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Optimization of Electrical Parameters for Production of Carbon Nanotubes in Arc Discharge Technique

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Abstract: Through extensive research for >2 decades on the production of Carbon Nanotubes (CNT) and optimization of its manufacture for the industrial applications, it is believed that they are the strong enough but most flexible materials known to humankind. It is known that carbon nanotubes could behave as the ultimate 1-dimensional material with remarkable mechanical properties. Moreover, carbon nanotubes exhibit strong electrical and thermal conducting properties. In the process of optimizing the production in line with the industrial application, the researchers have found a new material to act as an anode, i.e., coal which is inexpensive as compared to graphite. The production of carbon nanotubes in large quantities is possible with inexpensive coal as the starting carbon source by the Arc Discharge Technique. It is found that a large amount of carbon nanotubes of good quality can be obtained in the cathode deposits in which carbon nanotubes are present in nest-like bundles. This study primarily concentrates on the optimising such parameters related to the mass production of the product. It has been reviewed by the past researchers that through the process optimization, one of the main variables had been the electrical parameters. It has been shown in this study, through simplex process that based on the cost of the SWNT obtained by the Arc Discharge Technique, the voltage and the current should lie in the range of 30-42 V and 49-66 A, respectively. Any combination above the given values will lead to a power consumption cost beyond the final product cost in turn leading to infeasibility of the process.

Key words: Coal, carbon nanotubes, SWCNT, simplex, optimisation, India

INTRODUCTION

In 1985, Drexler proposed a molecular bearing consisting of two graphitic nanotubes of different diameter which are concentrically arranged. It was a virtual operation inside a computer. This dream, however has become more realistic by the discovery of carbon nanotubes. There had been revolutionizing researches on the production of carbon nanotubes from last 20 years and optimising its manufacture for the industrial applications. It has been thought that they are the strongest but most agile materials known to humankind and thus have potential to take part in new nanofabricated materials as additives. It has been shown that carbon nanotubes could behave as the ultimate 1-dimensional material with remarkable mechanical properties. Carbon nanotubes exhibit strong electrical and thermal conducting properties. Study of the past researches on the production of carbon nanotubes from coal revealed that most of the researches concentrate on producing CNT by arcing electrodes, produced separately by mixing the crushed coal with coal tar followed by molding process. However, the only process till date that has shown a positive adaptation to direct coal application is thermal plasma jet technique.

With the extensive research in the production of the carbon nanotubes, the requirement of optimising the process parameters are realised. This study concentrates on the optimising such parameters related to the mass production of the product. It has been found through calculation that the only determining parameter in the Arc Discharge Technique is the power of the equipment in terms of voltage and current and it is shown that on optimisation of these parameters, the cost of the process reduces drastically.

CNT PRODUCTION THROUGH ARC DISCHARGE TECHNIQUE

Carbon Nanotubes (CNTs) have been used in various fields of research due to their unique properties. There are various methods such as arc discharge, laser

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ablation, Chemical Vapour Deposition (CVD), template-directed synthesis and the use of the growth of CNTs in the presence of catalyst particles (Tsai *et al*., 2008). Special ambient gas is required for the fabrication of CNTs in order to prevent the oxidation of carbon at high temperature.

The production of carbon nanotubes in large quantities and other nanomaterials as by-products is possible with inexpensive coal as the starting carbon source by the Arc Discharge Technique (Qiu *et al*., 2002, 2003). It has been found that a large amount of carbon nanotubes of good quality can be obtained in the cathode deposits in which carbon nanotubes are present in nest like bundles. In the past decades, various alternate synthesis strategies and methods have been explored and developed in the hope of mass-producing cheap and high quality Single-Walled Carbon Nanotubes (SWNT). Compared to other methods, the Arc Discharge is the simplest, cheapest and easy to implement and it has been used because of its potential merits to make a massive production. The mineral matter in raw coals may also play an important part in the formation process of carbon nanotubes.

An approach of production of Single-Walled Carbon Nanotubes (SWNT) had been adopted (Qiu *et al*., 2004) where the coal is crushed and sieved with 150 μm mesh and mixed with coal tar and molded to form coal rods used for anode with a graphite cathode for the arc discharge process. Similar approach had been made by the same researchers for the production of Double-Walled Carbon Nanotubes (DWNTs) which were synthesized from coal in large quantity by Arc Discharge Method in hydrogen-free atmosphere (Qiu *et al*., 2007) and was systematically examined using scanning electron microscopy, transmission electron microscopy, high-resolution transmission electron microscopy and raman spectroscopy. In the case of coal-derived carbons, the breaking-up scheme involved in the Arc Discharge process significantly differs from that of graphite because of the striking difference in their textures. Coal or coal-derived carbons feature macromolecular structures rather than the lattice structure of graphite. In their chemical structures, there exist many weak binding linkages between carbon polymeric units such as polymerized aryl structures. In the fast paralyses process under arc plasma conditions, these weak linkages would be broken up rather easily to release a variety of reactive fragments of hydrocarbon molecules such as alkynes and aromatic species. However, the production of SWNTs has seen a typical use of an iron wire mesh utilised between the electrodes and the carbonaceous matter is found on the wire mesh.

