Economic and Environmental Tradeoffs in SWNT Production

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ABSTRACT

Assessment of economic and environmental attributes of nanomanufacturing during process development has significant potential to contribute to the quality and effectiveness of the processes, and will lead to development of competitive, safe and environmentally responsible manufacturing technologies. An economic comparison of Arc Ablation, CVD and HiPco processes was undertaken by developing cost models for each of these processes. Results revealed that HiPco is most economically viable for bulk production of pure single-walled carbon nanotubes, and cost drivers are identified to further reduce processing costs. Analyses using life cycle software indicate while HiPco shows the lowest costs, it also creates the highest environmental burden for the input parameters assumed. Since no data are yet available for environmental or health impacts of SWNTs, the results from this analysis can only indicate the impact of resource and energy use during processing.

Keywords: SWNT, nanotubes, economic, environmental

1 INTRODUCTION

Carbon nanotubes (CNTs) show extraordinary properties suitable for numerous applications. With a myriad of applications, the market size for nanotubes will be enormous in the next few decades. The CNT market is now valued at slightly less than $8 million, but is projected to grow $230 million by 2006. CNT production technologies for high volumes are under development, and there is evidence that low-scale production has already begun to serve niche markets. While the technological aspects of development are critical, economic and environmental aspects must also be evaluated comprehensively.

Currently research grade nanotubes are sold for research purposes and the overall production capacity is around 10-20 kg per year in United States [1]. By understanding the economic drivers for CNT production, researchers and system developers optimize manufacturing conditions and work towards the most economically viable process. This intersection of technical and economic performance is vital for the successful commercialization of new materials. Further, inclusion of the environmental performance as part of the “triple bottom line” is of significance to create a sustainable production system. While environmental compliance and performance are important factors in deciding which materials to utilize, cost often remains the bottom line.

However, potential consequences of manufactured nanomaterials on public health have become an issue of notable concern. In recent preliminary studies [2-3], researchers reported that single-walled carbon nanotubes (SWNTs) appear to damage lung tissue in mice. The researchers cautioned that more work is essential to fully understand the observed responses. Inhalation was the primary exposure route for classic small particles, but ingestion and dermal exposure could occur as possible routes, although there is little information on the effects of dermal contact. Another concern is bioaccumulation of nanoparticles. Although one of the potential positive implications of manufactured nanoparticles for the medical field is the ability of these particles to pass through cell walls, the consequences of implementation are unknown.

The threat of these “unknowns” has stirred controversy in the development of nanotechnology. An apprehensive public can be fueled either by promises of fantastic technology or by possibilities of doom, such as that envisaged by Bill Joy [4] where the world is dominated by superintelligent machines that achieve world domination. Dr. Vicki Colvin, Director of the Center for Biological and Environmental Technology at Rice University (an NSF-sponsored NSEC), has been offering a message of caution on both sides, and suggests that after technical information is in hand, better decisions can be made about technology development [5].

To boost the odds of nanotechnology’s long-term commercial success and public acceptance [6], the nanotechnology research community is proactive in exploring and assessing the environmental effects and potential risks. The research results presented here address this need.

The process based technical cost models developed through our research are used to calculate total cost of producing pure single wall carbon nanotubes (SWNTs) and do not incorporate the application of tubes in final products.

The models allow changes to base case assumptions to determine the cost driving process parameters, and further, are used to track life cycle inventories for environmental assessments. The results from these models are used to compare economics of competing technologies existing today i.e., Arc Ablation, Chemical Vapor Deposition (CVD), and High Pressure carbon monoxide (HiPco) processes. Selected results of the comparative environmental attributes of each process are also reported for specific base assumptions.

2 ECONOMIC COMPARISON

For all processes investigated, there are four process steps: synthesis, purification, inspection, and packaging. Purification (to separate SWNTs from other by-products) was assumed to include dispersion, sonification, and filtration without neutralization or rinse.

