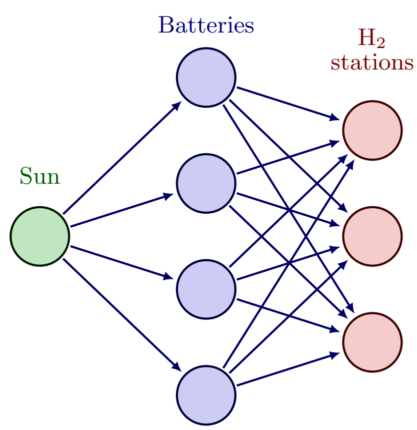
One such network is the system for generating hydrogen as a fuel for electric vehicles (HEVs). This simplified linear instance of such a system demonstrates the key features:

$$\underset{\text{Sun}}{\bullet} \xrightarrow[\text{PV cells}]{} \underset{\text{Battery}}{\bullet} \xrightarrow[\text{Electrolyser, Compressor}]{} \underset{H_2 \text{ fuelling station}}{\bullet}$$

This graphical abstraction of the system is useful for visualising the relationships between the various components. Moreover, it is possible to formalise the relationships between the components as a directed graph. Notice that the Sun, Battery and H_2 fuelling station are energy stores if an energy resource can be considered as an energy store of pseudo-infinite capacity. The PV cells, electrolyser and compressor are energy converters which take a single input and produce a single output.

Treating energy stores as graph vertices and energy converters as weighted graph edges provides a general approach that can be utilised to model the behaviour of broad class of energy conversion networks. This class can be further broadened by transforming other networks into this form, for example by edge subdivisions or adjusting edge weightings.

The attribute of generality is important for the model to be of utility for future investigation. One pertinent use case is a large-scale network of many HEV fuelling stations. It is especially crucial to be able to model the behaviour under critical conditions such as component failure. This is because the failure of a single component can have a significant impact on the performance of the entire system.



In the above example, the high connectivity and number of nodes per layer will likely prevent a single battery failure from entirely disabling its downstream components, but having a mathematical way to quantify the benefit of this connectivity is critical for determining the trade-off between economics and system performance.

The objective of this article is to develop a generalised model for analysing the behaviour of such energy conversion networks.

2 Methodology

2.1 Preliminaries

Consider a simple, directed graph defined as an ordered pair of vertices and edges $G = (V, E)$ where V is the vertex-set and $E \subseteq \{(x, y) : (x, y) \in V^2 \mid x \neq y\}$ is the directed edge-set, with vertices labelled to represent the *energy stores* and edges labelled to represent the *energy converters* of the energy system.

Definition 2.1. The *adjacency matrix* of G is $\underline{\underline{A}} \in \mathbb{R}^{V \times V}$ such that its entries satisfy

$$\underline{\underline{A}}_{ij} = [(v_i, v_j) \in E]$$

where $[\ \cdot\ ]$ is the Iverson bracket.

Definition 2.2. Similarly, the *weighted adjacency matrix* of G is $\underline{\underline{W}} \in \mathbb{R}^{V \times V}$ such that its entries satisfy

$$\underline{\underline{W}}_{ij} = w(i, j)\underline{\underline{A}}_{ij}$$

where $w(i, j)$ is the weight label of the edge (v_i, v_j).

Lemma 2.3. *G is connected iff $\nexists$ (i, j) such that*

$$\left(\sum_{k=1}^{|V|} \underline{\underline{A}}^k \right)_{ij} = 0$$

Proof. $\underline{\underline{A}}$ is a linear map between vertices and their neighbours so $(\underline{\underline{A}}^k)_{ij}$ is the number of k-walks from v_i to v_j. Hence the total number of walks from v_i to v_j in K steps or less is given by $\left(\sum_{k=1}^{K} \underline{\underline{A}}^k \right)_{ij}$. Now, if a walk between v_i and v_j exists, the shortest such walk must be in a number of steps less than or equal to the cardinality of V, that is, G is connected iff the number of walks in $|V|$ steps or less between every pair of vertices is non-zero. □

