Monte Carlo Multi-Criteria Risk Analysis of Single Wall Carbon Nanotube Production Processes Under Uncertain Manufacturing Costs, Occupational Health Risks, and Regulatory Standards

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ABSTRACT

Given the considerable uncertainty surrounding the occupational, consumer, and environmental, health and safety (EHS) risks of various nanomanufacturing processes, Monte Carlo (MC) models were developed to investigate the implications of these uncertainties on high pressure carbon monoxide (HiPco) nanomanufacturing processes. This paper illustrates the use of MC models to study the impact of inherent uncertainties and early EHS standards decisions on predicting long-term manufacturing costs, occupational health (OH) exposure risks, and associated tradeoffs. Until research progresses on the EHS risks of nanotechnology, these types of analyses can provide useful information for private and regulatory decision-makers and for guiding research priorities.

Keywords: uncertainty, occupational health risk, HiPco, Monte Carlo

1 INTRODUCTION

As commercialization of nanotechnology is proceeding quickly in the global market, the need for research to more fully understand the occupational, consumer, and environmental, health and safety (EHS) risks of nanotechnology has grown. There are indications that engineered nanomaterials may have negative properties that might present risks to human health [1]. Critical reviews on the toxicity of single wall carbon nanotubes (SWNTs) showed damage to lung tissue in mice [2], [3], but further research is needed to develop more definitive information about the EHS risks of nanotechnology.

In the Nanotechnology White Paper, the U.S. Environmental Protection Agency has announced its intent to develop a roadmap for assessment of EHS risks of nanotechnology [4]. A recent study undertaken by the National Institute for Occupational Health has suggested preliminary guidelines for working safely with nanomaterials [5]. Even though attention to EHS issues related to this emerging technology has been increased, and a strategy for EHS research was announced [6], risks of nanotechnology are likely to remain unclear for the foreseeable future since more research is necessary to definitively characterize risks of nanotechnology, provide guidance for safe handling of nanomaterials, and minimize workplace exposure. Monte Carlo (MC) simulation models therefore were developed to investigate the implications of inherent uncertainties on high pressure carbon monoxide (HiPco), a common carbon nanotube production method.

Uncertainties in the level and timing of possible required standard practices and associated full-scale production cost and occupational health (OH) exposure risk values are represented by probability distributions and chance events. Numerous uncertainties were examined for their impact on the expected values, variances, and probability distributions of production costs and OH exposure. Given the significant uncertainty in commercialization of nanotechnology, these models will allow development of a more informed understanding of the inherent tradeoffs. Moreover, such designs help to identify optimal manufacturing decisions and policy decisions for funding research priorities.

2 MODEL DESCRIPTION

Earlier process-based technical cost models [7] were developed and used to determine baseline cost estimates for arc ablation ($1,830/g), chemical vapor deposition ($1,586/g), and HiPco ($450/g) SWNT manufacturing processes, all assuming 50% synthesis reaction yield, 90% purification yield, no EHS standards, and a 10,000 g/yr production volume. Since the HiPco process resulted in significantly lower cost, Ok, Isaacs, and Benneyan [8] developed a MC model to assess the OH risks and production costs of SWNT HiPco processes associated with possible regulatory futures. Four general levels of occupational exposure control standards (i.e., none, low, medium, and high) were defined to represent the spectrum of possible nano-EHS standards, with Table 1 summarizing cost assumptions for each level.

If low, medium, or high levels of EHS standards are adopted, the HiPco production costs increase progressively to $460/g, $528/g, and $660/g, respectively. Variability and uncertainty in implementation costs and at each EHS level are represented by triangular distributions. Minimum and maximum possible manufacturing costs under each level of EHS standards are set ±10% of their corresponding most likely values, as summarized in Table 2.

Since no data are readily available regarding OH exposure for the HiPco SWNT manufacturing process, an arbitrary 0 to 10 scale was assumed to represent the level of exposure, again with uncertainty represented via the triangular probability distributions shown in Table 2. For example, if a company does not adopt any standards, it is assumed that the minimum, most likely, and maximum annual values for worker exposure are 7, 9, and 10 units per year, respectively. However, if low levels of worker protection were implemented, then the minimum, most likely, and maximum exposure amounts would decrease to 6, 8, and 9 units.

Implementation rates of EHS standards also have significant uncertainty depending on technology, new research on health risks, regulations, and political forces. Although different assumptions could be used in other analyses, "conservative" transition probability assumptions of the model are shown in Table 3. For example, the likelihoods of remaining at no standards level is high (0.95), whereas probabilities of imposing low, medium, or high levels of EHS standards are low (0.02, 0.015, and 0.015). If a low level of standards is imposed in some future year, the probability of remaining at this low level of protection in subsequent years again will be higher (0.4) than of transitioning to a medium or a high level standards (0.3). Once a medium level standard is introduced, the probabilities of remaining at this medium level or moving to a high level standards are equally high (0.5).

As the MC model executes, manufacturing costs and exposures under each level of EHS standards are randomly generated from the probability distributions shown in Table 2. This logic is implemented in such a way to ensure that exposure and cost progressively decrease and increase, respectively, as a facility implements higher levels of worker protection. Figure 1 summarizes the general logic of a Monte Carlo model.

