Optimization of operation of renewable electric energy sources based on fuel cells, accumulators and FV panels for small powers

29. září 2014

Motivation and introduction

For better understanding of the whole text, lets imagine a model problem, which we can follow through the entire work. Lets say, we want to make an energy independent unit - ecologic house, for example.

Lets add renewable energy source (fotovoltaic panels) and a system for storing energy. Batteries alone are not sufficient, because they would need to be changed, due to degradation. So lets add availible hydrogen technologies - electrolyzer, hydrogen tank, fuel cells. And, to finish the setting, backup energy unit (or electric grid). The goal is to determine the system parameters (and develop the strategy to do so) and power managment strategy in a manner to make the system independent as much as possible (minimizing the consumption of backup energy or energy from grid).

For now, lets look at the theoretical and practical tools needed to solve this problem - in the following part "research and previous works". Later we will return to our model problem, and we will use the tools to analyze the setting and rewrite it into mathematical formulation. Next we will state arising interesting questions, which we will try to answer - to complement other works.

Lastly, there will be a brief note about developed computer program.

Research and previous works

Lets summarize other works and interesting ideas from the relevant fields.

Optimization and hydrogen technology

Fuel cells and hydrogen technologies (as a part of renewable resources [MASb]), extend the possibilities of energy storage [eJ] and creates a possibility for research of various systems and using mathematical tools to model and optimize theese systems. One example of such a system are the standalone energetic units [Masa].

Some possibilities of optimization theese standalone systems are sumarized in [EU12], optimization of standalone energetic units and power managment strategies are being researched too [IVS+09].

Application of optimization in the theory of optimal control is described in the books [Eva], [Lew12], [War72]. An example of a method used for global optimization is an application of metropolis algorithm, so called Simulated Annealing [BM95] (that is used too for the design of electric circuits or

in chemistry [CD97]). There is even a method taking in account the uncertainity of data, Stochastic Annealing [PD95]. This method is used in [GPSV10] for optimization of the parameters of the control strategy.

Another interesting principle, the Pontryagin principle, is used to prolong the lifetime of such systems [XQL+13, ZXZ13, ZXP+14], or optimization problems are solved for vehicles [MKAD14]. In the article [CdAVvS06], there is proposed an optimal system even for the powerplant of SOFC type.

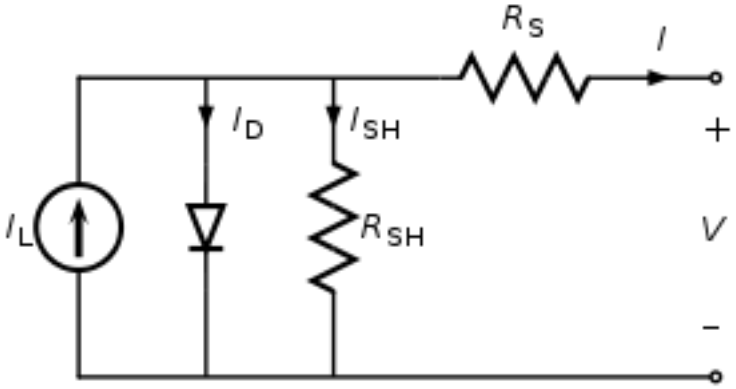
Needed to say, that often, new algorithms of global optimization are being used (ex. particle swarm, or genetic algorithms). For theese algorithms, the question of convergence is still an open problem (about this and another possibilities of algorithms is the text [Alv06]).

Models for batteries, fuel cells, electrolyzer, photovoltaics...

There are rich availible model descriptions, complex models (with PDEs) are used for complicated problems and for detailed desription of inside processes (for example in a battery), but theese models arent meant and suited for simulations. More simple models with less variables (for example like curve fitting) are better in case we need to evaluate the model more times (as in our case).

Photovoltaics

When looking at photovoltaic (PV) panels, if we want a better model than saying "general power source", we need to consider that the photoelectric effect (the power source) happens at the P-N junction, which is, of course, a diode, and that there is some ressistance present. Thats the reason, why the following equivalent circuit "5 parameter circuit" is used (there exists even the so called "7 parameter circuit" which has another diode in parallel to the first diode).