Economic analysis was undertaken using process based technical cost models that were developed for each process [7]. The models were developed based on scale-up from laboratory processes to high rate manufacturing. Since HiPco processes are proprietary, process assumptions were made based on available published literature. Development and use of processed based models allowed the ability to perform sensitivity analyses on different input assumptions to determine the extent to which each assumption affects the manufacturing cost.

For the base case arc process, during synthesis it is assumed that 4.5 % of the input carbon is converted to product for further processing, which resulted in a cost of \$2332/g of SWNT. In a best case scenario, 10% (or 20%) could be converted. The quantity of SWNTs in that product is assumed at 60%. With a purification yield at 70%, the resulting cost for production of 35,000 g is \$1550/g for 10% conversion, versus \$1200/g for 20% conversion, as shown in Figure 1.

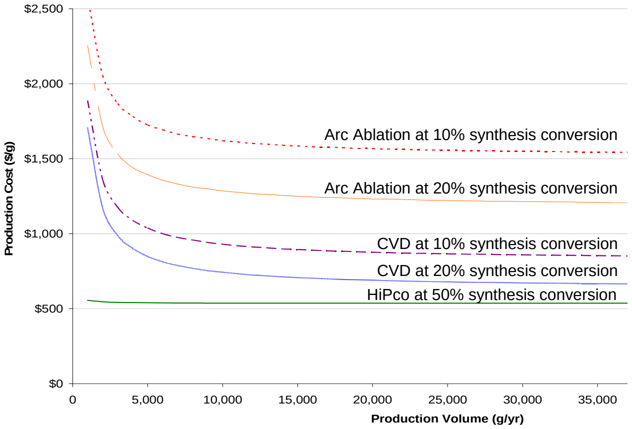

Figure 1: Comparison of SWNT production costs

Assessment of the CVD process similarly shows two curves in Figure 1. The synthesis reaction yield represents the amount of methane that reacts within the furnace to create SWNTs and other deposits. With a base case assumption of 2.95% for synthesis yield, a cost of \$1852/g SWNT results. However, if best conceivable synthesis reaction yields of 10% and 20% are assumed, the cost is reduced. The quantity of SWNTs in this product is assumed at 90%, which reflects current operating conditions. With commonly achieved higher purification yields of 90% for this product, the cost plateaus at 30,000 g with \$860/g for 10% conversion versus \$670/g for 20% conversion.

As a modification to CVD, the HiPco process (a continuous process, not batch as in previous two) has an improved synthesis reaction yield, in this case assumed to be 50%, which represents the amount of carbon monoxide that reacts with the catalyst to produce SWNTs. The synthesis conversion yield is high because it is assumed that the unreacted CO is recycled for reuse in the synthesis process. The quantity of SWNTs contained in the synthesis product is assumed at 97%, with a purification yield of 90%. Costs of \$536/g result, which compare with market prices. Without recycling, cost increases to \$750/g.

3 ENVIRONMENTAL COMPARISON

Environmentally conscious manufacturing initiatives are becoming more common in industry, not only due to impending environmental regulations and liabilities, but also because of increasing costs of pollution remediation. In addition, there is potential for manufacturing cost reductions by implementing pollution avoidance plans or source reduction, rather than the end-of-pipe pollution abatement schemes. To assess the consequences of products and processing technologies, life cycle analysis (LCA) has become one of the most actively considered techniques for the study and analysis of strategies to meet environmental challenges.

Life cycle analysis is typically presented as a three-step process [8-9]: 1) The identification and quantification of energy and resource use and environmental releases to air, water, and land (inventory analysis); 2) Technical, qualitative and quantitative assessment of the consequences on the environment (impact analysis); and 3) The evaluation and implementation of opportunities to reduce environmental burdens (improvement analysis).