EHS Standards Level	Costs (Exposure)		
	Minimum	**Most Likely**	**Maximum**
None	\$405 (7)	\$450 (9)	\$495 (10)
Low	\$414 (6)	\$460 (8)	\$506 (9)
Medium	\$475 (3)	\$528 (4)	\$581 (6)
High	\$594 (0)	\$660 (1)	\$726 (2)

Table 2: Assumed parameters for cost (\$/g SWNT) and exposure triangular distribution.

		Level of EHS Standards			
		None	**Low**	**Medium**	**High**
Engineering Controls					
General exhaust – Ventilation			24 hours, 1,000 cfm ventilation rate, \$10,000 capital cost, \$3,000/year operating cost	24 hours, 1,000 cfm ventilation rate, \$10,000 capital cost, \$3,000/year operating cost	24 hours, 1,000 cfm ventilation rate, \$10,000 capital cost, \$3,000/year operating cost
Fume hoods				\$4,000 capital cost for 6.25 ft^2 equipment and \$9,500 for 25 ft^2 equipment	\$4,000 capital cost for 6.25 ft^2 equipment and \$9,500 for 25 ft^2 equipment
Enclosure of processes					50% decrease in labor productivity, 50% extra equipment cost
Administrative Controls					
Annual worker training			8 hours of training, \$560/year instructor cost	8 hours of training, \$560/year instructor cost	8 hours of training, \$560/year instructor cost
Air monitoring			Monthly monitoring, equipment cost of \$20,000	Weekly monitoring, equipment cost of \$20,000	Biweekly monitoring, equipment cost of \$20,000
Medical monitoring					\$950/worker/year
Personal Protective Equipment					
Gloves	Latex		5 pairs/shift, \$0.06/pair		
	Nitrile			5 pairs/shift, \$0.09/pair	5 pairs/shift, \$0.09/pair
Respirators	Disposable		1/shift, \$0.70	1/shift, \$0.70	
	HEPA filters				1 pair/ 30 hrs, \$10/pair
Tyvek suits					1/shift, \$4

Table 1: Summary of assumptions for EHS standards.

EHS Standards Level (from)	Transition Probabilities (to)			
	None	Low	Medium	High
None	0.95	0.02	0.015	0.015
Low	0	0.4	0.3	0.3
Medium	0	0	0.5	0.5
High	0	0	0	1

Table 3: Assumptions for EHS transition probabilities.

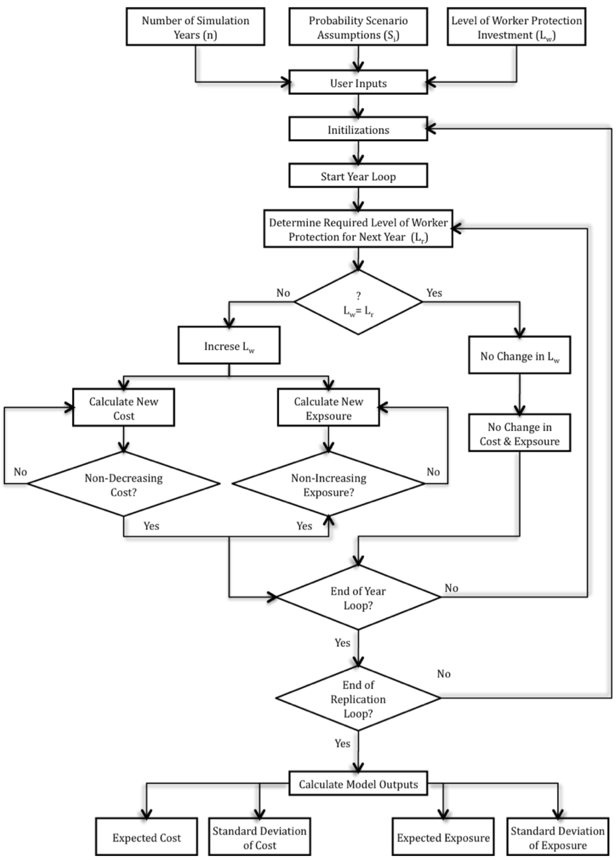

Figure 1: Monte Carlo logic flow.

3 POTENTIAL RESULTS FROM MC RISK MODELS

Assuming the conservative implementation rates given in Table 3, 10,000 replications of a 10-year simulation analysis window results in expected value and standard deviation of \$491/g and \$65/g for manufacturing cost and 7.1 units and 2.4 units for exposure, respectively. Note that in this type of analysis the expected value and standard deviation correspond to the most likely one-time outcome and the uncertainty in this one-time outcome, respectively. That is, the actual manufacturing cost will lie anywhere between roughly \$405/g and \$726/g (a range of \$321) and the actual exposure will lie anywhere between 0 and 10 units. These are large ranges for both possible per gram manufacturing costs and exposure amounts due to the amount of uncertainty assumed in the model.