Contruction details, like material used (single crystalline silicon, polycrystalline and semicrystalline, thin films, amorphous silicon, spheral) or additional tricks (concentrated cells, lens, antireflexive and other coating) affect the parameters and the efficiency.

The circuit supplies current $I = I_{pv}$ at voltage $V = V_{pv}$, I_L is generated current by photovoltaic effect and from that we subtract diode current and shunt current. This way we can derive the model:

- $I_{pv} = I_L - I_D - I_{sh} = I_L - I_0(\exp(\frac{V_{pv}+I_{pv}R_s}{\alpha})) - \frac{V_{pv}+I_{pv}R_s}{R_{sh}}$
- $I_L = C_1 G$, $I_0 = C_2 T^3 \exp(\frac{-E_{GO}}{kT})$
- $P_{pv} = V_{pv} I_{pv} \eta_{conv}$
- α curve fitting parameter (model requires test runs and measurements)
- G incident radiation

- T surface temperature
- E_{GO} band gap of the used PV material
- C_i constants
- $I_L$light current
- $I_D$diode current
- I_{sh}shunt current
- I_0diode reverse saturation current (comes from the Shockley's diode equation)
- V_{pv}, I_{pv}, operational voltage and current
- R_s, R_{sh}, parallel and shunt ressistors
- P_{pv}, η_{conv} output power and effectivity

Parameters used to characterize the output of the unit are short circuit current, open circuit voltage and maximum power point. Nice derivation is in the work [Ø.98] together with a method how to compute the parameters from manufacturers supplied information from datasheet and notes on behavior with changing temperature. Also, the efficiency of PV energy generation is said to be from 5 to 20%.

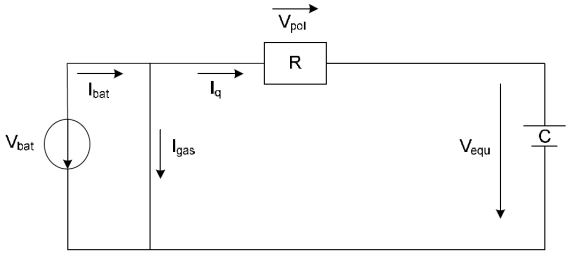
In a work focused on solar panels and water electrolysis [Olu11], there is deeper description and analysis and measurement of output power dependency on illumination and even thermal effects.

Needed to say, that detailed analysis of output power includes an observation [Vou11], that there is a maximal power point in the voltage current characteristic; this is ideally exploited by a microcontroller, traking this point. (In addition this book covers many interesting details, even about AC/DC converters.) Algorithms for tracking maximal power point are also being developed in [BHB04, SOBL06], even using neural networks is considered [CNCP11].

Battery

Why to use both batteries and hydrogen (tanks) to store energy? Batteries have higher efficiency, but cant store as much energy as we can with hydrogen. Moreover, the state of charge of batteries tends to decrease and batteries tends to lose quality over time. But using them as quick source, or buffer of energy, is generally a good idea, moreover in case, where electrolyzer works better at lower loads, battery can lower the load by taking it on itself.

The main variables for a battery model are the voltage and state of charge (SOC). Lets speak about a model of lead acid accumulator from [Vou11] - the model is valid for batteries charged more than 20 %, has relations for carging and discharging and parameters that need to becomputed experimentally. (Needed to say, that there exists models even for overcharged batteries and other specific cases.)



$$I_{bat} = I_q - \frac{Q_{bat,nom}}{10} g_0 exp(\frac{V_{cell}}{g_1} - \frac{g_2}{T_{bat}})$$

THe batter current is the reaction current (I_q) minus the gas current loses, that are modelled using nominal capacity of accumulator ($Q_{bat,nom}$ in Ah), cell voltage, temperature and gassing current parameters. The cell voltage is the equillibrium plus polarization voltage:

$$V_{cell} = V_{equ,0} + \frac{V_{equ,l} SOC}{100} + V_{pol}$$

The equillibrium voltage is approximated linearily by its value at $SOC = 0$ and slope $V_{equ,l}$, the polarization voltage is different for charging and discharging (with coefficients dependent on the battery):

$$\begin{aligned} V_{pol,ch} &= U_{ch} a_{ch} (1 - \exp(-\frac{I_{q,norm}}{b_{ch}}) + c_{ch} I_{q,norm}) \\ V_{pol,dch} &= U_{dch} (1 - \exp(-\frac{I_{q,norm}}{b_{dch}}) + c_{dch} I_{q,norm})(1 + (g_{100} - 1)\exp(\frac{SOC - 100}{k_{100}})) \end{aligned}$$

The indexes "ch" stand for charging and "dch" for discharging. The parameters g_{100}, k_{100} are height and slope parametes for fully charged battery ($SOC = 100\%$).

