ACS Sustainable Chemistry & Engineering

Research Article

pubs.acs.org/journal/ascecg

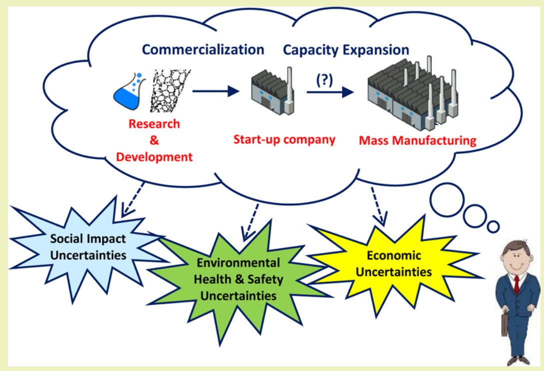
Multistage Stochastic Programming (MSP) Model for Carbon Nanotube Production Capacity Expansion Planning

Serkan Erbis, Sagar Kamarthi, Thomas P. Cullinane, and Jacqueline A. Isaacs*

Department of Mechanical and Industrial Engineering and Center for High-rate Nanomanufacturing, Northeastern University, 360 Huntington Avenue, Boston, Massachusetts 02115, United States

Supporting Information

ABSTRACT: Nanotechnology companies face uncertainties from several fronts including occupational safety regulation, demand for nanoproducts, and technology advancements. These uncertainties can prove to be a challenge for planning the production capacity expansion of engineered nanomaterials or nanoenabled products. Exploratory Monte Carlo simulation results indicate that these uncertainties have a significant effect on potential revenue and that there are opportunities for making optimal sustainable capacity expansion decisions by evaluating all possible future scenarios through optimization models. Accordingly, this work develops a multistage stochastic programming (MSP) model to determine the optimal timing of expansion, expansion size, process type, production volume, and also the occupational safety controls in the company to ultimately minimize the total production cost. This MSP model also helps decision makers to achieve sustainable manufacturing goals by reducing the unnecessary capacity expansion and occupational exposure.



KEYWORDS: *Nanotechnology, Monte Carlo, Simulation, Exposure, Uncertainties, Optimization, Carbon Nanotubes, CNTs*

■ INTRODUCTION

With increased understanding of the properties of carbon nanotubes (CNTs), CNT-enabled products have been proliferating in the market.[1] CNTs are used in various applications such as batteries,[2] microelectronics,[3] composite materials,[4] and nanoscale-sensors to identify contaminants.[5] According to the Project on Emerging Nanotechnologies, there are 1628 nanotechnology-enabled consumer products on the market as of September 2013, and 87 of these products use carbon-based nanomaterials.[6] The market share for nano-enabled products is estimated to grow at a minimum to \$3.3 trillion[7] in 2018. With an expected increase in demand for CNTs, the fabrication technology for mass-production of CNTs is likely to evolve.

Although applications using nanomaterials are quickly advancing, the environmental, health, and safety (EHS) risks of engineered nanomaterials used for these applications are not yet known with certainty. With increasing calls for nano-EHS studies during the 2000s,[8−10] the number of publications dealing with these issues has increased. Over a 12-year period between 2000 and 2011, more than 4800 peer-reviewed articles appeared in a wide range of journals, most of which focused primarily on nanotoxicology.[11] Existing studies indicate that there can be possible toxicity effects of nanomaterials and that the physicochemical properties influence the toxicity of the nanomaterials.[12] However, it is still uncertain how the properties of engineered nanomaterials influence their toxicity.[13] Although surveys of representatives in the nanotech industry show agreement that there is a high level of uncertainty in environmental and health risk of engineered nanomaterials, safety practices in industry do not always correspond with recommended safety practices and guidelines, perhaps due to lack of information about implementation, lack of regulation, budget constraints, or internal enforcement.[14] Unless there are strict protocols or regulations in place to protect workers and the environment, and until the potential EHS risk of nanomaterials becomes clearer, questions linger on how to expand the beneficial attributes of this technology without unintended consequences.

In 2010, only 25% of the global capacity of CNTs was produced. Although demand is expected to increase to 40−50% by 2016,[15] the global demand for CNTs is expected to remain below the supply level over the next five years.[16] However, with anticipated increased future demand for CNTs, start-up companies as well as small to medium enterprise companies in CNT markets may be deliberating strategic plans to expand their production capacities. An optimum investment strategy would be required to minimize the excess capacity (especially in short-term) and potential shortage in the long term.

