

Optimization Study of Hydrogen Gas Adsorption on Zig-zag Single-walled Carbon Nanotubes: *The Artificial Neural Network Analysis*

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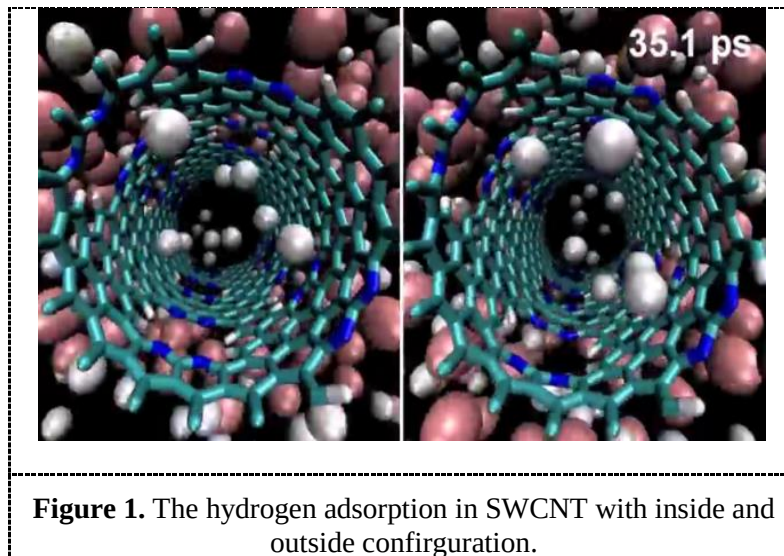
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Abstract. The use of hydrogen gas in fuel cell technology has a huge opportunity to be applied in upcoming vehicle technology. One of the most important problems in fuel cell technology is the hydrogen storage. The adsorption of hydrogen in carbon-based materials attracts a lot of attention because of its reliability. This study investigated the adsorption of hydrogen gas in Single-walled Carbon Nano Tubes (SWCNT) with chirality of (0, 12), (0, 15), and (0, 18) to find the optimum chirality. Artificial Neural Networks (ANN) can be used to predict the hydrogen storage capacity at different pressure and temperature conditions appropriately, using simulated series of data. The Artificial Neural Network is modeled as a predictor of the hydrogen adsorption capacity which provides solutions to some deficiencies in molecular dynamics (MD) simulations. In a previous study, ANN configurations have been developed for 77k, 233k, and 298k temperatures in hydrogen gas storage. To prepare this prediction, ANN is modeled to find out the configurations that exist in the set of training and validation of specified data selection, the distance between data, and the number of neurons that produce the smallest error. This configuration is needed to make an accurate artificial neural network. The configuration of neural network was then applied to this research. The neural network analysis results show that the best configuration of artificial neural network in hydrogen storage is at 233K temperature i.e. on SWCNT with chirality of (0,12).