A discrete model for a capacity of the battery is

$$Q_{bat,i} = Q_{bat,i-1} + I_q(t_i - t_{i-1}) = Q_{bat,nom} SOC_{i-1}/100 + I_q(t_i - t_{i-1})$$

The state of charge of the accumulator is a fraction of the current capacity at each time instant divided by its nominal capacity. So for SOC we have a model with efficieency (η_{ac}), discharge rate (σ_{ac}) and charge or discharge current I_{ac}.

$$SOC(t+1) = SOC(t)(1 - \sigma_{ac}) + I_{ac}\eta_{ac}(\Delta t)$$

SOC cant be directly measured, it needs to be derived from the model or indirectly from experiements.

Electrolyzer and Fuel cell

Electrolyzer and fuel cell both basically operate from simple chemical reaction:

$$H_2O \longleftrightarrow H_2 + \frac{1}{2}O_2$$

By adding electrical power, the reaction occurs from left side to the right, producing hydrogen and oxygen, whereas combining hydrogen and oxygen allows us to get the energy back. The first way is the basic function of electrolyzer and the latter is of the fuel cell. By Faradays law, the (molar) quantity of produced/consumed hydrogen is proportional to transfered charge.

Interesting details arise from the exact engeneering of both processes (parameters like temperature, material of electrolyte or membrane, catalyzators etc...), anyway the basic common variables are voltage, current and temperature.

It is good to note, that hydrogen has the best heating value (energy to fuel ratio). The higher heating value is $285.83\,kj\,mol^{-1}$, the pure standart heat formation of the product water. The lower heating value is $120\,MJ\,kg^{-1}$, calculated from the fact, that the product oxygen goes out unused as a steam (at said 150 °C). Electrolysis is not the only way to get hydrogen, other ways are being considered too, for example by reforming natural gases.

Electrolyzer

Common types of electrolyzers are alkaline based (operates using an alkaline solution) electrolyzers and proton exchange membrane electrolyzer.

As presented in [Vou11], there are many ways to the voltage - current model of the electrolyzer - regression, models based on analysis of processes on anothe, cathode and membrane (and calculating then V-I relationship by subtracting from the open circuit voltage the voltages of activation polarization and ohmic polarization), and even rigorous CFD models.

Butler Volmer equation In the work [Ø.98], it is noted, that at low voltages, the electrolyzer is more efficient, but generates small amounts of hydrogen. The Butler-Volmer equation is used to model the system:

$$I = I_{0e}(\exp(\frac{(1-\alpha_e)n_eF}{RT}(U-U_{eq})) - \exp(-\frac{\alpha_e n_e F}{RT}(U-U_{eq})))$$

With unknown parameters I_{0e}, α_e (symmetry factor) andU_{eq}. Hydrogen production rate is computed as follows:

$$n_{H_2} = \frac{N_{call} I_{el}}{nF}\eta_F$$

where F is Faraday constant and η_F is Faraday efficiency (relation between theoretical and actual electron transfer, often to be determined by experimental measure).

One empirical model

$$V_{elec} = V_{rev,elec} + \frac{r_1 + r_2 T}{A_{elec}} I_{elec} + (s_1 + s_2 T + s_3 T^2)\log(\frac{t_1 + t_2/T + t_3/T^2}{A_{elec}} I_{elec} + 1)$$

There exists even empirical model for the faraday's efficiency, that takes into account the fact, that with decreasing current and/or higher temperatures, the parasitic currents increase (because of the electrolyte).