A possibility of the production of carbon nanotubes from heavy hydrocarbon resources had been proposed (Kidena *et al*., 2008). Before the use of heavy hydrocarbons, pure compound, toluene was used as the pure substrate to establish the reaction system for the production of carbon nanotubes. Toluene was fed by a mist-spray feeding system with a carrier gas as 9:1 mixture of nitrogen and hydrogen at 100 mL min^{-1} and following the reaction at 750°C catalysed by 9.8% (by weight) ferrocene, carbon nanotubes were found in the carbonaceous product deposited on inner wall of a quartz tube and at the exit of the tube. The product was observed by scanning electron microscopy and analyzed by temperature-programmed oxidation experiments to identify the presence of carbon nanotubes. Based on the reaction system and reaction conditions with toluene, the production of nanotubes was examined by using heavy hydrocarbons such as asphaltene and maltene fractions from natural asphalt. Under selected reaction conditions including the reaction temperature and the amount of the catalyst, carbon nanotubes with a diameter of 30-60 nm were found.

OPTIMISATION OF VOLTAGE AND CURRENT USED IN THE CARBON NANOTUBE PRODUCTION

It is known that voltage and current constitute the power requirements for an electrically operated machine. Same in the case of the production of CNT from the Arc Discharge Method, the electrical power signifies the characteristics of the arc that is generated between the two electrodes in this case, one coal-based and the other, graphite. For the optimisation process, the total cost of the input materials must be lesser than that of the output product.

It is seen from the past experimental research (Yu *et al*., 2003; Williams *et al*., 1999), the research done on Bituminous and Anthracite coal samples. From the domestic coal, cost fixed by Coal India Ltd., the coal costs are as shown in Table 1.

Table 1: Basic price of run of mine non-long-flame non-coking coal (In Rs. ton^{-1})

Field/Co.	A	B	C	D	E	F	G
ECL	3690	3590	1680	1350	1010	790	560
ECL/Mugma	3690	3590	1950	1610	1290	960	620
ECL/Rajmahal	-	-	-	-	1330	1130	910
BCCL	3690	3590	1630	1350	1080	860	610
CCL	3690	3590	1590	1300	1030	820	590
NCL	3690	3590	1430	1200	960	750	560
SECL	3690	3590	1370	1140	950	740	560
MCL	3690	3590	1370	1140	950	740	560

A = Graphite/High quality Anthracite, B = Anthracite (C:H>30), C = Anthracite (C:H~26-30), D = Semi-anthracite, E = Semi-bituminous, F = Bituminous, G = Low quality Bituminous

For Anthracite and Bituminous coal, researchers choose Grade B and F, respectively (Krishnan, 1940). Therefore, the cost would be \$72 and \$23 ton^{-1}, respectively if researchers take the maximum cost of the above grades from different companies.

The coal-based electrode specifications for the Arc Discharge Process are found from the experimental research in the past. With the aim of the maximum cost involved in the production of the coal-based electrode, the electrode with maximum volume is selected as it is the electrode that involves the maximum amount of coal and thus the cost. Out of the several independent researches the specification of diameter 10 mm and length 200 mm is chosen as it gives the maximum volume as compared to the other electrodes in the other researches.

Therefore, electrode volume = $\pi/m\ d^2 \times l = \pi/4 \times 10^2 \times 200 = 15707\ mm^3 = 1.57 \times 10^{-5}\ m^2$. Bank density of coal is 1346 kg m^{-3}. So, bank weight of the powdered coal used = $1.57 \times 10^{-3} \times 1346 = 0.021$ kg. Maximum cost of the coal is taken to be \$0.07 kg^{-1}. Therefore, cost of the coal used 0.07×0.021 = \$ 0.0014. The cost of power is to be calculated next. In a typical experiment (Williams *et al*., 1999), the current was taken to be 100 A and the voltage was taken to be 36 V. Therefore, Power = $V \times l = 30 \times 100$ = 3000 W = 3 kW. The rate of anode feed in the experiment is taken to be 10 mm for 2 h. The length of the electrode in the experiment is 75 mm. So, the total experiment time equals 15 h. For that time, the 45 units of electricity is consumed (1 kWh = 1 unit of consumed electricity). As per the regulations of Calcutta Electricity Supply Corporation (CESC), the rate in the corresponding dollar values are \$0.054 $unit^{-1}$ for the 1st 25 units consumed then at the rate of \$0.066 $unit^{-1}$ for the next 35 units. Therefore, Total cost = $25 \times 0.054 + 20 \times 0.066$ = \$2.67.