Lemma 2.4. *G is weakly connected iff $\nexists$ (i, j) such that*

$$\left(\sum_{k=1}^{|V|} \left(\underline{\underline{A}} + \underline{\underline{A}}^\top \right)^k \right)_{ij} = 0$$

Proof. A directed graph is weakly connected if its underlying undirected graph is connected. Since $A^\top$ is the adjacency matrix for the graph with the same vertices as G and reversed edges compared to G, the adjacency matrix $\underline{\underline{A}}'$ for the underlying undirected graph of G has the same zero-entries as $\underline{\underline{A}} + \underline{\underline{A}}^\top$, that is to say

$$\forall i, j : [\underline{\underline{A}}'_{ij} = 0] \Leftrightarrow [(\underline{\underline{A}} + \underline{\underline{A}}^\top)_{ij} = 0]$$

Hence the result follows from the previous lemma. □

This latter lemma serves as a useful tool for asserting the weak connectivity of a graph in the model since disconnected graphs will be considered to be separate systems.

2.2 Ideal Behaviour

To develop the model, first begin by examining the ideal case without constraints or energy losses. Consider a single vertex $v_i \in V$ representing an energy storage unit (e.g., a H_2 fuelling station) labelled with its stored energy $u_i = u_i(t)$:

$$\xrightarrow[\text{Net power in}]{} \overset{u_i(t)}{\bullet} \xrightarrow[\text{Net power out}]{}$$

In the ideal case the flow of energy through the vertex from and to its neighbours is unrestricted and immediate. During a time interval Δt

$$\Delta u_i(t) = u_i(t + \Delta t) - u_i(t) = -\overbrace{\sum_{j=1}^{N} \underline{\underline{W}}_{ij} u_i(t)}^{\text{energy out}} + \underbrace{\sum_{j=1}^{N} \underline{\underline{W}}_{ji} u_j(t)}_{\text{energy in}}$$

Future references to this result will omit the explicit declarations of $\underline{u}$ being a function of time for brevity, however these terms should still be understood to be time-dependent. It is also useful to sanity-check that this result is consistent with the First Law of Thermodynamics:

Lemma 2.5. $\forall\ \underline{\underline{W}}, \underline{u} : \sum_{i=1}^{N} \Delta u_i = 0$

Proof.

$$\sum_{i=1}^{N} \Delta u_i = \sum_{i=1}^{N} \left(-\sum_{j=1}^{N} \underline{\underline{W}}_{ij} u_i + \sum_{j=1}^{N} \underline{\underline{W}}_{ji} u_j \right) = \sum_{i=1}^{N} \sum_{j=1}^{N} \underline{\underline{W}}_{ji} u_j - \sum_{j=1}^{N} \sum_{i=1}^{N} \underline{\underline{W}}_{ij} u_i = 0$$

$\square$

Thus this process conserves $\|\underline{u}\|$ and is diffusive.

2.3 Non-Ideal Behaviour

The model considers the following non-idealities:

- **Maximum storage capacity** $u_{i_{max}}$ such that $0 \leq u_i \leq u_{i_{max}}$.
- **Maximum energy transfer rate** $\underline{\underline{P}}_{ij}$ such that $0 \leq \underline{\underline{W}}_{ij} u_i \leq \underline{\underline{P}}_{ij} \Delta t$ where $\underline{\underline{P}}_{ij}$ is the maximum possible power transfer through the edge (v_i, v_j).
- **Energy storage self-discharge**: loss of energy stored over time.
- **Power transfer inefficiency**: losses during energy conversion.

The constraints on maximum energy and power can be handled by applying bounds to some of the terms in the prior result.

$$\Delta u_i = \min \left(u_{i_{\max}} - u_i, \begin{array}{l} -\sum_{j=1}^{N} \min(\underline{\underline{W}}_{ij} u_i, \underline{\underline{P}}_{ij} \Delta t) \\ +\sum_{j=1}^{N} \min(\underline{\underline{W}}_{ji} u_j, \underline{\underline{P}}_{ji} \Delta t) \end{array} \right)$$

It is now no longer guaranteed that $\sum_{i=1}^{N} \Delta u_i = 0$ because the system is no longer closed.