$$\eta_F = B_1 + B_2 \exp(\frac{B_3 + B_4 T_{el} + B_5 T_{el}^2}{i})$$

Fuel cell

The exact process happens in this way:

$$\begin{aligned} H_2 &\rightarrow 2H^+ + 2e^- \\ \frac{1}{2}O_2 + 2e^- &\rightarrow O^{2-} \\ 2H^+ + O^{2-} &\rightarrow H_2O \end{aligned}$$

And the calculation for the amount of hydrogen produced is (from [Olu11]), where ϵ is the fuel cell efficiency:

$$n_{H_2} = \frac{1}{\epsilon} \cdot 0,01866 \frac{mol}{hr \cdot Amp},\ m_{H_2} = \frac{1}{\epsilon} \cdot 3,77 \cdot 10^{-5} \frac{kg}{hr \cdot Amp}$$

The simplest way to model fuel cell V-I relationship is to look at it as a reverse electrolyzer, this course is followed by the following model from [Vou11].

First empiric model Takes into account the overvoltages (ohmic and activation), but not effects of mass. The model computes the cell voltage V_{cell} using open circuit voltage E, current density i, model parameter b, current at the inflection point of the V-I curve I_d and slope Δ at the linear stage of ohmic overvoltage:

$$V_{cell} = E + \frac{b}{\ln(1/I_d\, i)} - (\Delta - \frac{b}{4I_d})\, i$$

The parameters ($K \in \{E,\, I_d,\, b,\, \Delta\}$) vary with fuel cell temperature T and oxygen partial pressue p_{O_2}:

$$K = K_1 + K_2 T + K_3 T \ln(p_{O_2})$$

It is said, that this model is suitable more for low voltages and powers. But can be used even for electrolyzer (p_{O_2} is then the operating pressue for the electrolyzer at which the oxygen is produced).

Second empiric model This model takes into effect even the mass transport limitation. For computation of a cell voltage V_{fc} and open circuit voltage V_o, the following applies:

$$\begin{aligned} V_{fc} &= V_o - a_T \log(i) - ir + m \exp(il) \\ V_o &= V_{rev,FC} + B \log(i_o) \end{aligned}$$

Where $V_{rev,FC}$ is the reversible voltage, i the current density, i_0 and B the Tafel parameter, a_T the Tafel slope, r the resistance (in $\Omega \cdot cm^2$), finally the model parameters m, l representing the overvoltage due to mass transport limits. All theese parameters can depend on temperature.

Hydrogen and oxygen then flows according to equations (by Faradays law):

$$H_{2,g} = \frac{nI}{2F\eta_F},\; O_{2,g} = \frac{nI}{4F\eta_F}$$

All theese models are empirical and are important only because of their low computational complexity. For greater complexity, there are of course more sophisticated models using partial differential equations. There is also a nice book about fuel cells, that examines every aspect of fuel cell design and explains the details of how fuel cells works [LDM03]. larminie2003fuel

Lets add a word about the storage of hydrogen. The possibilities for storage are to store it at the output pressue of the electrolyzer, or at higher pressue or liquidified. Theese possibilities are covered in most of presented resources and citations. If we wanted to store the hydrogen in any other way than at the output pressue, we would need to add the compressor into the equation (like it is done in).

Optimization and optimal control

Optimization is a rich field with many subproblems arising from the specific problems settings. Optimal control is applied optimization together with variational calculus and has similar subproblems.

As (global) optimization is concerned about finding the minimum of a function with number of parameters, optimal control theory takes this idea to the next step and solves minimum of a functional ("objective function" or "cost function" J that consists of final time objective and integrated Lagrangian) of a dynamic system, evolving in time, controlled by a function (system dynamics).

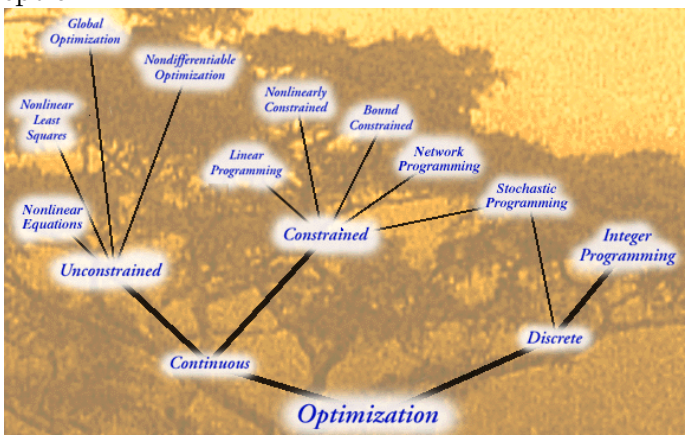
$$\text{minimize } J = \phi(x(T), T) + \int_0^T L(x, u, t)\, dt \qquad \text{...cost function / objective function}$$
$$\dot{x} = f(x, u, t) \qquad \text{...system dynamics}$$
$$x(0) = x_0$$
$$g(x, u, t) \leq 0 \qquad \text{...constraints}$$