Figure 2 and Table 4 summarize the joint probability distribution obtained from the MC model of per gram manufacturing costs and exposure for a HiPco process, as well as the inherent tradeoff between production costs and workplace exposure. As illustration, the probability that production costs and exposure will simultaneously be between \$450 to \$475/g and 8 to 9 units, respectively, is 0.132, which is the largest shown joint probability volume. The marginal probability that the total cost (independent of exposure) will be less than \$550/g is fairly high (roughly 80%), whereas the marginal probability that exposure (independent of cost) will exceed 7 is roughly 60%. However, Figure 3 shows that the two measures are very highly correlated, with a correlation coefficient of r=-0.934, i.e., with low exposure becoming less likely as production costs decrease. Given the current significant uncertainty in EHS standards and health risks, similar analyses could be performed using different assumptions to provide further insights regarding worker protection, plant design, and technology investments.

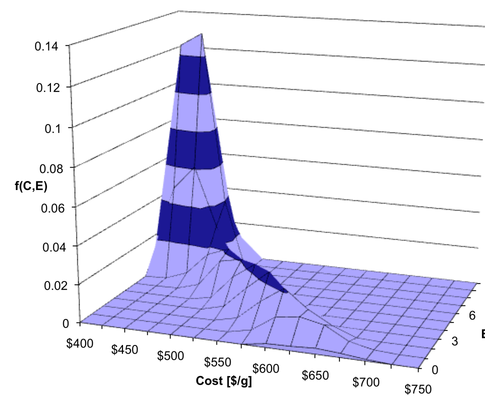

Figure 2: Joint probability density of HiPco SWNT manufacturing costs and exposure.

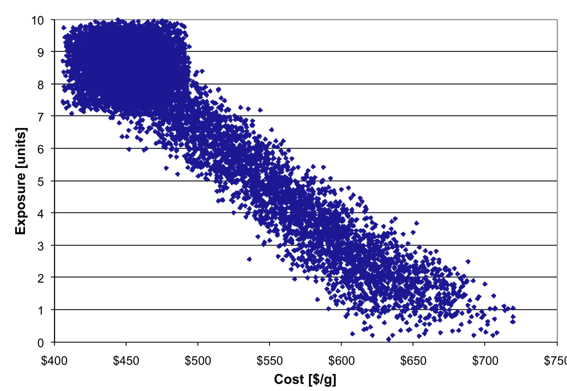

Figure 3: Correlation of 10-year annualized cost and OH exposure.

Ranges	0 < E ≤ 1	1 < E ≤ 2	2 < E ≤ 3	3 < E ≤ 4	4 < E ≤ 5	5 < E ≤ 6	6 < E ≤ 7	7 < E ≤ 8	8 < E ≤ 9	9 < E ≤ 10	Total
400 < $ ≤ 425	0	0	0	0	0	0	0	0.011	0.028	0.020	0.059
425 < $ ≤ 450	0	0	0	0	0	0	0.001	0.048	0.125	0.081	0.255
450 < $ ≤ 475	0	0	0	0	0	0	0.005	0.061	0.132	0.080	0.278
475 < $ ≤ 500	0	0	0	0	0	0.004	0.017	0.029	0.040	0.020	0.110
500 < $ ≤ 525	0	0	0	0	0.002	0.018	0.021	0.007	0	0	0.048
525 < $ ≤ 550	0	0	0	0.003	0.015	0.021	0.008	0	0	0	0.047
550 < $ ≤ 575	0	0	0.003	0.015	0.023	0.008	0.001	0	0	0	0.050
575 < $ ≤ 600	0	0.003	0.013	0.025	0.009	0.001	0	0	0	0	0.051
600 < $ ≤ 625	0.002	0.011	0.022	0.01	0.002	0	0	0	0	0	0.047
625 < $ ≤ 650	0.002	0.013	0.012	0.003	0	0	0	0	0	0	0.030
650 < $ ≤ 675	0.003	0.01	0.005	0	0	0	0	0	0	0	0.018
675 < $ ≤ 700	0.002	0.003	0.001	0	0	0	0	0	0	0	0.006
700 < $ ≤ 725	0.001	0.001	0	0	0	0	0	0	0	0	0.002
725 < $ ≤ 750	0	0	0	0	0	0	0	0	0	0	0
Total	0.010	0.041	0.056	0.056	0.051	0.052	0.053	0.156	0.325	0.201	1

Table 4: Joint probability distribution of HiPco manufacturing costs and exposure amounts.

4 CONCLUSIONS

Assessing the tradeoffs between manufacturing costs and occupational health consequences of nanotechnology production processes is especially difficult given the limited data on the health effects of nanoparticles. This paper illustrates the use of Monte Carlo models to study the impact of these uncertainties on the inability to predict long-term occupational health exposure risks, manufacturing costs, and inherent tradeoffs. Results underscore the observation that, given the extreme amount of uncertainty in the exposure risks and costs of different levels of protection, policy and manufacturing decisions should not be based on expected values alone. Until research progresses on the EHS risks of nanotechnology, these types of analyses can provide useful information for private and regulatory decision-makers and for guiding research priorities.

ACKNOWLEDGMENT

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