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Dynamic Modelling of a Metal Hydride Reactor During Discharge Through Artificial Neural Network Regression

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INTRODUCTION & AIM

With hydrogen as a clean but hazardous energy carrier, solid-state hydrogen storage in the form of a metal hydride has come forth as a safe and low-pressure storage solution with competitive volumetric energy density. In this technology, hydrogen is stored in a hydride-forming metal, in this study specifically AB5-type metal hydride, through exothermic absorption, which can then be discharged through endothermic desorption. This results in a complex batch system where hydrogen discharge is caused by high-temperature fluid heating the reactor and, by extension, the metal hydride bed. This, in turn, increases the hydrogen pressure of the gas surrounding the metal hydride bed, which is then released through a regulator to achieve the desired pressure of the discharge hydrogen. This discharge dynamic system, as a result, is notoriously hard to model and predict.

In general, hydride-forming metal reactors are modelled using lumped parameter models. In this approach, mass conservation, energy conservation and reaction kinetics are of great importance. Regarding the reaction kinetics, the sorption-chemical reaction isotherms play an important role. Thus, an isotherm model to represent accurate isotherm data is also key.

For the proposed modelling approach, certain simplifications are introduced, including the assumption that the gas acts as an ideal gas, local thermal equilibrium, and adiabatic conditions. Further simplifications can be made, such as constant thermal and physical properties. For this purpose, the finite element method allows these models to be adapted easily to different reactor geometries with accurate results.

Artificial neural networks have been utilised for optimisation, tracking and modelling purposes. More specifically, digital twins are a transformative technology which allows for the accurate prediction and diagnosis of systems. Furthermore, digital twins can be used to enhance the design process as well as increase the lifespan of systems, specifically in the case of energy storage applications

METHOD

Experimental equipment to validate this study was supplied by HySA-Systems under the umbrella of the University of the Western Cape. Figure 1 represents a schematic diagram of the experimental setup filled with $LaNi_{4.9}Sn_{0.1}$ hydride-forming metal. This unit is an industrial unit, used to compress hydrogen, installed at a mine in the Northwest. Thus, tests were then performed at normal operational conditions so as not to disrupt the operation of the mine. For the discharging validation data, the desired gas pressure delivered by the unit was set at around 16 bar on the regulator, and to achieve that, steam of 135 °C to 145 °C was used.

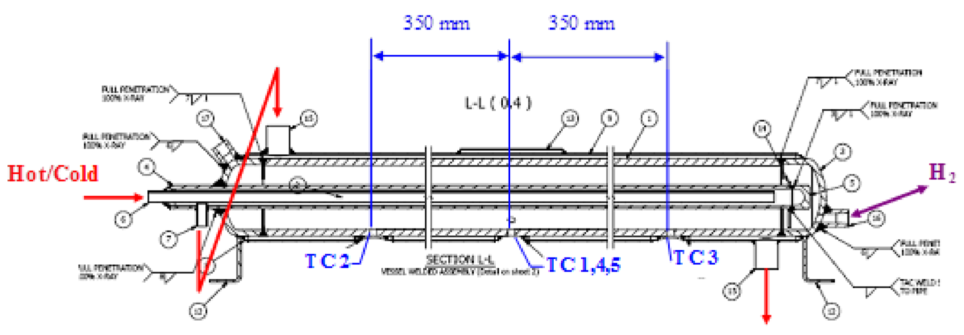

Figure 1: Schematic diagram of a hydride-based hydrogen compressor

For the finite element model, COMSOL Multiphysics was used with an ideal gas assumption. Considering the bed expansion, the assumption was made that 25% volumetric expansion is linearly proportional to concentration. Finally, gas in bed transport was considered to follow Darcy's law and a porous heat transfer model was used. Figure 2 shows the performance of the model.