Special Issue: Sustainable Nanotechnology 2013

Received: February 18, 2014
Revised: May 14, 2014
Published: June 13, 2014

Investment decisions involve risks—sometimes high, sometimes low. A list of trade-offs can be translated to monetary metrics as a means to weigh the consequences of alternative decisions. For engineered nanomaterials, there are additional uncertainties that must be considered, including the immediate and long-term consequences for human health and the environment. Given the uncertainties associated with these types of investments, investors are likely to struggle with decisions on production capacity expansion. Production scale-up planning tools that are employed to quantify decision trade-offs must be modified to include consideration of uncertainties in CNT manufacture. To be effective, a decision tool should determine an optimum periodic expansion of capacity to meet a growing demand and at the same time minimize the investment and exposure risks in nanomanufacturing. Uncertainties in the future demand for CNTs, in future available technologies for producing CNTs, and in future regulations for CNT production should be considered as scenarios in order to minimize the investment and exposure risks. A multistage stochastic program (MSP) model was therefore created to optimize the capacity expansion strategy over multiple time periods. The advantages of this approach include the ability to model the probability space of possible events or scenarios (instead of using the expected values of scenarios) and the ability to make corrective decisions depending on the scenarios that occurred in the preceding periods. Results from the MSP model offer recommendations on making the trade-offs for planning capacity expansion, improving production technologies, and investing in occupational safety. Further, the MSP model provides information leading to efficiencies for more sustainable manufacturing by minimizing the unnecessary capacity (including materials and energy usage) and protecting workers' safety.

Literature Review of Stochastic Programming Models Applied to Capacity Expansion Planning. Capacity expansion planning problems have been studied by researchers since the 1960s. Manne[17] developed the first mathematical model for the capacity expansion problem under the assumption of both deterministic and random demand. The author used the Bachelier–Wiener diffusion process to show that the expected discounted cost and optimal expansion sizes over an infinite horizon increases as the variance for demand increases. Freidenfelds[18] reformulated the stochastic capacity expansion model as an equivalent deterministic model, assuming that the demand is a birth–death process. Davis et al.[19] proposed a mathematical model based on the stochastic control theory to solve the capacity expansion problem with uncertain future demand (discrete), nonzero lead times, and random costs. Bean et al.[20] developed a capacity expansion model to meet a stochastically growing demand that is assumed to be either nonlinear Brownian motion or a non-Markovian birth and death process.

The use of scenarios to model the uncertainty in capacity expansion planning has significantly increased with the use of stochastic programming and improvements in computation power. Fine and Freund[21] studied the product–flexible manufacturing capacity investment decisions and formulated a two-stage stochastic programming model. Malcom and Zenios[22] developed a robust stochastic programming model for capacity expansion problems in power systems. Wagner and Berman[23] created five different stochastic optimization models for planning the capacity expansion for convenience stores using an algorithm[24] based on Lagrangian relaxation and knapsack problem structure. Liu and Sahinidis[25] developed a two-stage stochastic programming model for planning capacity expansion and solved the model by using Benders' decomposition algorithm. They also compared stochastic programming and fuzzy programming approaches and showed that the stochastic programming approach is more efficient than a fuzzy programming approach in terms of finding a feasible solution. Barahona et al.[26] addressed a capacity expansion planning problem in semiconductor manufacturing and formulated a two-stage stochastic mixed integer programming model. Bertnard et al.[27] developed a bilevel model for the optimal investment problem in generation capacity. The bilevel model was transformed to a single-level model by using Karush–Kuhn–Tucker optimality conditions, and the single-level model was reformulated as a two-stage stochastic model to optimize the investment time and size. Li and Ierapetritou[28] formulated a two-stage stochastic integer programming model for planning capacity expansion in a process industry. The augmented Lagrangian approximation and scenario decomposition algorithm were employed to solve the two-stage stochastic model.

A multistage approach has also been applied to capacity expansion planning problems. Rajagopalan et al.[29] studied capacity expansion planning and technology replacement in growing markets with an uncertain technological breakthrough. A multistage model was developed for the problem and solved by using a dynamic programming strategy. Chen et al.[30] addressed technology selection and capacity expansion and formulated a MSP model. Ahmed and Sahinidis[31] created a MSP model for planning capacity expansion in multiple production facilities. The model optimizes the capacity expansion size, type, and capacity allocations to meet the unanticipated growing demand. Later, Ahmed et al.[32] expanded Ahmed and Sahinidis' work[31] by adding inventory balances and developed a framework-based heuristic algorithm and a branch and bound algorithm.