To handle self-discharge losses and energy conversion losses, consider an arbitrary energy conversion p_{xy} with efficiency η_p. For simplicity, assume in this example that p_{xy} is the only edge out of v_x and assume initially that p_{xy} is ideal, that is, $\eta_p = 1$.

$$v_x \xrightarrow{p_{xy},\ \eta_p=1} v_y$$

If p is not, in fact, ideal, then we can model this by partitioning some power off into an energy wastage sink. Suppose it is 70% efficient:

$$\begin{tikzcd} v_x \arrow[rr, "{p_{xy},\ \eta_p=70\%}"] \arrow[dr, dashed, "30\%"] & & v_y \\ & \text{energy sink} & \end{tikzcd}$$

Additionally, suppose that v_x has a self-discharge rate of $10\%/\Delta t$. Then the net useful power out of v_x is $\eta_p(p_{xy} - \frac{0.1}{\Delta t} u_x)$. To keep the graph simple, combine the two edges representing power loss into a single one.

$$\begin{tikzcd} v_x \arrow[rr, "{p_{xy},\ \eta_p=63\%}"] \arrow[dr, dashed, "27\%"] \arrow[dr, dashed, bend right, "10\%"'] & & v_y \\ & \text{energy sink} & \end{tikzcd} \rightleftharpoons \begin{tikzcd} v_x \arrow[rr, "{p_{xy},\ \eta_p=63\%}"] \arrow[dr, dashed, "37\%"] & & v_y \\ & \text{energy sink} & \end{tikzcd}$$

Now that the model has been extended to handle non-idealities, it is possible to consider the behaviour of the system over time through numerical integration by successive summation of Δu_i.

3 Results

Returning to the initial simple linear system considered

$$\text{Sun} \xrightarrow[\text{PV cells}]{} \text{Battery} \xrightarrow[\text{Electrolyser, Compressor}]{} H_2 \text{ fuelling station}$$

applying the model to this system yields some interesting results, with data about photovoltaic performance sampled for Cyprus. Assumptions about system component characteristics were taken to be the same as Olympios et al. [1]. The modelling and optimisation was implemented in *Python*.

The model was applied in the context of a techno-economic optimisation problem. The *L-BFGS-B* algorithm was used to minimise the total budget required to sustain the system for a given number of HEV consumers. The results for the optimal budget allocation between system components is given in Figure 1. Note that the solution η given is relative to the output of the PV cells.

# HEVs	Min. budget (€)	Solution η	PV capacity (kW)
1	70.8k	0.55	4.6
10	715k	0.55	46
100	6800k	0.55	460

Figure 1: *Table of results for the optimal budget allocation between system components.*

It was not possible to simulate 1000 HEVs due to size constraints from the PV data API.

The optimal solution η was found to be independent of the number of HEVs. This is likely at least partially due to weaknesses in assumptions made while implementing the model. Although the model itself is generalised, when applied to this problem, assumptions about linearity in component behaviour clearly impact the results.

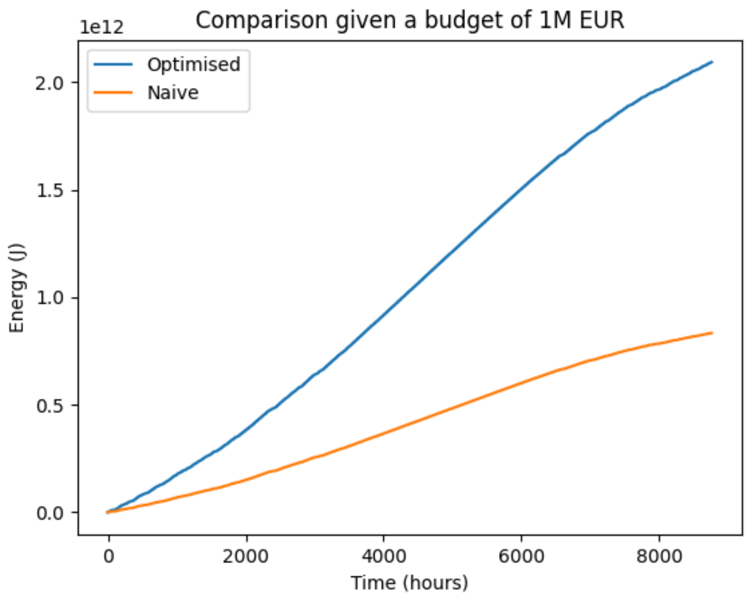
Additionally, the optimum solution found is possibly a local minimum rather than a global minimum due to temporal constraints on the optimisation workflow. The PV capacity per car required matches a rough back-of-the-envelope calculation taking the average daily mileage of a car to be 40km and fuel consumption to be 0.08kgH_2/km.