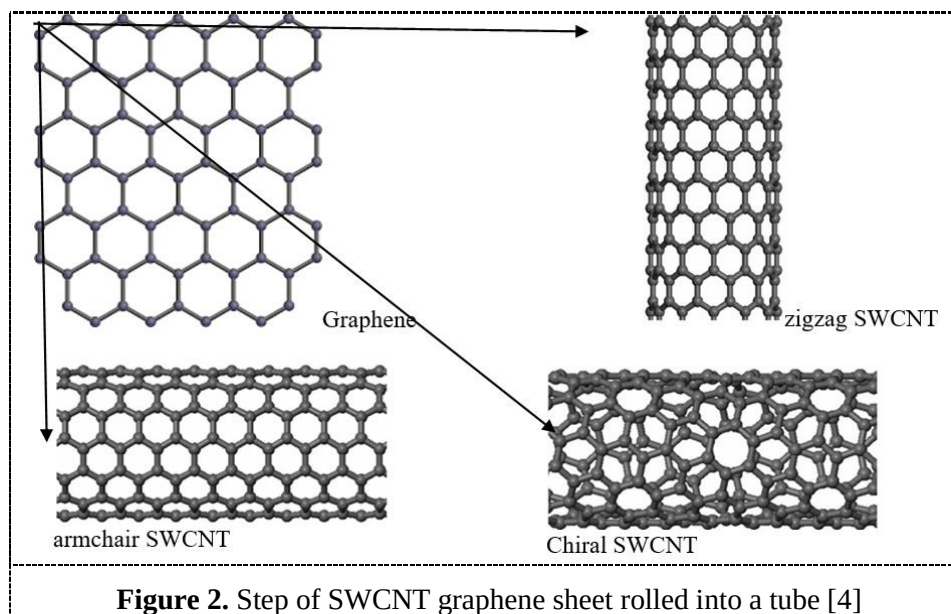
1. Introduction

The most potential energy for future that environmental friendly with massive of quantity in this universe is hydrogen [1]. However, the problem is about how to keep hydrogen gas on storage cover up by single-walled carbon nano tube (SWCNT) as adsorbent [2, 3]. SWCNT is a structure of nano tube with one carbon graphene builder, which is optimum in adsorbed hydrogen with inside and outside of the nano tube as illustrated in Figure 1.





SWCNT rolled by three type rolling method as showed in Figure 2 [4]. It is result a different tube. SWCNT that rolled by zig zag model was selected for this research because more effective to adsorb hydrogen with it peaks form.



With rolling zigzag method, SWCNT, as the adsorbent of hydrogen gas with various chirality or diameter of tube giving difference result on the adsorption capacity [5]. In the figure 1, the molecular dynamic simulation of hydrogen adsorption by SWCNT is showed. Molecular dynamic simulation (MDS) is a simulation method that used for simulating the adsorbed hydrogen by CNT on storage [6, 7]. Actually, the experiment and simulation has conducted an observation of the adsorption hydrogen by SWCNT [3, 8, 9]. And there has shortcoming from both research methods. Then it is cover up by artificial neural network (ANN). Neural network is a tool on MatLab software data apps that one of its function is used for predict hydrogen storage capacity on different pressure condition precisely without conducting simulation [10].

In the previous research, ANN was modeled, as an effort to preparing ANN to be a smart prediction tool that resulting good output. There is a configuration of ANN is needed [11]. So in the previous research neural network configuration was observed [12]. The result is an ANN configuration to predict hydrogen storage capacity called weight percent (wtp) without simulation was found. This configuration is for three variances of hydrogen temperature storage which is 77k, 233k, and 298k resulting difference configuration but with same optimum neuron that is neuron 10 [13]. The configuration of ANN formed with 3 scale range variance for wtp data clarity, 2 type of training set and validation set election variance, and 4 neuron election [14]. The best configuration that is chosen from each temperature is the configuration that resulting wtp value closer to both the experiment and simulation wtp resulted. The configuration that formed shown in Table 1 – Table 3.

Table 1. The error result with scale of 100-1000 and first election variant at temperature 77K.

	(a). Error result of training output			(b). Error result of validation output		
	RMS	CV	R2	RMS	CV	R2
N3	0.140146	2.414148	0.999436	0.338206	6.149633	0.996284
N5	0.140146	2.414148	0.999432	0.318123	5.784464	0.9967209
N7	0.112371	1.935687	0.999635	0.343534	6.246516	0.996686
N10	0.111936	1.928196	0.99964	0.332033	6.037397	0.996374

The focus of attention from Table 1 is the value of coefficient of determination parameter (R2) and the best regression neuron that is neuron 10 i.e 0.999641. Then the graphs of target and validation data are presented in Figure 3.