Review papers on capacity expansion planning are useful for researchers to explore the current state-of-the-art in modeling and determine the research needs in capacity expansion planning. Luss[33] reviewed the capacity expansion planning models in the literature and discussed the major issues in capacity expansion. The main decisions in a capacity expansion problem were identified as expansion size, expansion time, and expansion locations (and/or capacity types). Later, Julka et al.[34] reviewed the multifactor capacity expansion models for manufacturing plants and concluded that the mathematical models in the literature did not capture all aspects of production capacity expansion and that actual industry case studies are limited.

Several studies explored CNT production expansion planning and CNT production planning. Earlier, Ok et al.[35] developed a decision support tool based on a desirability function to find the most beneficial of the six predetermined expansion strategies. Each expansion strategy includes five criteria such as facility size, expansion capability, throughput, EHS protection, and EHS uncertainty. The desirability optimization method determines the most desirable expansion plan by using importance weights for each criteria and desirabilities for the values for each criteria in each strategy. However, the model provides decisions for only one-time capacity expansion, and the results are based on the expert opinion. Moreover, Ok et al.[35] did not consider the uncertainties in demand for CNTs or future available technologies for CNT production, which are believed to affect the long-term profit. Later, Chen et al.[36] created a nonlinear and chance constraint programming model to calculate the production volume for fixed capacity and occupational safety practices in order to maximize the total profit and minimize occupational exposure risk. Uncertainties in occupational safety risk of CNTs were considered by using chance constraint parameters. However, the model does not capture the future demand or technological evolution uncertainties. Further, the model was limited to make a production volume decision based on fixed capacity and occupational safety practices for one time. It does not provide expansion and production planning decisions over multiple time periods.

The present study differs from that of Ok et al.[35] and Chen et al.[36] with regard to modeling approach, decision variables, and uncertain parameters considered in the model. The present study explores use of a MSP model for a CNT production capacity expansion planning problem. The MSP approach offers the ability of modeling the probabilistic space of possible events by using scenarios and provides decisions for each scenario. Therefore, the decision maker can make corrective decisions depending on the possible events that occur in previous periods. Uncertainties in future demand for CNTs, future technological evolutions in CNT production, and future regulations (occupational exposure limits for CNTs) are considered by using various scenarios in the model. In addition, the model in this study was developed to optimize expansion strategy (number of process lines), final capacity, and production volume decisions for CNT production and determine the appropriate occupational safety practices based on the production volume over multiple time periods for each scenario. Ok et al.[35] and Chen et al.[36] did not capture the future demand and technological evolution uncertainties and did not provide expansion, production volume, and occupational safety decisions over multiple time periods for different demand, technological evolution, and regulation scenarios.

As previously mentioned, MSP models were applied to capacity expansion planning problems for manufacturing plants. However, there is no study in the literature where a MSP approach is specifically applied to CNT production capacity expansion planning. The model in this study was developed by considering the uncertainties (e.g., future demand for CNTs, technological evolution for CNT production, future regulations for CNT production) specifically associated with CNT production industry. Moreover, constraints associated with occupational exposure were included in the model. In previous studies, only one parameter (either demand or technological evolution) was assumed to be uncertain, and occupational safety (or exposure) metrics were not captured.

Because the uncertainties considered in this study are believed to be valid for other nanomaterials and nanoenabled products, the model could be applied to other nanotechnology related products. The model can also be modified for other engineered nanomaterials and nanoenabled products if additional factors need to be considered. The MSP model described in the following section was run with the input values associated with CNT production; results from the model provide insights to companies in the CNT industry.

■ METHODS

In this section, the MSP model for CNT production capacity expansion planning problem is formulated. The MSP approach[37] is suitable for problems involving multiple scenarios and uncertainties at decision points. To explore the problem, initially a Monte Carlo (MC) simulation model was developed (Supporting Information). The simulation model examines how the expenditures (including the lost revenues) of CNTs manufacturing companies vary when companies face uncertainties in demand for CNTs technological evolution for CNT production and occupational safety regulations. It also investigates how the total expenditure is affected by different investment strategies. The output of the simulation model shows that total production expenditure is sensitive to stochastic parameters in the model. Moreover, it is observed that an optimum expansion decision set over multiple time periods for different future scenarios is needed to minimize the expected production cost. These observations confirm that MSP is a good approach to model and study the CNT production expansion planning problem. In the following section, the MSP approach is presented for a CNT manufacturing expansion planning problem.

