Neural Network Based Modeling of Metal-hydride Bed Storages for Small Self-sustaining Energy Supply Systems

M. Stark, G. Krost, *Member, IEEE*, D. Lemken, B. Oberschachtsiek

***Abstract*-- The electrical supply of remotely located objects - such as telecommunication relay stations, alpine huts, or farms and small settlements in developing countries - requires autonomously operated micro-grids, favorably based on renewable energy sources. For decoupling of fluctuating renewables based generation and consumption, energy storage is needed. Hydrogen paths, especially those based on metal-hydride beds, have proven well as long term energy storage in particular for such small supply systems, combining the advantages of low operating pressures and no storage losses. The performance of such metal-hydride bed storages plays an important role in designing and operating the complete energy system; rather, physical modeling of them for simulative system studies is awkward in consequence of the high grade of non-linearity and the multitude of internal parameters to be considered, which are partly unknown. Therefore, neural network based modeling of metal-hydride bed storages was successfully developed and verified, which is described in the present paper.**

***Index Terms*— fuzzy system, hydrogen storage, metal-hydride beds, neural network, renewable energy, self-sufficient power systems**

I. Introduction

Renewable energy sources like wind or photovoltaic provide an eligible possibility for supplying remotely located small scale energy systems without an existing link to the public grid. The fluctuating energy supply of renewable sources however necessitates the decoupling of power generation and consumption by means of long and/or short term energy storage. In this respect, hydrogen represents an interesting option for long term energy storage, in particular in the form of metal-hydride beds; these can arbitrarily be combined with accumulator based short term storage when indicated.

Various principal configurations are supposable for autonomous, decentralized energy systems for which a renewable energy supply offers an opportunity; some of them are for instance:

- remotely located telecommunication base stations (up to 2.5 kW) [1], [2];
- solitary buildings such as alpine huts, summer residences or small farms (up to 5 kW) [3], [4];
- farms and small settlements in developing countries (above 5 kW) [5].

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The cardinal components of such small self-sustained renewable energy based electrical supply systems are shown in Fig. 1.

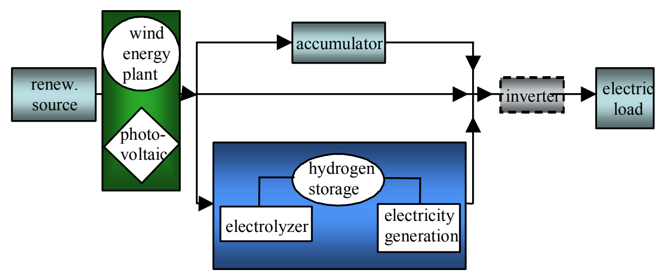

Fig. 1: Self-sufficient electrical power supply structure.

Depending on local conditions such as solar irradiation and wind profiles, available space for allocation, as well as expected load shapes, the proper renewable source is chosen. Small wind generators suitable for the considered applications are commercially available, and photovoltaic panels can be individually composed to arbitrary peak power output.

Since renewables based generation usually does not coincide with load profiles, energy storage is essential. For the adjustment of day/night cycles or load peaks (short term) customary accumulators are an eligible option. Long term storage is needed for bridging calm wind periods, bad weather periods or seasons (winter time for PV); for this purpose hydrogen has proven well as a storage medium. Hydrogen can be produced by electrolyzers which are commercially available; re-conversion to electricity is possible either by means of a combustion engine driven generator set or a fuel cell.

The relatively low energetic efficiencies of devices in the storage paths (estimated at approx. 75 % for the accumulator, approx. 60 % for the electrolyzer and approx. 35 % for electricity re-generation) plays a minor role, especially under the aspect that the generation is renewables based. Furthermore, this and also the relatively high investment cost of such plants are justified by the fact that such small-scale detached electricity supply is only considered if a solid public grid is either completely unavailable or only accessible under disproportionate investment cost, as given in the examples mentioned above.