In free final time, the function ϕ is not present.

Problems from calculus of variations can be formulated as an optimal control problem, so the ideas from this field apply in optimal control too. Moreover, optimal control theory has methods for solving the problem of controllability and observability and the presence of noise.

Basic terms

Optimization problems have many subclasses (as the picture shows) and optimal control is not an exception.



So, in formulating the problem, there are many decisions that need to be made, or many features, that can be adressed. To get a grasp of the field, lest summarize the most common features (more details can be found in the book [BBBB95]).

bertsekas1995dynamic

First, the problem can be formulated in **finite time** or **infinite time**, or the **time can be varied** too ("free time, fixed endpoint" problem vs "fixed time free endpoint"). The model can be **continuous** or **discrete**, not only in **time, but also in states**. Lastly, we can account for **statistical uncertainities**. When we add probabilty to the problem, we will be dealing with markov chains theory.

The goal, control policy, can be made **open loop** or **closed loop** formulation. Closed loop does care for values and decisions in intermediate states, whereas open loop control has the control function predetermined in advance and not relying on intermedate states and values. Methods for solving optimal control problems are **dynamic programming**, **Hamilton Jacobi Bellman (HJB) equations** and **Pontryagin maximum principle** (or minimum principle, it doesn't matter and is called by both names in literature). Only some of the problems can be solved analytically, for example the class of **linear quadratic control** problems, that can be solved through Riccati equations.

Hamiltonian of the system

May problem formulations could be efficiently written using Hamiltonian of the system. We will use it too, so lets state the Hamiltonian as a Lagrangian (from cost function) plus adjoint variable times system dynamics.

$$H(x, u, \lambda, t) \quad = \quad L(x, u, t) + \lambda^T f(x, u, t)$$

The adjoint variable comes from the idea to take the system dynamics as a constraint and to introduce lagrangian multipliers, that enables us to switch from constrained optimization to unconstrained (as in [Eva, Lew12]) or from HJB equations (there are two ways to get the equations presented later, one gives the name "adjoint variable" to one of the derivatives, so it is conveniet to use the name). It is essential for formulations, that will come later. Lets just note here, that Hamiltonian is constant for systems with parametres undependent on time.

Dynamic programming

Dynamic Programming is a principle well known for problems, that can be decomposed into smaller subproblems. The principle is easy - if the optimal solution of a problem can be composed from optimal solutions of subproblems, we can use this information to build the solution. Whenever this is true (needs for example additive cost function), we just dont need to search the whole state space, but we can construct the solution by constructing subsolutions one from another in a clever order. One example from other field is the problem of finding the shortest path in a graph.

Dynamic programming needs discretized problem formulation, but going to the limit gives rise to the HJB equations.

Hamilton-Jakobi-Bellman equations

HJB eq. are partial differential equations of the problem (here we need the Hamiltonian), the last equation is just system dynamic written using Hamiltonian:

$$
\begin{aligned}
J^\star(x(T),T) &= \phi(x(T),T) \\
-\frac{\partial J^\star}{\partial t} &= \min_u H(x,u,J_x^\star,t) = \min_u H(x,u,J_x^\star,t) = L(x,u,t) + J_x^\star f(x,u,t) \\
\dot{x} &= \frac{\partial H}{\partial \lambda} = f \qquad \text{...state equation}
\end{aligned}
$$

When using this apporach, the first step is to solve to get the optimal value function first and from that the other values. Hamilton-Jakobi-Bellman equations from optimal control gave life to the theory of viscosity solutions, more can be found in articles [BCD08, Dra, LZ13]. Theese equations can be solved using finite element methods, but their stability is said not to be good.