Along with calculating costs for each process step, the models can accurately track life cycle inventories for materials and energy. These data are shown in Table 1. The inventory is computed by performing mass balance over the production steps and does not represent any industry, geography or data from any regulatory body. Because the technology is at developmental phase, obtaining information is very difficult due to proprietary issues. Hence, the inventories of chemicals used and released have been determined using mass balance and allows identification of potential releases in industrial scenarios.

Using the inventories as input parameters to SimaPro™ software [10], each alternative was evaluated for its environmental attributes. SimaPro™ assesses the life

Table 1: Life Cycle Inventory for Production of 1g SWNT

Inputs			Outputs		
Arc Ablation					
Synthesis					
Iron powder	13.48	g	Carbon rod	94.97	g
Yttrium powder	3.40	g	Carbon powder	50.53	g
Sulfur powder	1.82	g	Helium	173.39	g
Carbon powder	1.70	g			
Helium	173.39	g			
Carbon rod	127.88	g			
Total energy	382.23	kWh			
Purification					
Triton X100	0.03	g	Scrap membrane	1.19	g
Nitric acid	1,342.88	g	DI water after rinse	9,524.00	g
PTFE membrane	1.19	g	Filtrate	3,439.57	g
DI water	11,619.28	g			
Total energy	30.03	kWh			
CVD					
Synthesis					
Ammonum	0.002	g	Methane Gas	40.90	g
Magnesium	3.30	g	Hydrogen Gas	42.36	g
Colbalt	0.02	g	Argon Gas	839.36	g
Cirtic Acid	0.13	g			
Methane	42.14	g			
Hydrogen	42.36	g			
Argon	839.36	g			
Total energy	763.15	kWh			
Purification					
Triton X100	0.01	g	Scrap membrane	0.62	g
Nitric acid	696.31	g	DI water after rinse	4,938.40	g
PTFE membrane	0.62	g	Filtrate	1,783.01	g
DI water	6,024.85	g			
Total energy	17.43	kWh			
HiPco					
Synthesis					
Catalyst $Fe(CO)_5$	0.08	g	CO	10.44	g
Catalyst CO	9.29	g	Argon	0.06	g
CO	2.29	g			
Argon	0.06	g			
Total energy	388.15	kWh			
Purification					
Triton X100	0.01	g	Scrap membrane	0.57	g
Nitric acid	646.06	g	DI water after rinse	4,582.00	g
PTFE membrane	0.57	g	Filtrate	1,654.26	g
DI water	5,590.04	g			
Total energy	12.96	kWh			

cycle inventory information provided by the process based technical cost models. Using databases provided with the software that determine the impact of releases, SimaPro™ can evaluate process impacts on the environment, by comparing different materials used for a specific application, different methods used in a specific process, or using different valuation methods. Results from SimaPro™ are classified into various categories of environmental or health burdens, based on the databases of environmental impacts of the inventories. Since no data are available in these databases for evaluation of the environmental or health impacts of SWNTs, the results from this software and subsequent analysis can only indicate the impact of materials and energy use.

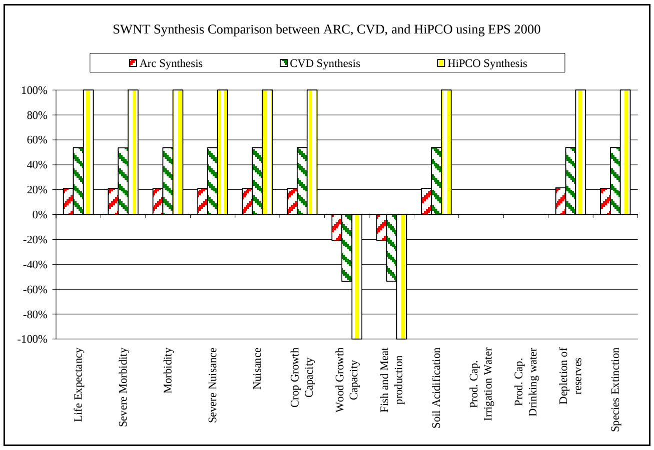

Figure 2: Comparison of environmental attributes for ARC, CVD, and HiPco using EPS 2000