So the total input cost for the production of CNT is \$2.67 (neglecting the cost of coal as too small as compared to the power consumption cost). Now, the cost of the carbon nanotubes as per standards shown in Table 2. The amount of CNT produced in experiment is about 20 mg (Williams *et al*., 1999). Thus, the total cost comes to be $20/1000 \times 83$ = \$1.66 Therefore, it can be understood that as the input cost is greater than the output cost, optimisation is essential in this case.

Optimising the power:

$$\text{Power} = V \times l$$

$$\log p = \log V + \log l$$

$$\text{Taking, } \log P = x_1;\ \log V = x_2;\ \log I = x_3$$

In all the experiments, minimum voltage and current are taken as 30 V and 50 A, respectively:

$$V \geq 30,\ L \geq 50,\ \log V \geq 147,\ \log l \geq 1.69$$

$$x_2 \geq 1.17,\ x_3 \geq 1.69,\ x_1 = x_2 + x_3,\ x_2 \geq 1.47,\ x_3 \geq 1.69$$

Considering the power consumption rate as \$0.054 $unit^{-1}$. The total power can be calculated as:

$$15 \times 2.7 \times P = 0.81P$$

For optimum result:

$$0.81P \leq 1.66$$

$$P \leq 1.66/0.81 = 2.05\ kW = 2050\ W$$

$$\log P \leq 3.31,\ x_1 \leq 3.31$$

Applying simplex algorithm:

$$\text{Min } x_1 = x_2 + x_3$$

Subjected to the constraints:

$$x_2 + x_3 \leq 3.31,\ x_2 \geq 1.47,\ x_3 \geq 1.69$$

Solving it by graphical method is shown in Fig. 1. Researchers in Fig. 1 take equalities for the above constraints:

$$x_2 + x_3 = 3.31,\ x_2 = 1.47,\ x_3 = 1.69$$

The arrows shown on the particular line denoted the lesser than equal to and greater than equal to zone for the particular constraint line. The area enclosed by the three constraint lines gives the range of feasibility of the variables. Therefore, researcher can conclude that the enclosed region with the three lines, fit the feasible

Table 2: Carbon nanotube price list (All costs in \$)

	SWNT			MWNT (Diameter in mm)					
Package (g)	High purity*	Arc CNT*	DWNT (High purity*)	<10	10-20	10-30	20-40	40-60	60-100
1	210	83	210	75	40	28	28	28	28
10	1600	700	1600	600	300	190	190	190	190
50	6850	3050	6850	2200	1300	700	700	700	700
100	12400	5500	12400	3300	2000	930	930	930	930
500	Call	Call	Call	10000	6700	3000	3000	3000	3000
1000	Call	Call	Call	10000	8800	4000	4000	4000	4000*

*The high purity CNT (>90% pure) is not achievable by Arc Discharge Method as per different researches and thus the cost of the Arc CNT, made from Arc Discharge Method is always less than the former. However, DWNTs are not the common by-product from the Arc Discharge Method; Tsai *et al.* (2008)

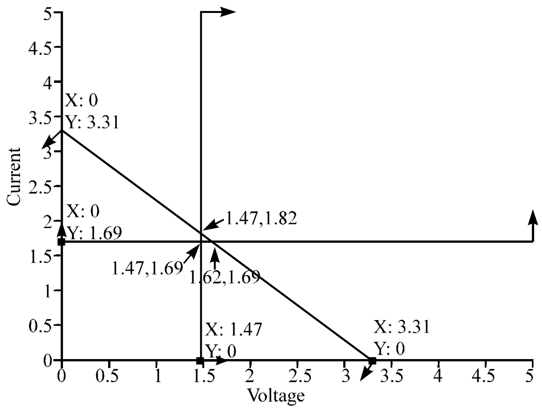

Fig. 1: Solution graph of simplex optimisation process

solution range (Max x_2 = 1.62, Max x_3 = 1.82). The optimal range of the voltage and current can be defined as (by antilog of the results obtained):

$$V = 29.5\sim 41.68\ V,\ I = 48.97\sim 66.07\ A$$

CONCLUSION

An optimisation of the main process parameters, i.e., voltage and current, pertaining to the arc discharge process discussed in the study. The result focuses on the feasible and optimum range of the parameters, based on the cost of the SWNT obtained as the product. It can be certainly perceived through calculation that if the voltage or the current cross the optimal range, the power consumption is increased and thus, the input cost is aggravated resulting in infeasibility of the production line. However, still more scopes remain as the major assumptions viz., the cost of power consumption is only confined to the unit power consumption cost fixed by CESC can be made universal by programming the algorithm mentioned before and a detailed analysis of the optimization by various other processes may lead to many valuable information in this virgin field.

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