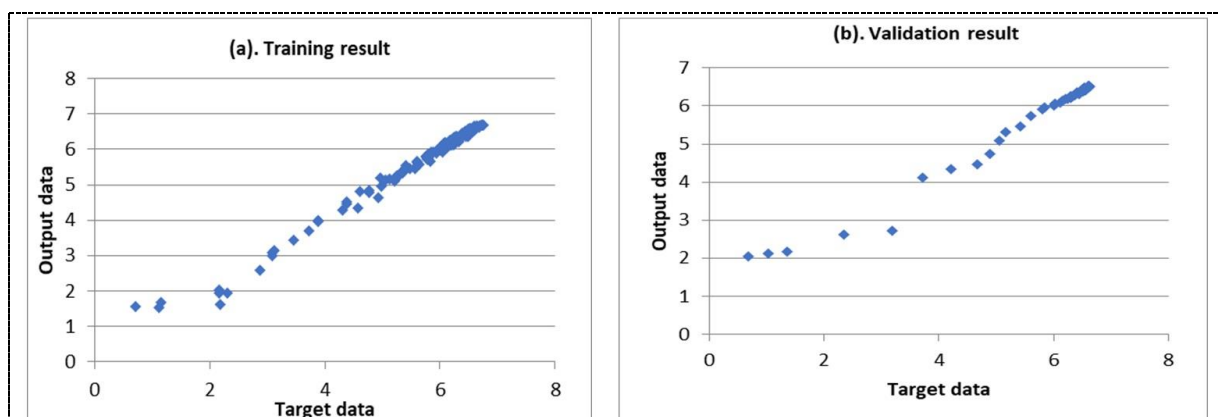


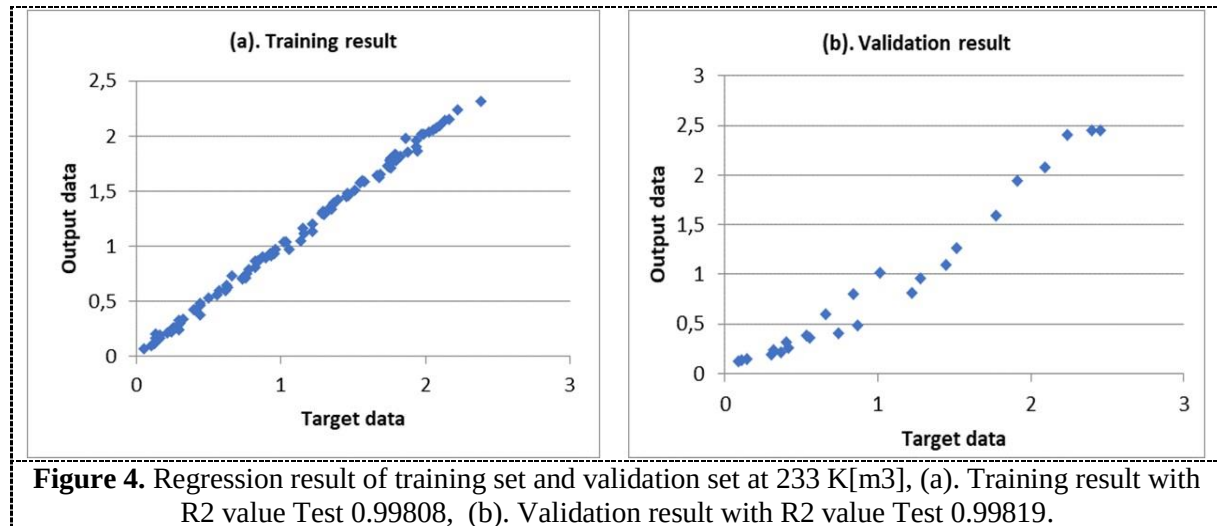
Figure 3. Regression result of training set and validation set at 77K[m3], (a). Training result with R2 value Test 0.9948, (b). Validation result with R2 value Test 0.97903.

The configuration for temperature of 233 K is shown in Table 2.

Table 2. The error result with scale of 100-10000 and first election variant at temperature 233K

	(a). Error result of training output			(b). Error result of validation output		
	RMS	CV	R2	RMS	CV	R2
N5	0.000957422	0.086474	0.998832	0.092853	9.040775	0.994739
N3	0.00375281	0.338953	0.995352	0.157781	15.37459	0.98192
N7	0.000830143	0.074978	0.998985	0.091785	9.814819	0.9949889
N10	0.000534122	0.048242	0.99935	0.190719	18.07104	0.974673

It can be shown in Table 2 the same result as 77 K temperature, that the best regression neuron is neuron 10 configuration. The graphs of target and validation data at temperature 233 K are presented in Figure 4.



The result for temperature 298 K is presented in Table 3 and Figure 5. The result of the best configuration is also neuron 10.

Table 3. The error result with scale of 0-100 and second election variant at temperature 298K.