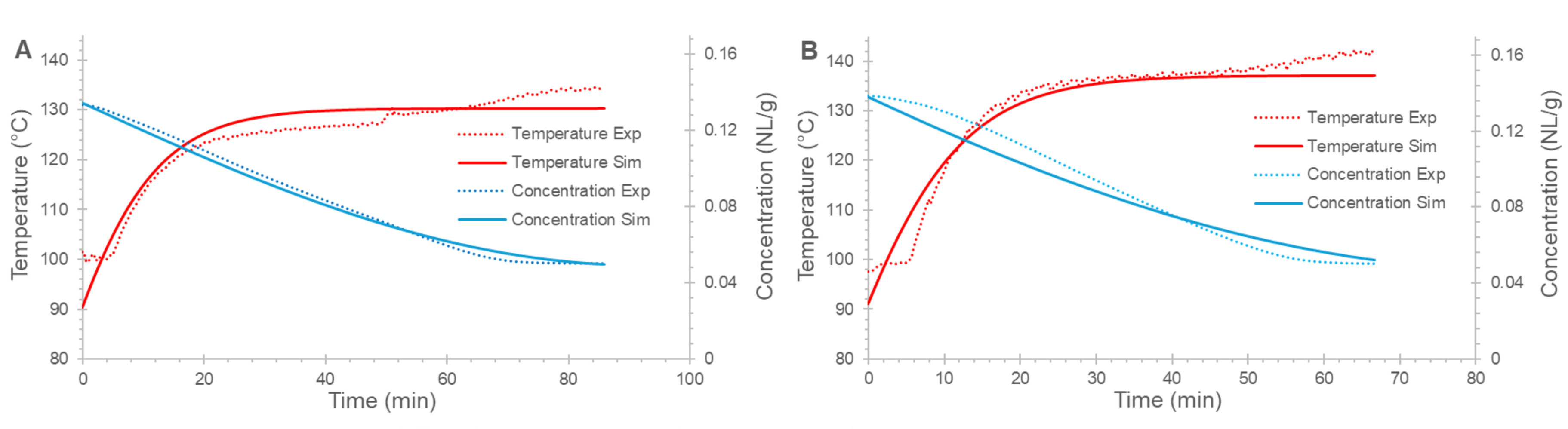

Figure 2: Computational fluid dynamics validation with time versus concentration and temperature with (A) discharge gas pressure at 16.4 bar with heating fluid at 135 °C and (B) discharge gas pressure at 16 bar with heating fluid at 142 °C

This model was then used to generate training data by varying the operational input parameters and measuring the dynamic output. This data was then used to train an artificial neural network using the desired gas pressure, heating fluid temperature, and time as inputs and concentration as the variable the neural network would predict. These neural networks would vary in layer count and hidden neuron count using a ReLU activation and the Levenberg-Marquardt training algorithm. For this, both MathWorks MATLAB and TensorFlow were used with a 70-15-15 Training-Testing-Validation split.

The trained models would then be re-validated against the experimental data, and performance would be analysed in terms of R-squared and mean-squared-error, which can be considered measures of precision and accuracy of the model. Using simulated data to train the neural networks bypassed the need for extensive and expensive experimental trials.

RESULTS & DISCUSSION

Figure 3 shows the final mean squared error of the nine different neural network architectures when evaluated on the experimental data regarding the discharge state. This is a fully connected neural network with one to three hidden layers and 5, 10, or 20 neurons on each hidden layer. While the mean squared error of all nine neural network architectures lies in the same range, the lowest observed mean squared error architecture with the least level of complexity is the two-layer architecture, with ten hidden neurons on each hidden layer. It should, however, be noted that the single-layer architecture is a contender as well, only being beaten by the two-layer architecture at five, then outperforming the two-layer architecture at ten and twenty neurons on each hidden layer.