MSP Modeling Approach. A start-up company that produces carbon nanotubes is considered for the model. The company needs to expand its capacity to meet the growing demand for CNTs. The hypothetical start-up company considered here produces both low purity single-walled carbon nanotubes (SWCNTs) (as-produced) and high purity SWCNTs (refined through a series of purification processes) in one facility. Currently, the company produces low purity SWCNTs and high purity SWCNTs with two separate synthesis production lines (such as HiPCO process, CVD, or ARC) and is interested in expanding its production capacity to meet the expected growing demand. However, there are budget and space constraints for expansion. Production rate per hour is also limited due to occupation exposure limits. Occupational safety controls can be upgraded to increase the production rate. The company needs to make optimal expansion strategy decisions to minimize the total expenditure of the company and the revenue lost due to unmet demand. The objective of the model is to minimize the total production cost, which includes the capacity expansion, manufacturing, storage (inventory), shortage (unmet demand), and occupational safety cost.

Percentage increase in demand, probability of technological improvement, and occupational safety regulations are considered as the stochastic parameters in the model. Given these uncertainties, the company is expected to determine an optimal expansion strategy to minimize its total cost and lost revenues. Hence, the model is programmed to determine the optimal values for the following decision variables: timing for expansion, expansion size (number of production lines), technology type, capacity allocation for each product, and occupational safety level. The following assumptions are made in creating the stochastic programming model:

(1) The demand for CNTs is nondecreasing over time.

(2) The improved synthesis methods and the new synthesis methods that give higher CNT yields and release fewer CNTs into the work environment are available with certain probability. This assumption is supported by the fact that both the existing and new CNT synthesis methods are emerging through ongoing research and development efforts. For instance, CVD process has been upgraded many times by the researchers to increase its production rate.[38]

(3) More stringent regulations for occupational exposure of CNTs are likely in the future. As mentioned earlier, there is significant uncertainty regarding the environmental, health, and safety (EHS) risks of engineered nanomaterials. Since 2010, SWCNTs and multiwalled carbon nanotubes (MWCNTs) have

been subject to Pre-Manufacture Notices (PMNs) within the context of the Toxic Substance Control Act (TSCA).[39] The companies that intend to manufacture, import, or process either SWCNTs or MWCNTs are required to notify the U.S. Environmental Protection Agency (EPA) at least 90 days prior to initiating those activities. In addition to this regulation, in 2013, NIOSH[40] suggested a recommended exposure limit (REL) of 1 μg/m^3 elemental carbon as a respirable mass 8-h time-weighted average (TWA) concentration, although NIOSH[41,42] recommended limits of 7 μg/m^3 in 2010. Nakanishi[43] proposed 30 μg/m^3 (8-h TWA) as an occupational exposure limit for CNTs in 2011. Nanocycl[44] recommended 2.5 μg/m^3 (8-h TWA) as an exposure limit for MWCNTs in 2009, whereas Aschberger et al.[45] proposed 2 μg/m^3 (8-h TWA) for MWCNTs and 1 μg/m^3 (8-h TWA) for SWCNTs in 2010. Although NIOSH's recommendation is not a regulation, 1 μg/m^3 is assumed to be the limit in the model for the high level regulation that could come into effect in the future.

(4) The production volume and 8-h working time are included in the calculation of CNTs concentration in the working environment in each period to determine the occupational safety level. According to NIOSH,[46] the exposure risk of nanomaterials depends on three factors: volume of nanomaterial handled or produced, physical form of the nanomaterial, and production duration. As one or more of these factors changes to affect higher exposure risk, more efficient exposure control measures are needed. To estimate the occupational safety level, the formula below is adopted from Chen et al.[36] but modified to calculate the 8-h time-weighted average concentration of CNTs (μg/m^3) in air

$$E = \frac{Q \times \varepsilon \times f}{V \times \text{Day} \times \text{Hour}}$$

where E is the concentration of CNTs (μg/m^3) in the work space, Q is annual production (g/year), ε is the emission coefficient, f is the conversion factor (1,000,000 from g to μg), V is volume of the working space, Day is the number of working days per year, and Hour is the number of working hours per day. A constraint to ensure that the 8-h TWA concentration of CNTs in the air (μg/m^3) is smaller than the 8-h TWA exposure limits (μg/m^3) is used in the model.