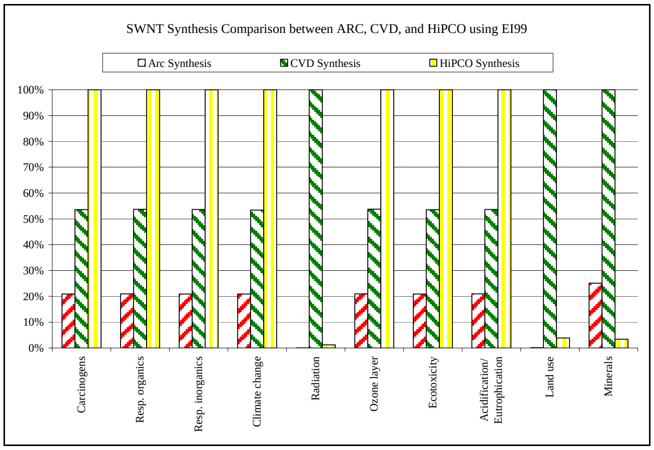

Figure 3: Comparison of environmental attributes for ARC, CVD, and HiPco using EI99

EPS 2000 and EI 99 are two of the methods for valuation of impact data that are available within SimaPro™. EPS 2000 (Environmental Priorities Systems 2000) was developed by researchers at Chalmers Institute in Sweden [11] with impact categories identified from five safe guard subjects: human health, ecosystem production capacity, abiotic stock resource, biodiversity and cultural and recreational values. EI 99 (Environmental Impact

1999) was developed by PRé consultants [12] in the Netherlands with three impact (damage) categories: human health, ecosystem quality and resources.

For the assumed input parameters and the use of the valuation methods EPS 2000 and EI 99 (Figures 2 and 3, respectively) available in SimaPro™, the synthesis process is found to be more environmentally detrimental for all alternative processes. This is attributable to electricity consumption, with HiPco showing the highest environmental burden for the assumed synthesis conversion rates. Although the two valuation methods track environmental burdens by different methods, it is interesting to note that they both appear to indicate that for the assumed inputs, the environmental burden related to electricity consumption by HiPco processing is higher.

4 SUMMARY

For Arc Ablation assuming a purification yield at 70%, the resulting cost for production could be as low as $1550/g for 10% conversion, or $1200/g for 20% conversion. For the CVD process, the cost could be as reduced to $860/g with 10% conversion rates, or even $670/g for 20% conversion rates. But these manufacturing costs are not likely to compete with HiPco costs of $536/g. Of course, these costs do not reflect the technical quality of the SWNT product.

Although the HiPco process appears to be more economically viable for production of single-walled CNTs, its environmental burden is higher than ARC and CVD processes, which are 21% and 54% of the HiPco burden, respectively. The "burden" is not reflected in the SWNT manufacturing cost as the price of electricity has remained low. Further, since no data are available in the SimaPro™ databases for evaluation of the environmental or health impacts of SWNTs, the results only indicate the impact of materials and energy use.

The HiPco process shows higher environmental impact due to contributions from electricity production. HiPco is a continuous process unlike ARC and CVD, which are batch processes. For batch processes, as the synthesis yield increases, the amount of product produced in a single batch increases (i.e., synthesis yield = X/Y where X increases). As more product is obtained per batch, the number of batches and hence the quantity of electricity used over the production volume are both reduced. With the HiPco continuous process, the yield is varied in the model by changing parameters related to the recycling of CO during the production process (i.e., synthesis yield = X/Y where Y decreases), however, the time for producing the assumed production volume remains constant, which requires an equivalent total electricity. Therefore as CVD batch process yields improve, the environmental burden of CVD is reduced below HiPCO, although CVD costs remain higher. HiPco shows the highest environmental burden because the electricity use during manufacturing is driving the environmental burden. With appropriate energy management of an industrial system, this disadvantage can be overcome.

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