In order to achieve high utilization and reliability in practical operation and management of such self-sufficient systems, appropriate selection and dimensioning of system components is mandatory. This task however requires knowledge and experience from various domains such as electrical, process and chemical engineering and is therefore complex and time consuming. In this regard a tool is under development which considers knowledge of the previously mentioned domains as well as the characteristics and specifics of available system components, their operational interactions and safety restrictions. The tool comprises three successive steps for the plant layout:

a) component selection by an expert system [6];
b) dimensioning of components by simulation and optimization;
c) development and subsequent verification of an appropriate operation concept, the latter also based on simulation [7].

Obviously, for both proper dimensioning (b) as well as the verification of an appropriate operation and control strategy (c), high fidelity simulation of the entire plant under consideration of realistic load and generation profiles is required. While proper simulation models for most of the devices involved such as wind and solar generation, accumulators, gas engine driven generators etcetera is available from previous work (e.g., [8]), viable physical modeling of metal-hydride bed hydrogen storage is barely available. Reasons for this are the distinct non-linearity, the high number of influencing quantities as well as reluctance of manufacturers to reveal product specific details. Therefore, a *neural network* based metal-hydride bed storage model was developed which was trained with own-made measurements of parameters which are accessible externally; this will be described in the following.

II. Hydrogen storage

Hydrogen is a promising medium for energy storage as it offers several advantages such as

- acceptable volumetric storage density,
- lossless storage (except liquefaction) even under adverse conditions like low temperatures and
- cycle stability.

Different technologies are applicable to hydrogen storage, but only two concepts are interesting for small scale applications:

- storage of gaseous hydrogen in pressure tanks (CGH2, physical method);
- storage of hydrogen in chemically bonded form (metal-hydride storage, chemical method);

For pressurized storage (up to 70 MPa) a compressor is required, the energy demand of which has negative impact on system efficiency. The main advantage of metal-hydride storages is the low filling pressure of less than 3 MPa; in case an electrolyzer is used the operating pressure of which matches the filling pressure of the hydrogen storage, a compressor can completely be spared.

In metal-hydride beds hydrogen atoms are intercalated into interstitial sites and bond in a constant chemical metal-hydrogen compound [9]. The process of the absorption is exothermic and reversible (1):

$$\text{Metal + Hydrogen} \underset{\text{Desorption}}{\overset{\text{Absorption}}{\rightleftarrows}} \text{Metal Hydride + Heat} \qquad (1)$$

Compared to tanks for pressurized and liquefied hydrogen gas, in consequence of the low storage pressure metal-hydride beds are at least adequate with respect to safety. As the absorption reaction is exothermic, for the desorption process heat has to be supplied; in case of leakage the storage will "freeze" and therefore provides further safety. Beyond that, metal-hydride beds offer a higher volumetric energy density than compressed gas; the lower gravimetric density is not relevant for stationary applications regarded here.

Few existing simulation models for metal-hydride storage describe physical emulation, but they are mostly type specific and based on information about the inner geometry of the storage vessels as well as the composition of storage materials [10], [11]; for commercially available metal-hydride storages such information is often kept confidential. Furthermore, for physical modeling the knowledge of the interior temperatures of storage material is mandatory, which cannot be measured. For these reasons the simulation model proposed here is based on a black box approach, using neural networks combined with fuzzy technology. For training purposes of the neural network data sets had to be provided by practical measurements, purely reflecting externally accessible parameters such as

- storage pressure,
- ambient temperature,
- surface temperature of storage vessel,
- loading respectively unloading condition,
- hydrogen flow rate,
- capacity in % by weight and
- time response of load-/ unload process.

III. Experimental setup for hydrogen storage investigation

For the identification of external characteristic properties of metal-hydride vessels – needed for neural network training – an experimental setup has been erected providing the following features:

- operation of low temperature metal-hydride storage tanks;
- hydrogen pressure up to 10 MPa;
- hydrogen flow rates from 0.01 to 20 Nl/min;
- ambient air temperature of tested storage tank adjustable in the range from -20 °C to 70 °C.