A Multiperiod ($t \geq 3$) Stochastic Programming Model. A MSP model is created to determine a capacity expansion planning strategy for companies in the nanotechnology sector with consideration of various scenarios. For the three-period model, the initial expansion decision is made in the first period. After the second period's demand is fulfilled, regulations (exposure limit) and technological evolution (whether a new generation of an existing process is available) are observed (Figures S3 and S4, Supporting Information), and then second period decisions (on production amounts, occupational safety level, and second period expansion decisions) are made. If new generation processes become available for use in the second period, the decision maker has an option of investing in these new processes.

The following notation and input parameters are used in the multistage stochastic mixed integer programming model:

i = index of product types $\in \{1,2, ..., a\}$
t = index of period $\in \{1,2, ..., T\}$
j = index of process type $\in \{1,2,..., (T-1)\}$
k = index of demand scenarios $\in \{1,2,..., b^{(T-1)}\}$
m = index of occupational safety regulation scenarios $\in \{1,2, ..., c\}$
c = integer that depends on the number of different regulation scenarios and number of periods in the model
n = index of occupational safety level $\in \{1,2, ..., d\}$
l = index of technology level scenarios $\in \{1,2, ..., e^{(T-2)}\}$
A = space limit (number of production lines)
B = budget for expansion (\$)
ε_j = emission coefficient for process type j
V = volume of working space (m^3)
R_{ji} = annual production rate of a process type j for product i (gram/year) with one 8-h shift working 365 days each year
p_k = probability of demand scenario k
π_l = probability of technology scenario l
q_m = probability of regulation scenario m
G_{11} = initial number of lines of process type 1 in period 1
F_n = exposure limit adjustment coefficient for occupational safety level n
D_{itk} = demand for product i in period t in demand scenario k (gram)
L_{tm} = exposure limit in period t in regulation scenario m (μg/m^3)

$$W_{jtl} = \begin{cases} 1, \text{if process type } j \text{ is released in period } t \\ \text{in technology improvement scenario } l \\ 0, \text{otherwise} \end{cases}$$

C^X_{11} = setup cost for 1 line of process type 1 in period 1 (\$/line)
C^Z_{jtl} = setup cost for 1 line of process type j in period t in scenario l (\$/line)
C^Q_{jit} = cost for producing product i with process type j in period t (\$/gram)
C^I_t = inventory cost for storing product i in period t (\$/gram)
C^S_{itl} = shortage cost for product i due to unmet demand in period t in technology scenario l (\$/gram)
C^F_n = cost for occupational safety level n (\$/gram)

The following decision variables are optimized in the model:

X_{11} = expansion decision (number of lines of process type 1) in period 1
Z_{jtkl} = expansion decision (number of lines of process type j) in period t in demand scenario k in technology scenario l
P_{jitkl} = number of lines of process type j used to produce product i in period t in demand scenario k in technology scenario l
Q_{jitkl} = production volume of product i produced by process type j in period t in demand scenario k in technology scenario l (gram)

$$Y_{ntklm} = \begin{cases} 1, \text{if the safety level is } n \text{ in period } t \\ \text{in demand scenario } k \text{ in technology scenario } l \\ \text{in regulation scenario } m \\ 0, \text{otherwise} \end{cases}$$

EHS_{ntklm} = occupational safety cost for safety level n in period t in demand scenario k in technology scenario l in regulatory scenario m

These next variables are calculated based on the decision variables:

I_{itkl} = inventory level for product i in period t in demand scenario k in technology scenario l (gram)
S_{itkl} = shortage level for product i in period t in demand scenario k in technology scenario l (gram)

The equations to solve the capacity expansion planning problem using a MSP model are provided:

$$\text{Minimize}\left[X_{11}C_{11}^{X}+\left(\sum_{k=1}^{b^{T-1}}p_k\sum_{l=1}^{e^{T-2}}\pi_l\sum_{j=1}^{T-1}\sum_{t=2}^{T-1}Z_{jtkl}C_{jtl}^{Z}\right)\right] \quad \text{Expansion Cost}$$

$$+\left(\sum_{k=1}^{b^{T-1}}p_k\sum_{l=1}^{e^{T-2}}\pi_l\sum_{i=1}^{a}\sum_{t=2}^{T}I_{itkl}C_t^{I}+S_{itkl}C_{itl}^{S}\right) \quad \text{Inventory and Shortage Cost}$$

$$+\left(\sum_{k=1}^{b^{T-1}}p_k\sum_{l=1}^{e^{T-2}}\pi_l\sum_{j=1}^{T-1}\sum_{i=1}^{a}\sum_{t=2}^{T}Q_{jitkl}C_{jit}^{Q}\right) \quad \text{Production Cost}$$

$$+\left(\sum_{k=1}^{b^{T-1}}p_k\sum_{l=1}^{e^{T-2}}\pi_l\sum_{m=1}^{c}q_m\sum_{t=2}^{T}\sum_{n=1}^{d}EHS_{ntklm}\right) \quad \text{Occupational Safety Cost}$$