The converse problem was also studied, that is, maximising the number of HEVs that can be sustained for a given budget. The naive approach of an equal budget allocation is given as a baseline for comparison in the accompanying graphical figures in Figure 3.

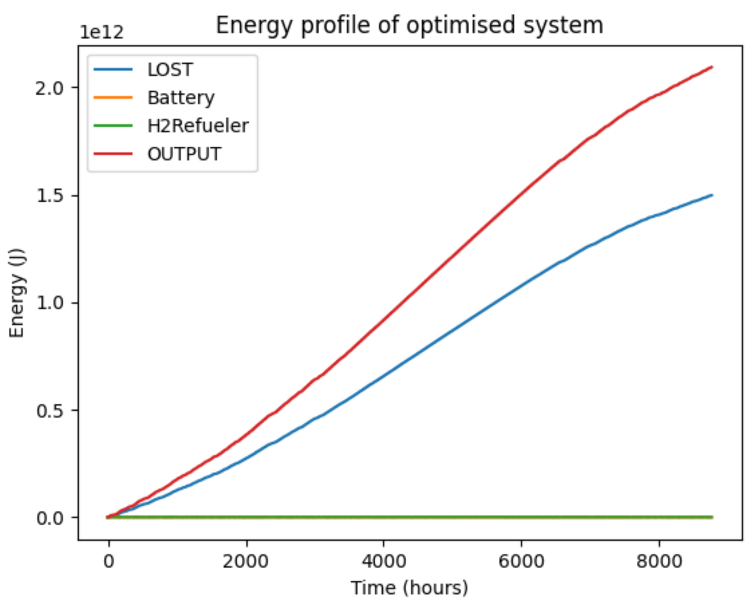
PV (€)	Battery (€)	Electrolyser (€)	H_2 station (€)
645k	244k	107k	3.90k

Figure 2: *Table showing optimal budget allocation for 1M€.*

Indeed, using the same budget the optimised budget allocation more than doubles the system output of H_2. Nevertheless, the skewed ratio in Figure 2 is potentially an indication of either the implementations's failure to capture the non-linearities in the system or the failure of the optimisation algorithm to find the global minimum.



(a) H_2 output over time for optimised and naive budget allocations.



(b) Energy distribution through the system over time for optimised budget allocations.

Figure 3

4 Conclusion

A general model was developed and implemented for the purpose of analysing the behaviour of energy conversion networks. Using a simple linear system as a demonstration, the model was applied to a techno-economic optimisation problem with sensible assumptions about component characteristics and yielded sensible results. As a rough guide—in this simplified linear system transforming solar energy into hydrogen fuel, the total budget required is at minimum 70.8k€ per hydrogen electric vehicle, of which enough should be spent on photovoltaic cells to generate at least 4.6kW of PV capacity per HEV. This work is easily extendable and extensible for future investigation into the feasibility of using hydrogen as a fuel for electric vehicles. Such future investigations would be aided by using more accurate characteristic curves for component attributes when applying this model to more complex systems.

References

[1] Andreas V. Olympios, Alexandros Arsalis, Fanourios Kourougianni, Antonio M. Pantaleo, Panos Papanastasiou, Christos N. Markides, and George E. Georghiou, *Technology design and operation optimisation of integrated electricity-heat-cold-hydrogen systems in buildings*, Proceedings of the 18th SDEWES conference, 24/09/2023 to 29/09/2023. To be presented at the 18th SDEWES Conference 2023 in Dubrovnik.