In Fig. 2 the test bench is shown schematically. The hydrogen to be absorbed is supplied by a pressurized gas cylinder. The control of mass flow and pressure is achieved by an interaction of mass flow meters and pressure regulators. The temperature control for the ambient air temperature of the test bank is accomplished by a thermostat.

During desorption a pressure reducer decreases the high hydrogen pressure supplied from the storage down to a range typically needed for fuel cells or gas engines (0.02 – 0.3 MPa). The hydrogen flow rate is controlled by mass flow controllers in a range between 0.01 and 10 Nl/min, which is equivalent to a hydrogen power output of 1.8 to 1800 W_{th}.

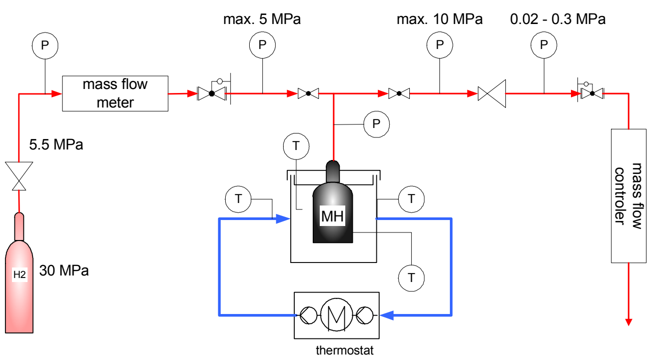

Fig. 2: Schematic of metal-hydride test bench.

Exemplarily some experimental measurement results of a commercially available storage with a reversible storage capacity of about 60 g hydrogen are shown: Fig. 3 exhibits the filling level of the storage. The setting value of the hydrogen flow rate for the *absorption* – loading the storage – was adjusted to 5 Nl/min, the ambient temperature was controlled to be 20°C and the storage was loaded with a filling pressure of 1.6 MPa corresponding to 16 bar.

In the first temporal phase of Fig. 3 the hydrogen flow into the storage vessel matches the pre-set target value. As mentioned before, the absorption is an exothermic process, therefore the temperature of the storage material increases and the internal storage pressure rises. Once the internal storage pressure attains the filling pressure – representing the realistic operation pressure of an electrolyzer – the hydrogen flow into the storage tank collapses. At this point the second phase of the absorption begins. With the same setting values, the storage is filled with a much lower, slightly decreasing hydrogen flow. Due to the reduced flow, the storage temperature decreases as less exothermic energy is released, and more hydrogen can be stored. The internal storage pressure increases slightly until the maximum filling level is reached.

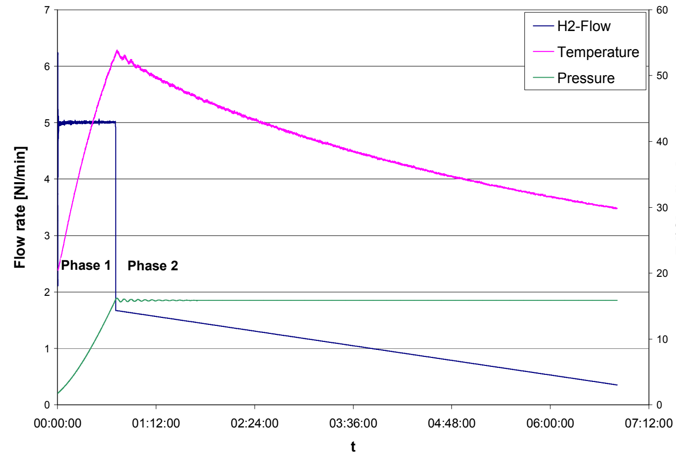

Fig. 3: Absorption with 5 Nl/min (measurement).

The *desorption* process – unloading – is shown in Fig. 4. For this example, again a hydrogen flow rate of 5 Nl/min had been chosen with a cooling bath temperature of 25°C.