Subject to

$$\sum_{i=1}^{a}P_{1i2kl}\le(G_{11}+X_{11})\quad\forall\, k,l \tag{1}$$

$$P_{ji2kl}=0\quad\forall\, i,k,l,j\neq 1 \tag{2}$$

$$\sum_{i=1}^{a}P_{ji(t+1)kl}\le G_{11}+X_{11}+\sum_{\tau=2}^{t}Z_{j\tau kl}W_{j\tau l}\quad\forall\, j,k,l;\ t=2,...,T-1 \tag{3}$$

$$G_{11}+X_{11}+\sum_{j=1}^{T-1}\sum_{\tau=2}^{t}Z_{j\tau kl}W_{j\tau l}\le A\quad\forall\, k,l;\ t=2,...,T-1 \tag{4}$$

$$X_{11}C_{11}^{S}+\sum_{j=1}^{T-1}\sum_{\tau=2}^{t}Z_{j\tau kl}C_{j\tau l}^{Z}\le B\quad\forall\, k,l;\ t=2,...,T-1 \tag{5}$$

$$Q_{jitkl}\le P_{jitkl}R_{ji}\quad\forall\, j,i,k,l;\ t=2,...,T \tag{6}$$

$$\frac{[\sum_{j=1}^{T-1}\sum_{i=1}^{a}Q_{jitkl}(\epsilon_j)]10^6}{V(365)(8)}\le L_{mt}(\Sigma_{n=1}^{d}Y_{ntklm}F_m)\quad\forall\, k,l,m;\ t=2,...,T \tag{7}$$

$$\Sigma_{n=1}^{d}Y_{ntklm}=1\quad\forall\, k,l,m;\ t=2,...,T \tag{8}$$

$$EHS_{ntklm}\ge\left[\sum_{j=1}^{T-1}\sum_{i=1}^{a}Q_{jitkl}\right]C_n^{F}-M(1-Y_{ntklm})\quad\forall\, k,l,m,n;\ t=2,...,T \tag{9}$$

$$I_{i2kl}-S_{i2kl}=\sum_{j=1}^{T-1}P_{ji2kl}-D_{i2k}\quad\forall\, i,k,l \tag{10}$$

$$I_{itkl}-S_{itkl}=\sum_{j=1}^{T-1}P_{jitkl}-D_{itk}+I_{i(t-1)kl}\quad\forall\, i,k,l;\ t=3,...,T \tag{11}$$

$$X_{11},P_{jitkl},I_{itkl},S_{itkl},Z_{jtkl},Q_{jitkl}\ge 0\quad\forall\, j,i,k,l;\ t=2,...,T \tag{12}$$

$$X_{11},P_{jitkl},I_{itkl},S_{itkl},Z_{jtkl},Q_{jitkl}\in Z\quad\forall\, j,i,k,l;\ t=2,...,T \tag{13}$$

$$Y_{ntklm}\in\{0,1\}\quad\forall\, k,l,m,n;\ t=2,...,T \tag{14}$$

Nonanticipativity constraints for the three-period model are included in eqs 15−19:

$$Z_{j21l}=Z_{j22l}=Z_{j23l};\ Z_{j24l}=Z_{j25l}=Z_{j26l};\ Z_{j27l}=Z_{j28l}=Z_{j29l}\quad\forall\, j,l \tag{15}$$

$$P_{ji21l}=P_{ji22l}=P_{ji23l};\ P_{ji24l}=P_{ji25l}=P_{ji26l};\ P_{ji27l}=P_{ji28l}=P_{ji29l}\quad\forall\, j,i,l \tag{16}$$

$$Q_{ji21l}=Q_{ji22l}=Q_{ji23l};\ Q_{ji24l}=Q_{ji25l}=Q_{ji26l};\ Q_{ji27l}=Q_{ji28l}=Q_{ji29l}\quad\forall\, j,i,l \tag{17}$$

$$Y_{n21lm}=Y_{n22lm}=Y_{n23lm};\ Y_{n24lm}=Y_{n25lm}=Y_{n26lm};\ Y_{n27lm}=Y_{n28lm}=Y_{n29lm}\quad\forall\, l,m,n \tag{18}$$

$$Y_{n2kl1}=Y_{n2kl2}=Y_{n2kl3};\ Y_{n2kl4}=Y_{n2kl5}\quad\forall\, k,l,n \tag{19}$$