Pontryagin principle of maximality, PMP

The last step - or method - principle of maximality (Pontryagin principle of maximality, PMP), can be derived using the HJB equations (as in [BBBB95]). Using that, we get to formulate equations for adjoint variable - the first equation is pontryagin maximum principle and the second we get by differentiating HJB equation, as in [Die11]. The last condition is the transversality condition for fixed time free endpoint problem.

$$
\begin{aligned}
u^\star(t,x,\lambda) &= \arg\min_u (H(x,u,\lambda,t))\phi(x(T),T) \\
-\dot{\lambda} &= \frac{\partial H}{\partial x} = \frac{\partial f^T}{\partial x}\lambda + \frac{\partial L}{\partial x} \\
\lambda(T) &= \nabla\phi(x(T),T)
\end{aligned}
$$

As was said, we get the same results even from the perspective of taking the system dynamic as constraint for lagrange multipliers.

- HJB Equations - tabulation in state space
- Indirect methods, Pontryagin - solve boundary value problem
- Direct Methods - change to nonlinear programming
  - Single shooting - discretized controls to NLP
  - Multiple shooting - controls and node start values discretized
  - Collocation - disretized controls and states

Obrázek 1: Numerical optimal control tree

In the presence of state constraints $x \in R = \{x \in \mathbb{R}^n, g(x) \leq 0\}$, PMP is formulated a bit differently [Eva] - we need to define a function

$$c(x,u) = \nabla g(x) \cdot f(x,u)$$

and the costate equation becomes:

$$-\dot{\lambda} = \frac{\partial H}{\partial x}(x,u,t) + \mu \frac{\partial c}{\partial x}(x,u)$$

While the PMP now states the existence of the function $\mu : [0,T] \to \mathbb{R}$.

Needed to say, that PMP equations are only necessary condition for optimality, so analytical proof of existence and uniqueness is needed.

All theese analytic methods will give us equations, to solve the equations is a concern of numerical optimal control.

Numerical optimal control

Numerical optimal control can be, again, used to solve continuous or discretized problems. Heavily relies on the problem analysis and follows the said methods. It would seem, that it is sufficient to just solve HJB PDR's, but it is not used everytime. The problem is the, so called, curse of dimensionality - when state and/or control, has many components, the problem becomes exponentially hard to solve. Suggested remedy, in the article [Die11], is, for example, to approximate value function by neural network methods.

The main classes are **indirect methods** (first optimize then discretize) and **direct methods** (first discretize, then optimize). Indirect methods results in algorithms similar to ODE solvers, but the resulting system can be badly conditioned or unstable. Direct methods just rewrite the problem to the area of nonlinear programming problem and then apply convenient solver.

There are three main cases of direct methods - single shooting, Multiple shooting and collocation.

Single shooting discretizes the control to piecewise constant function and uses numerical integrator for the evaluation of the cost function (ODE). This way we get a finite dimensional optimization problem, which can be solved by any nonlinear programming algorithm.

Suggested, for example, is Sequential quadratic programming, SQP, [BT95]. It is a method for solving nonlinear problems with second derivatives; uses repeated subsolutions of quadratic programming problems. When we are speaking about this subject, lets say the main keywords for algorithms used for differentiating the ODEs (theese derivatives are needed for the algorithms): External Numerical Differentiation (END), Variational Differential Equations, Automatic Differentiation, Internal Numerical Differentiation (IND).

Single shooting algorithm is usefull, but the stability can sometimes depend heavily on starting value.

Collocation discretizes both the control function and state function and approximates the integral. We get larger system for nlnlinear programming, but the good news is that the system is sparse (in the meaning, that the Jacobians have many zero elements). Collocation can treat better even unstable systems, but refining the grid results in new problem with higher dimensions.

Multiple shooting discretizes the control, as single shooting, and additionally the time scale. So it is multiple shooting, because it is like running single shooting algorithm again from the starting times t_i. Of course we need to add constraints for continuity (the end values from the previous interval to be the same as the starting values on the next interval). Multiple shooting is only block sparse, but is easy to paralelize and can treat even unstable systems well.