The desorption process can be divided into two phases, too. Firstly the storage is emptied with the pre-set hydrogen flow rate. Storage temperature and pressure decrease until a state is reached at which the required flow of hydrogen cannot be released by the storage medium any more. The hydrogen flow collapses, and at this point the second phase begins. Due to the diminished hydrogen flow – which still decreases slightly – the storage temperature rises again: to gain a longer constant hydrogen flow at the setting value, the storage has to be warmed up.

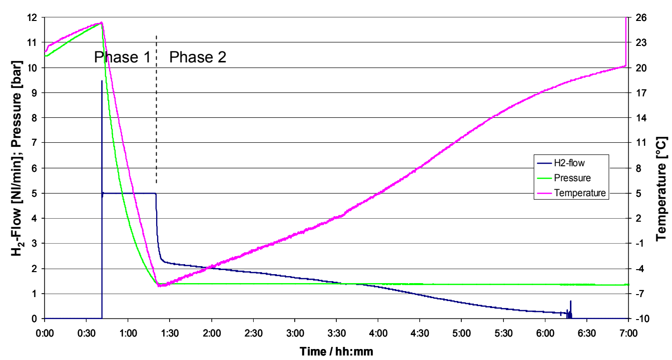

Fig. 4: Desorption with 5 Nl/min (measurement).

It can clearly be seen from Figs. 3 and 4 that both loading and unloading are rather non-linear processes, whereby the inflection points can reasonably be explained by the internal physical and chemical processes [9], [12], [13].

In Fig. 5 absorption measurements with flow rates of 10 Nl/min and 5 Nl/min are comparatively shown. It is evident that the set value for the flow rate of 5 Nl/min can be maintained more than twice the time as for 10 Nl/min in consequence of the slower increase of temperature, which constitutes another non-linear characteristic. In order to gain a longer lasting flow rate at desired value, parallel use of several metal-hydride vessels seems advantageous.

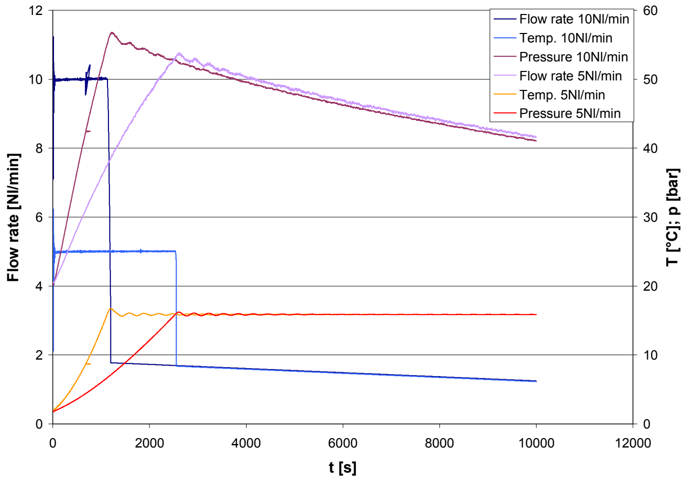

Fig. 5: Absorption at a flow rate of 10 Nl/min and 5 Nl/min (measurement).

Furthermore, in Fig. 6 the influence of different initial filling levels (as examples 68% and 37 %, respectively) of the vessel on the achieved flow rates at given set values is shown. Obviously, the time interval during which the pre-set flow rate can be maintained depends not only on the set flow rate value itself and the storage temperature at the begin of the desorption respectively absorption, but also on the actual filling level of the vessel. Furthermore, the pressure inside the hydrogen vessel depends on the filling level and in its turn influences the ratio between pressure and temperature, by which the begin of the above mentioned second phase of desorption / absorption processes is defined. As both the upper pressure boundary (16 bar, electrolyzer output pressure) and the lower pressure boundary (1.4 bar, to prevent negative pressure inside the vessel) are fixed, the ratio of temperature and pressure cannot be used as state descriptor for the begin of this second phase. Rather, the ratio between temperature and filling level gives information about the begin of the second phase of desorption /absorption. Thus, the initial filling level has also to be considered in the model.