	(a). Error result of training output			(b). Error result of validation output		
	RMS	CV	R2	RMS	CV	R2
N3	0.055917	6.441731	0.996896	0.077435	8.337538	0.995263
N5	0.036758	4.230856	0.998657	0.066016	6.81065	0.996264
N7	0.030488	3.512508	0.999078	0.036559	3.904285	0.998822
N10	0.026574	3.060571	0.9993	0.120471	13.18335	0.984872

As the previous result from other temperature, on this temperature, neuron 10 showing it best regression where the R square closer to 1 than the other neuron.

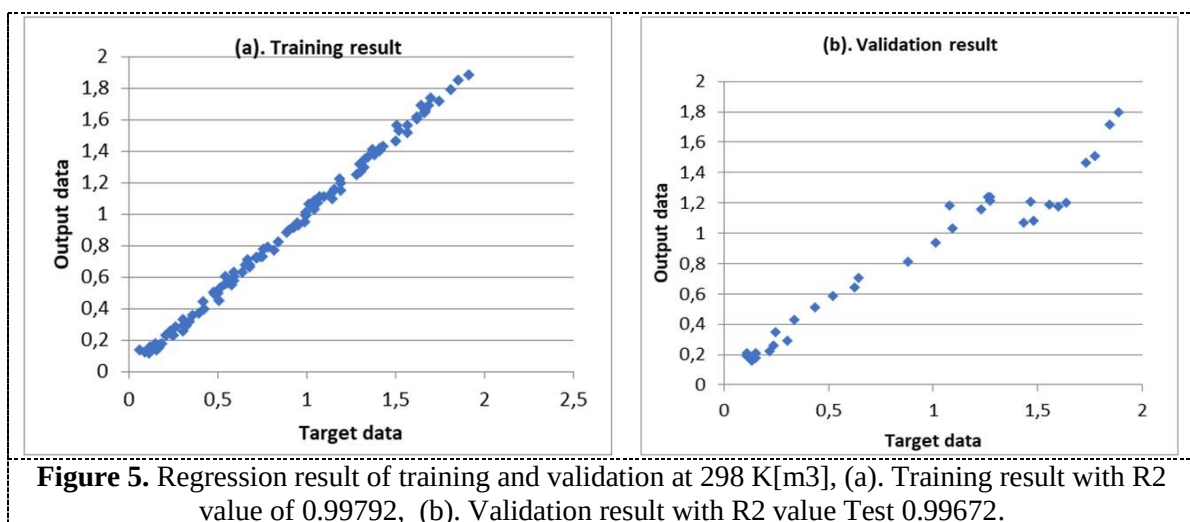


Figure 5. Regression result of training and validation at 298 K[m3], (a). Training result with R2 value of 0.99792, (b). Validation result with R2 value Test 0.99672.

In this research the configuration has been tested to predict wtp for ideal pressure. Hydrogen storage ideal pressure is the pressure that used in hydrogen storage in gas form. The pressure that conditioned to keeping hydrogen gas on storage has range 0-120 bar according to the previous research on hydrogen storage. More than 120 bar is limit closer to compressed tank pressure. It is unsuitable to implement the compressed tank on this purpose vehicle that is light weight vehicle, such as vehicle. Less than 0 bar or closer to -100 bar is the pressure on liquid gas storage. Hydrogen liquid storage absolutely no effective implemented for land transportation like vehicle.

(0,12), (0,15), and (0,18) chirality of SWCNTs were observed to find the optimum chirality to adsorb the hydrogen gas [15]. This chirality has used on previous research finding neural network configuration. And now this configuration is implemented to find the optimum chirality on optimum temperature in hydrogen adsorption.

2. Experimental

2.1. Computation method

With each best neural network configuration for each temperature, the testing method is used. On the three variances of temperature and chirality that used in the previous research that is temperature 77K, 233K, and 298K with (0,12), (0,15), and (0,18) chirality of SWCNT[16]. The required pressure is inputted with range 0-120 bar, the approachment of wtp resulted is analogically [15]. Data is grouped according with neural network characteristic.

2.2. Training ANN on MatLab

After the data has grouped, the process is training on MatLab with neural network tools. It is applied for each chirality on each temperature. For the final step is analyzing the optimum chirality on the optimum temperature consider from wtp resulted from the pressures inputted equally for dependent variables.