Numerous implementations of numerical optimal control are availible, namely [HFD11]. Houska2011a

Solution

In this section we will apply the theory and methods to our setting and problem (trying to focus on issues, that were not answered in other works).

Our contribution Now, lets emphasize, that other existing works tried to model the problem using discontinuous functions and optimized only the system parameters (for minimial cost) for given power managment strategy or optimized only the the power managment strategy (or decision constants of the said strategy). So lets ask the question:

- How will the perception of the problem change for continuous formulation of equations?
- Will there be a case, when it is not valid to suppose, that for all system parameters the optimal control strategy is still the same?

So our aim will be to optimize the global parameters against the cost (using global optimization algorithms) but for each test case (values of variables) use the methods of optimal control theory to find the best control strategy.

At the end, we will discuss how can we use ideas from other works (for example to switch from Simulated Annealing to Stochastic annealing) or how to use the designed method in practical setting.

In the scope of this work, there will be developed an implementation computing the values for an exact desired setting.

Mathematical formulation

Formulation of the optimal control strategy

Since we are using continuous formulation of equations, we are able to follow the optimal control theory for continuous cases (thats one difference from other works).

Simple model using power We need to rewrite the setting using mathematical formulation - to express the boundary conditions, the state variables $x(t)$, the performance index $J()$, the control function $u(t)$ and the dynamics of the system $f(x, u, t)$ (using notation consistent with the optimal control theory).

Lets express every variable in energy, Joules.

Because we have two state variables - the state of charge of the accumulator $SOC(t)$ and the stored hydrogen $S(t)$. So our state is two dimensional real valued function $x(t) = (x_1(t), x_2(t)) = (SOC(t), S(t))$. Theese quantities are bounded by $SOC(t) \leq SOC_{max}$ and $S(t) \leq S_{max}$, bounds to maximal battery charge and maximal hydrogen stored (in means of power we used to create the hydrogen).

The boundary condition is $P_{src}(t) = P_{in}(t) - P_{demand}(t)$, difference between input power and power demand.

The control function u is a two dimensional function of time and will define the power flow (so its units will be Watts):

- the first component tells us about charging/discharging the battery:

$$(\dot{SOC})(t) = P_{batt}(u_1) - \sigma SOC(t)$$

Using this equation we can model the less than one efficiency by setting $P_{batt}(u_1) = u_1\eta_{batt}$ and the result of auto discharge σ.

- $u_1 > 0$ ... We are charging the battery, using the power u_1. There is a bound, how much power can we give to the battery $u_1 \in [P_{batt+min}, P_{batt+max}]$
- $u_1 = 0$ ... Battery disconnected
- $u_1 < 0$ ... We are discharging the battery, getting the power $-u_1$. There is a bound, how much power can we get from battery $-u_1 \in [P_{batt-min}, P_{batt+-max}]$

- The second component tells us about the flow of hydrogen:

$$(\dot{SOC})(t) = P_{H_2}(u_2)$$

Again, here we can model the efficiency ($P_{H_2}(u_2) = u_2\eta_{H_2}$) and even nonlinear characteristics of the efficiency. Definitely the term will be different for u_2 positive and negative, because this equation models two different devices:

- $u_2 > 0$ ... The electrolyzer is turned on, using the power u_2. There is a bound, how much power it can convert $u_2 \in [P_{H_2+min}, P_{H_2+max}]$
- $u_2 = 0$ ... No change in hydrogen supply
- $u_2 < 0$ ... The fuel cell is turned on, giving us the power $-u_2$. There is a bound, how much power can we get $-u_2 \in [P_{H_2-min}, P_{H_2-max}]$

This design follows the wise rule, that the electrolyzer and fuel cell should not operate simultaneously (because that would be a waste of power). The bounds are for example the technical specifications set by manufacturer.