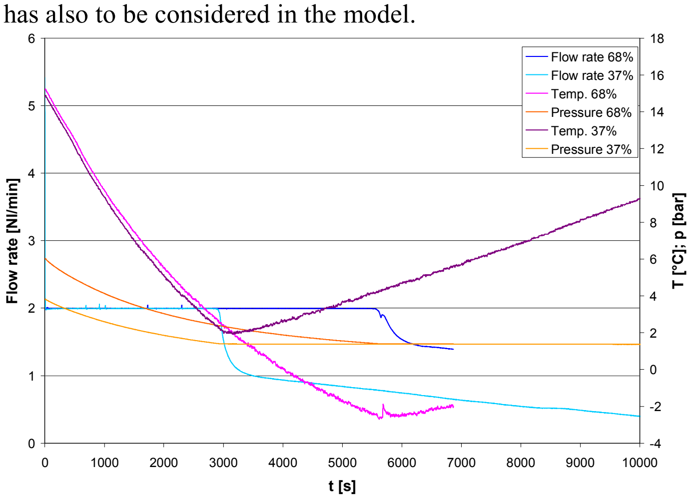

Fig. 6: Flow rates at 68 % and 37 % of filling pressure (measurement).

Similar measurement series as all those shown here have been conducted under varied flow rates, pressures, temperature conditions and initial filling levels, altogether constituting the training sets for the neural network based simulation model described in the following.

IV. Neural Network Based Metal-Hydride Storage Model

Both the high level of non-linearities which turned out in the measurements as shown above, as well as the mentioned unavailability of internal parameter data encouraged to develop a recurrent *neural network* based model for the metal-hydride energy storage; but nevertheless the resulting structure is rather complex.

Since the absorption and desorption processes – loading and unloading – differ significantly, they are considered individually by identically structured, but individually parameterized models, Fig. 7. For each of both processes a cluster of pairs of two separate feed-forward type neural networks with external recurrence loop – representing the two temporal phases of the processes as described before and marked in Figs. 3 and 4 – has been established and trained with relevant measured data sets for desorption of a fully loaded storage, see Fig. 7, upper part; the respective recurrent neural-network pairs within each cluster were trained at different pre-set hydrogen flow rates up to 15 Nl/min. According to the pre-set hydrogen flow rate, the output values of the particular flow-rate related neural-network pairs are non-linearly weighted by means of a fuzzy system, and thus finally lead to the time dependent actual values of hydrogen flow rate and temperature relevant to the pre-set flow rate as schematically shown in Fig. 7, right side.

In a special way the impact of the initial filling level is considered, which determines the transition between temporal phases one and two: the modeling – exemplarily described here for desorption – is based on the trained neural structure for a completely filled hydrogen vessel. By means of the actually given real filling level at desorption begin, from a characteristic diagram the temperature T_X is determined at which the second desorption phase begins, and compared to the actual temperature output value T given by the first phase neural network, see center of Fig. **7**. As long as the first phase neural network is activated, the second phase network is internally bypassed, and the first phase output of temperature and hydrogen flow is directly given to the final output. But when the output temperature of the first phase network attains the value T_X, then the first phase model is triggered to deliver its set of output data as initial values to the recurrent neural model of the second phase, and this is activated. For the hydrogen flow as well as the storage temperature this model provides appropriate results at the final output. The pressure, however, depends on the initial filling level of the vessel, too. For the calculation of the pressure at an arbitrary filling level at desorption begin, weighting of two neural network outputs provides a good solution: one neural structure is trained with the data for completely filled storage as described before, and another one having the same assembly with the data of a nearly empty storage, see lower part of Fig. 7. By non-linear fuzzy evaluation of the output pressures of the two neural structures any initial filling-level dependent pressure developing can be derived.