3. Result and Discussion

On chirality (0,12) that showing by Figure 6 (a), conditioning storage with temperature 77K wtp value going to be constant after pressure given more than 50 bar and increasing on the pressure more than 140 bar. Meanwhile, on temperature of 233K, wtp value going steadily increases according to the increasing of pressure value. And on 298K, the wtp is going to be constant after given pressure more than 10 bar.

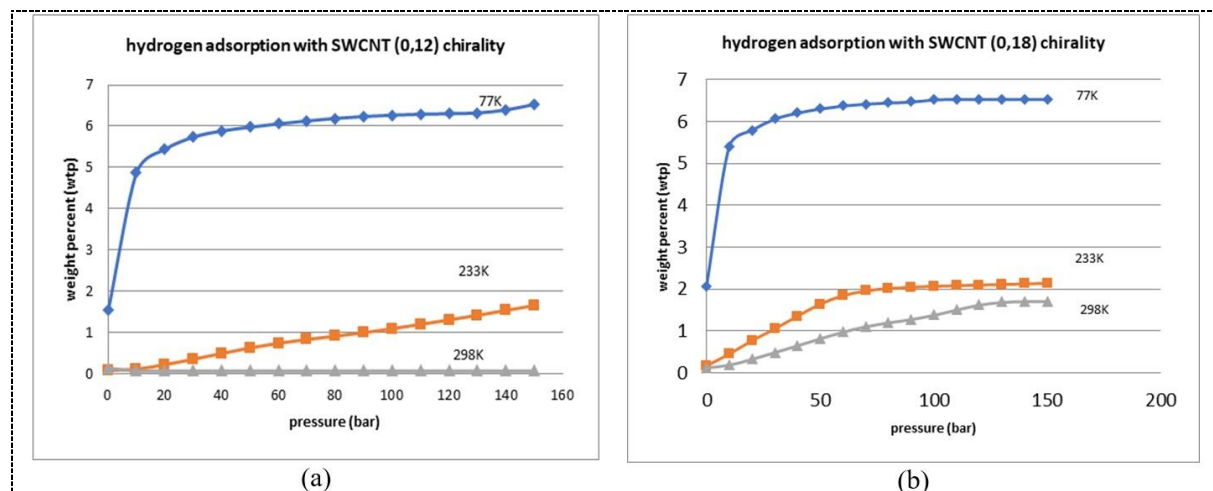


Figure 6. Weight percent (wtp) value with SWCNT; (a). (0,12) chirality, (b). (0, 18) chirality.

Figure 6 (b) shows graphic formed by chirality (0,15), conditioning storage with temperature 77K giving the wtp value highest than given by chirality (0,12). The weight percent (wtp) value chirality (0,15) on the pressure more than 30 bar has getting wtp more than 6, while the wtp on chirality (0,12) getting wtp value more than 6 on the pressure more than 70 bar. Then on temperature 233K wtp value is going constant on the pressure more than 100 bar. And on 298K, the wtp is going increase with a bit difference.

The last is graphic resulted by chirality (0,18) on Figure 8 showing that conditioning storage with temperature 77K, wtp 6 has got on pressure just more than 20 bar, it is easier to got then on chirality (0,15). Then on temperature 233K wtp value is going constant on the pressure more than 60 bar. And on 298K, same graphic on chirality (0,15) is resulted on chirality (0,18) too, the wtp is going to increase with a bit difference.

The results shown in Figure 6-8 are obtained from molecular dynamics simulations using the LAMMPS program developed by the Department of Energy (DoE) United States [7, 17, 18]. For setting the molecule in initial condition used packmol program [19].

4. Conclusion

Conditioning storage on 77K resulting wtp value that higher than other temperature. From Figure 6, Figure 7, and Figure 8 showing that conditioning storage with temperature 77K as increasing the chirality so the wtp value is easy to get with low pressure. In conclusion the recommended temperature and chirality that optimum to adsorb hydrogen from this observation is use SWCNT chirality 18 with storage temperature on 77K. Regression result of training set and validation set at 298 K[N3], (a). Training result with R^2 value Test 0.99792, (b). Validation result with R^2 value Test 0.99672.

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