So, once again and nicely written, the dynamics of our system is:

$$\begin{aligned} \dot{x} &= f(x,u,t) \\ \begin{bmatrix} \dot{SOC}(t) \\ S(t) \end{bmatrix} &= \begin{bmatrix} P_{batt}(u_1) \\ P_{H_2}(u_2) \end{bmatrix} + \begin{bmatrix} -\sigma \cdot SOC(t) \\ 0 \end{bmatrix} \end{aligned}$$

To finish our formulation, we want to find the minimizing control function $u^\star$ (and the corresponding minimizing trajectory $x^\star$ and costate $\lambda^\star$ - will be introduced later) to minimize the performance index

$$J = \phi(x(T),T) + \int_0^T L(x,u,t)\,dt = 0 + \int_0^T |P_{src} - P_{batt} - P_{H_2}|\,dt$$

Thats exactly the (squared) power, we are outputting to the net (or withdrawing from) over selected time interval $[0,T]$. We are not interested in the final value (even not in minimizing any function of the final state) so it is classified as final state free problem.

The Hamiltonian of our system, using $\lambda \in \mathbb{R}^2$ as lagrange multipliers is

$$\begin{aligned} H(x,u,\lambda,t) &= L(x,u,t) + \lambda^T f(x,u,t) \\ &= |P_{src} - P_{batt} - P_{H_2}| + \lambda_1(P_{batt}(u_1) - \sigma \cdot SOC(t)) + \lambda_2 P_{H_2}(u_2) \end{aligned}$$

By the way, because our state equations does not depend on time, our Hamiltonian is constant.

Additionally, in the presence of state constraints $x \in [0, SOC_{max}] \times [0, S_{max}] \iff \{x \in \mathbb{R}^2,\ g(x) \le 0,\ g(x) = -((x_1 - 1/2 SOC_{max})^2 + 1/4 SOC_{max}^2)((x_2 - 1/2 S_{max})^2 + 1/4 S_{max}^2)\}$, we need to define a function $c(x,u) = \nabla g(x) \cdot f(x,u)$

Conditions for minimum Other (necessary) conditions for minimum are: (state equation, costate equation, boundary conditions)

$$\dot{x} = \frac{\partial H}{\partial \lambda} = f \quad \text{...state equation}$$
$$-\dot{\lambda} = \frac{\partial H}{\partial x} = \frac{\partial f^T}{\partial x}\lambda + \frac{\partial L}{\partial x} \quad \text{...costate equation}$$
$$x(t_0) = (0,0) \quad \text{...boundary condition}$$
$$(\phi_x + \psi_x^T \nu - \lambda)^T|_T dx + (\phi_t + \psi_t^T \nu + H)^T|_T dT = 0 \quad \text{...boundary condition prototype}$$
$$\lambda^T|_T dx + H^T|_T dT = 0 \quad \text{...boundary condition in our case}(dT = 0)$$
$$\lambda_i(T) = \frac{\partial \phi}{\partial x_i}(x(T), T)$$
boundary condition for costate (for free final state)
$$\lambda_i(T) = 0 \quad \text{boundary condition for costate in our case}$$

Pontryagin minimum principle Because values of control function are bounded (maybe even discrete for degenerated intervals), we need to use Pontryagin maximum principle (we are dealing with constrained input problem) "the Hamiltonian must be minimized over all admissible u for optimal values of the state and costate." If we had continuous control function, the problem could be tackled by more traditional approach using derivative of Hamiltonian with respect to u.

In other words $H(x^\star, u^\star, \lambda^\star, t) \geq H(x^\star, u, \lambda^\star, t)$ for all admissible u. (We have this instead of the stationary condition $0 = \frac{\partial H}{\partial u} = \frac{\partial L}{\partial u} + \frac{\partial f^T}{\partial u}\lambda$)

In the presence of state constraints, we have (instead of $-\dot{\lambda} = \frac{\partial H}{\partial x} = \frac{\partial f^T}{\partial x}\lambda + \frac{\partial L}{\partial x}$ ...costate equation).

Hamilton Jacobi Bellman The equation for developement of the optimal cost (computed backwards) is

$$\begin{aligned} J^\star(x(T), T) &= \phi(x(T), T) \\ -\frac{\partial J^\star}{\partial t} &= \min_u H(x, u, J_x^\star, t) = \min_u H(x, u, J_x^\star, t) = L(x, u, t) + J_x^\star f(x, u, t) \end{aligned}$$

And to get $u^\star$ using HJB and Minimum principle:

$$u^\star(t, x, \lambda) = \arg\min_u (H(x, u, \lambda, t))\phi(x(T), T)$$

Existence and uniqueness

Numerical approach

Implementation and results

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