The objective function minimizes the total production cost, which includes the expansion cost in period 1 plus the expected expansion, inventory, shortage, manufacturing, and occupational safety cost in period $t \ge 2$. Constraint 1 ensures that the summation of the number of production lines used to produce each product i in period t ($t = 2$) should be smaller than the total number of production lines in the facility in period t ($\underline{t} = 2$). Constraint 2 ensures that the number of process type j ($j \neq 1$) is zero in period 2. Constraint 3 ensures that the summation of the number of production lines used to produce each product i in period t ($t \ge 3$) should be smaller than the total number of production lines in the facility in period t ($t \ge 3$). Constraints 4 and 5 ensure that the expansion does not violate budget and space limits. Constraint 6 ensures that the total volume of product i does not exceed the capacity allocated for that product. Constraint 7 determines whether the exposure associated with production quantity, emission coefficient, volume of working space, and working hours per year exceeds the resulting multiplication product of exposure upper limit and safety factor. Constraint 8 determines the occupational safety level. Constraint 9 calculates the occupational safety cost. Constraints 10 and 11 calculate the shortage and inventory for each product. Constraints 12 and 13 ensure that all the variables are non-negative integers. Constraint 14 sets the binary variable. Nonanticipativity constraints 15−19 are used in the MSP model to ensure that all of the scenarios with a common history have the same decisions up to the current time when the model is run for three periods. A detailed explanation of the model (cost functions) is presented in the Supporting Information.

■ RESULTS AND DISCUSSION

To parametrize the MSP model, reasonable ranges for the current and future CNT production technologies (Table S4, Supporting Information) were obtained through discussions with CNT industry experts. By considering the approximate ranges for CNT production lines in Table S4 of the Supporting Information, the data in Table S5 are generated. Data used to run the two-period model and the three-period model are shown in Tables S6–S11 of the Supporting Information. The emission coefficient data for the current technologies in Tables S7 and S9 of the Supporting Information are adapted from Chen et al.,[36] and it is assumed that the emission coefficient value is the same for all products. As mentioned previously, the emission coefficient decreases as the technology advances. There are four occupational safety levels that the company can invest in to decrease the occupational exposure. Occupational safety control levels and costs from Ok et al.[47] are modified for use in the model (Tables S10 and S11, Supporting Information).

Although the model described in the previous section can be run for three or more planning periods ($t \geq 3$), the model must be simplified to obtain results for the two-period planning cases. The equations for the simplified version of the model are included in the Supporting Information. Either model is run using IBM ILOG CPLEX Optimization Studio,[48] which is an optimization software package that solves mathematical programming models.

The simplified model was used for the two-period capacity expansion planning case. Input values in Tables S6, S7, S10, and S11 and Figure S4 of the Supporting Information were used to obtain the results in Figure 1 (also see Table S12, Supporting Information). Given the probabilities and model inputs for the present case, the company should invest in two production lines of the SWCNT synthesis process in the first period. After the demand and occupational exposure limit are observed, the production quantities and occupational safety level and resource decisions are made. For example, if demand scenario 2 and regulation scenario 3 occur in the second period, the occupational safety level should be 4 in the facility, and 11,680 g of high purity SWCNTs and 0 g of low purity SWCNTs should be produced.

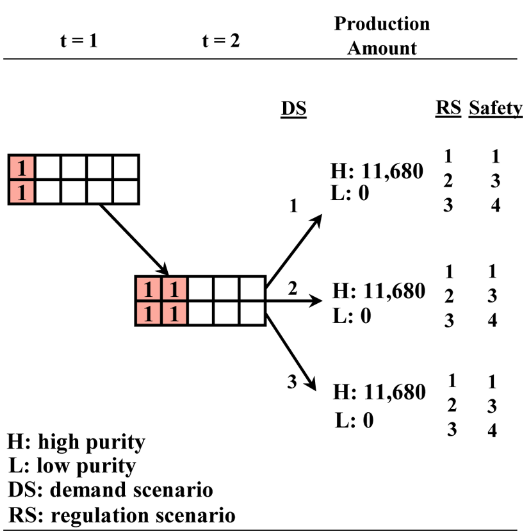


Figure 1. Results for two-period planning for each demand and regulation scenario recommended capacity expansion by two process lines. An optimal safety level should be selected as 1, 3, or 4 if a regulation scenario 1, 2, or 3 occurs, respectively.