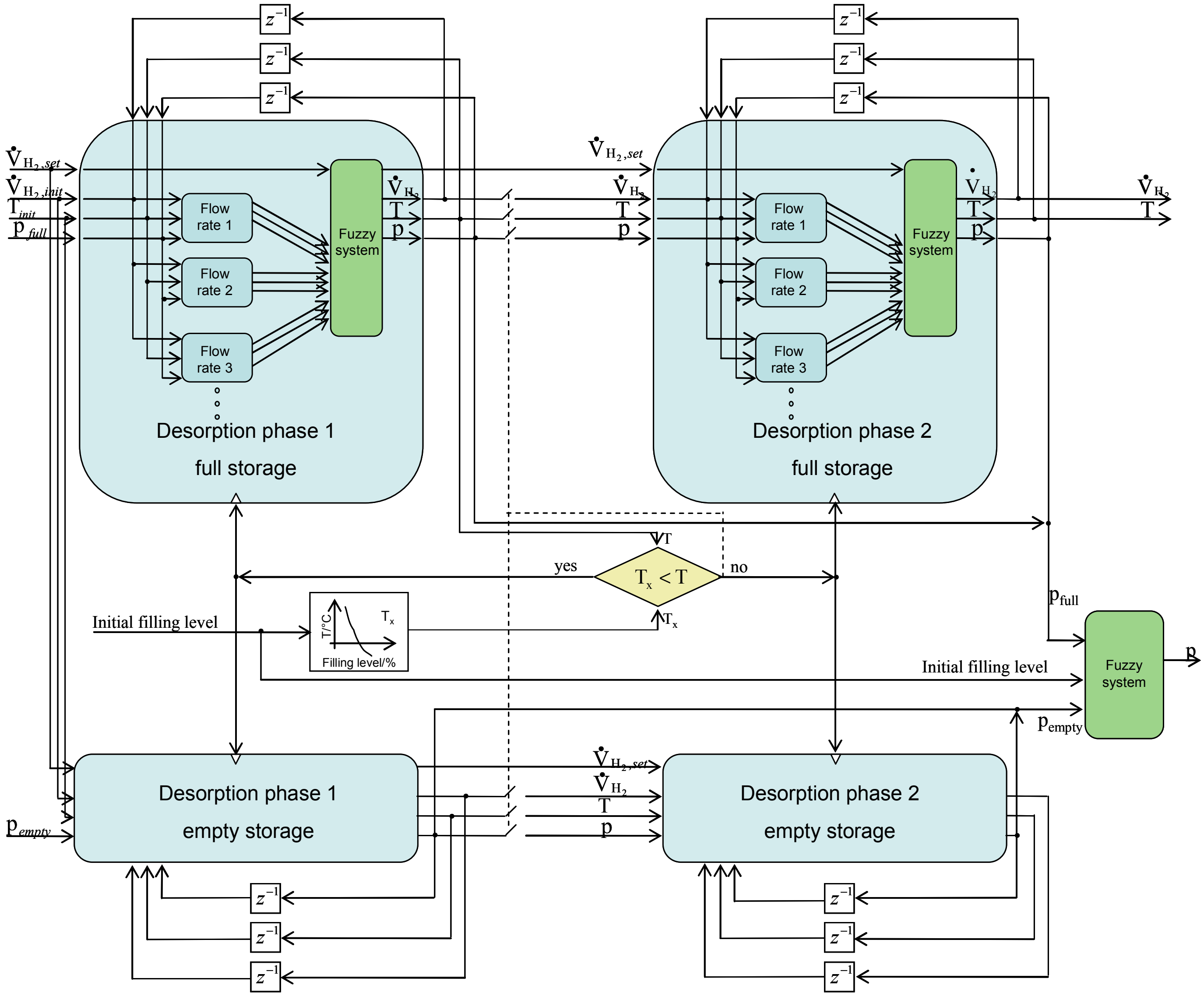

Fig. 7: Recurrent neural network based model of metal-hydride storage desorption; the absorption model has the same structure but different (trained) parameters; the inner structures of neural networks for empty storage (bottom of figure) are identical to those of the full storage as completely shown above.