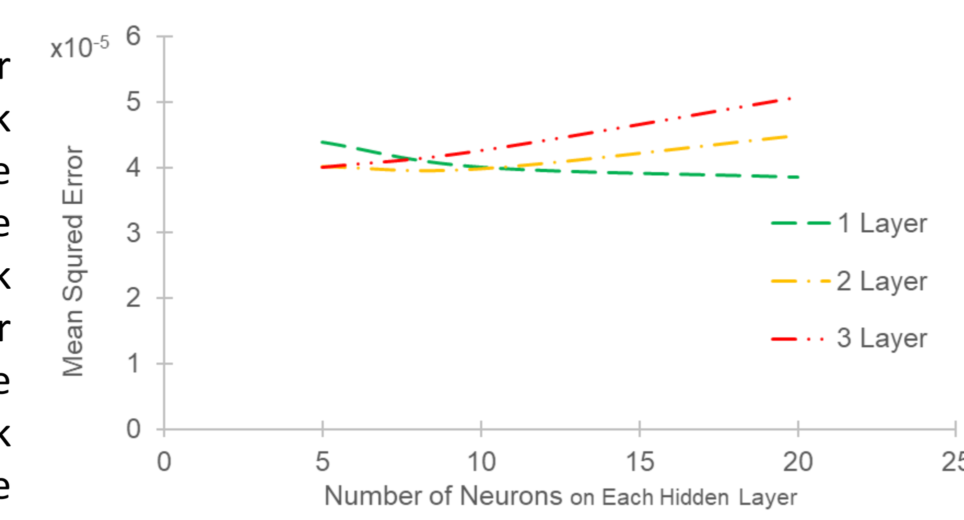

Figure 3: Mean-squared-error performance of the different neural network architectures when tested on the experimental data

Figure 4 represents the R-squared performance of the nine neural network architectures when tested on the experimental data regarding the discharge state. This R-squared is observed during the linear regression of model-predicted values and the experimentally observed values. During this application, this may be referred to as the adjusted R-squared statistic, as it does not measure the fit of the model on the dynamic data but only considers the predicted and observed data. This R-squared statistic measures how closely the model-predicted and experimentally observed data reflect each other; thus, a value closer to one is desired. It can be observed that the three-layer architecture with twenty neurons on each hidden layer has overfitted, performing much worse than the other architectures in this analysis. The rest of the architectures performed equally in this analysis.

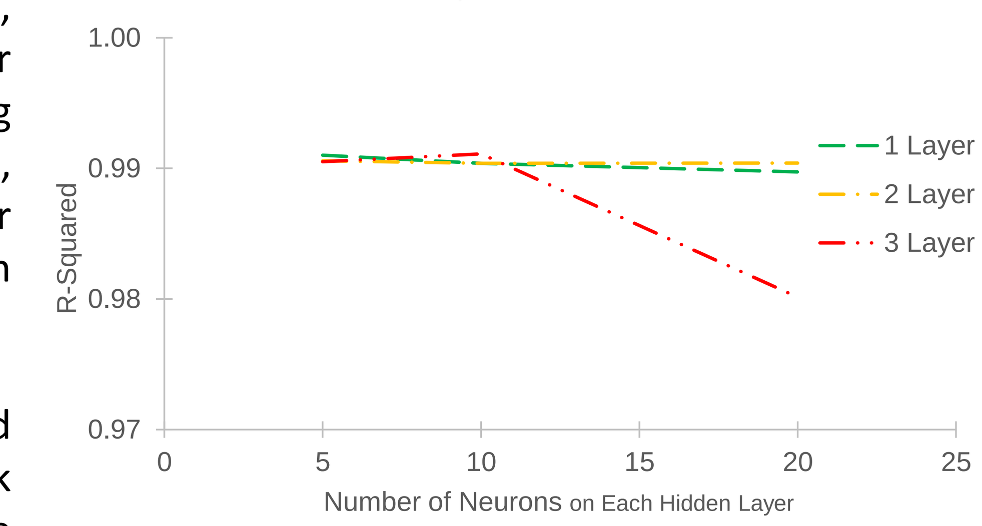

Figure 4: R-squared performance of the different neural network architectures when tested on the experimental data

Figure 5 represents the linear regression of the model-predicted values against the experimentally observed data. Specifically, for the two hidden layers, ten neurons on each hidden layer neural network architecture, which was determined to be the best performing neural network architecture for desorption. The R-squared in this instance was determined to be 0.99039.