In total, rather complex and interlaced neural network based structures for both absorption and desorption came into existence as conclusively sketched in Fig. 8; the reasonable performance of them was verified by various test runs as exemplarily shown in the following.

V. Model Verification

Fig. 9 shows the viable results of the neural modeling for an example *absorption* test data set (flow rate of 5 Nl/min, start filling level 10 %) in comparison with corresponding measurement results. The filling pressure was adjusted to 16 bar, thus realistically representing the operation output pressure of an electrolyzer. The blue colored graphs show the hydrogen flow rate, in deep blue the simulation and in light blue the measurement results. The red lines display the temperature profile and the lilac the pressure, respectively.

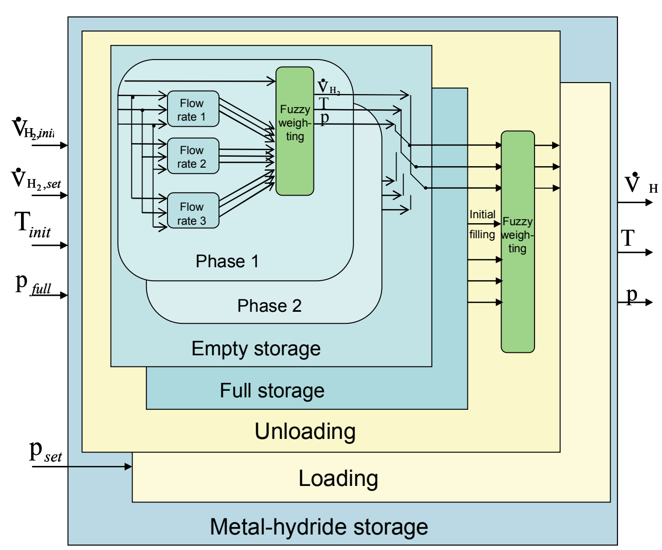

Fig. 8: Sketch of assembly of neural network based storage model.

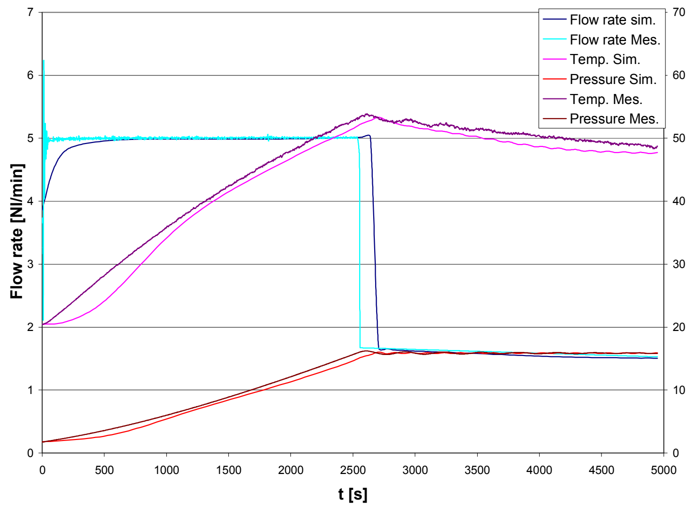

Fig. 9: Comparison of neural network modeling and measurement results at an absorption flow rate of 5 Nl/min.

In a similar way neural network based modeling of *desorption* proves to be sufficiently accurate as shown in Fig. 10 for a pre-set hydrogen flow rate of 5 Nl/min and start filling level of 97 %.

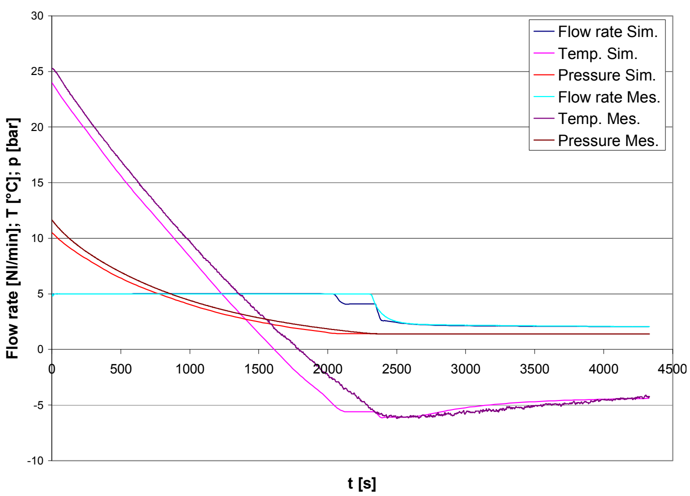

Fig. 10: Comparison of neural network modeling and measurement results at a desorption flow rate of 5 Nl/min.

In contrast to definite almost full/empty start filling conditions as depicted in Figs. 9 and 10, respectively, Fig. 11 shows the desorption results for the neural modeling for an intermediate start filling level of 68 %, a set flow rate of 2 Nl/min, a surface temperature of 15 °C and a filling pressure of 16 bar. In dark blue the simulation flow rate and in light blue the measured flow rate is shown. As it can be seen, also in this intermediate case the simulation results represent the measurements with sufficient accuracy; the same applies to the temperature and pressure profiles. Similar results were achieved for other parameter sets.

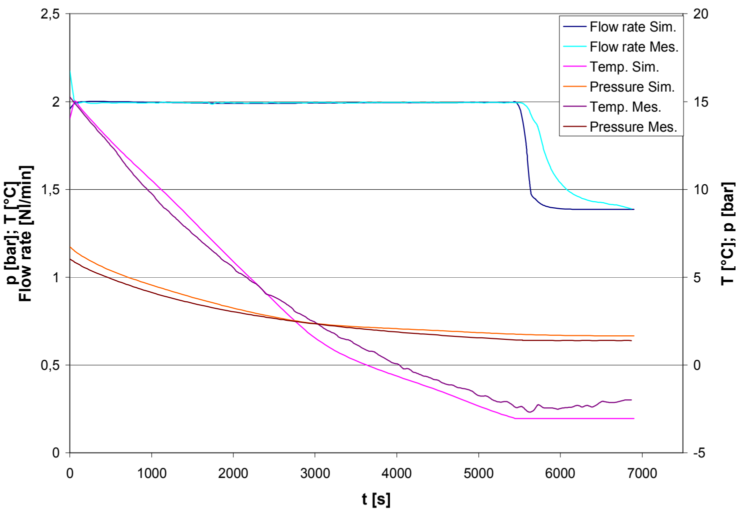

Fig. 11: Comparison of neural network based modeling and measurement results at a desorption rate of 2 Nl/min at a filling level 68 %.

Despite the strong non-linear characteristics of metal-hydride storage performance, and without having any internal data or measurements of the vessel available, evidently the neural network based approach, trained with pure externally measured data sets, provides reasonable modeling accuracy for their proper use in simulating complete self-sufficient small energy systems.

VI. Conclusion and Outlook

Proper design and operation strategy derivation for small self-sustained and renewables based electricity supplies such as for telecommunication bases or remote buildings requires an accurate system simulation. In contrast to available physical models for most constituting components of such systems, an applicable metal-hydride storage model was still missing since the grade of non-linearity is high and too many parameters are unknown or cannot be identified. For this reason, a neural network based modeling approach has been established. It was trained with measurement data of purely externally accessible quantities and delivers eligible accuracy to be applied for simulations in the frame of a tool which will

- facilitate the design of self-sustaining energy systems with reasonable operational performance;
- contribute to the development of new application areas of renewable energies;
- support the launch of fuel cell technology by easing engineering of the hydrogen path at reduced cost.

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