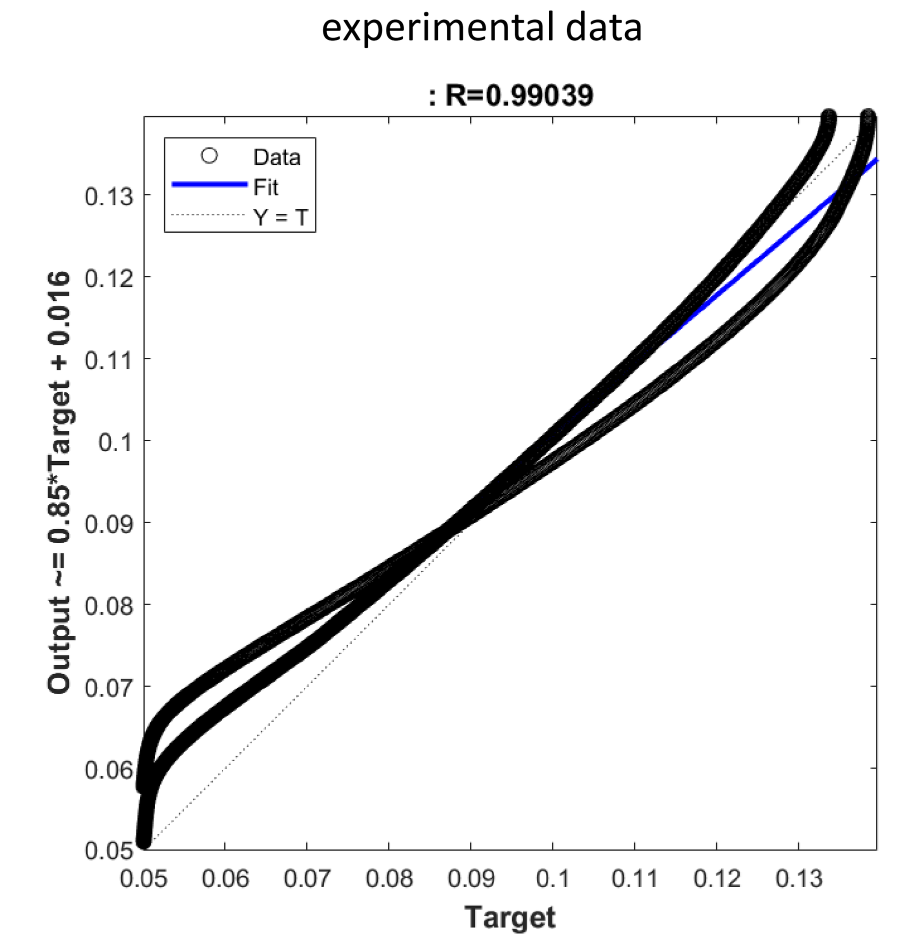

Figure 5: Regression of the two-layer, 10-neurons on each hidden-layer network architecture model predictions against experimental data

The two distinct curves that formed seem to be the two different experimental trials, having differing degrees of accuracy for the whole of the dataset. While within the bounds of accuracy, this indicates the model is not perfect.

CONCLUSION

The best-performing artificial neural network model achieved a regression coefficient of 0.9999 and a mean squared error of less than 10-5 during training. Likewise, the best-performing neural network model validation using the experimentally observed data achieved a regression coefficient of 0.99 and a mean squared error of less than 10-4. This proves that neural networks can model the complexity of metal hydride reactors during discharge, specifically the HySA-systems Metal Hydride reactor prototype.

FUTURE WORK / REFERENCES

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