For the three-period model, there are nine demands, six regulations, and two technological improvement scenarios. A total of 108 scenarios (= 9 × 6 × 2) are considered for capacity expansion decisions in the three-period MSP model (Figures S5 and S6, Supporting Information). In the three-period planning problem, there are technological improvement possibilities in the second period. Therefore, the company should consider the possibility of technological improvement in the second period, while making capacity expansion decisions in period 1.

The results for the three-period planning are shown in Figure 2 (also see Table S13, Supporting Information). On the basis of the input data (Tables S8–S11 and Figures S5–S6, Supporting Information), the company should invest in two production lines in the first period. After the occupational exposure limit, demand, and new technology availability are observed, resource decisions are made in period 2. For instance, if demand scenario 4 occurs and there is a new technology released in the second period, then the company should invest in three production lines of process technology 2. The production volume for each product and occupational safety decisions for each scenario (108 scenarios) and period (t = 2 and t = 3) are also optimized by using the model, but they are not shown in Figure 2.

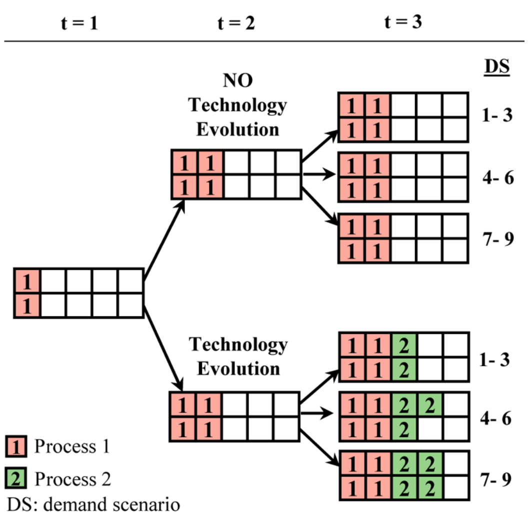


Figure 2. Results for three-period expansion planning for each demand and technology scenario recommended capacity expansion by two process lines using technology 1 in the first period. No expansion is needed if no technology evolution occurs in the second period. If a technology improvement does occur, then expand the capacity by 2, 3, or 4 process lines with technology 2, if the demand scenarios 1–3, 4–6, or 7–9 occurs, respectively.

Design of experiment analysis is conducted to investigate which of the factors have significant effect on total expenditures of the company. The factors determined for the analysis include stochastic parameters (e.g., demand, regulation, and technological evolution), expansion budget, and facility size (e.g., maximum of number production lines). The high, low, and base level values of the factors are shown in Tables S14–S17 of the Supporting Information. For stochastic parameters, different

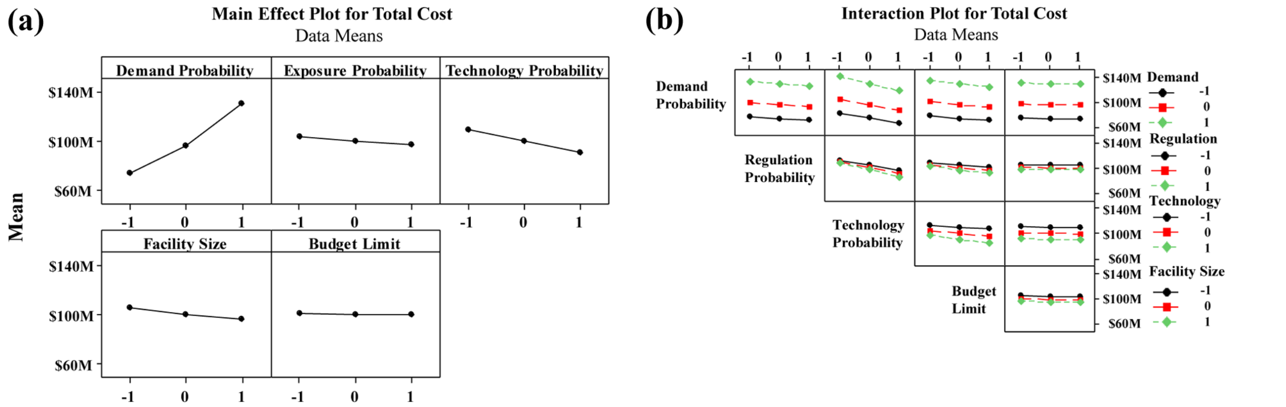


Figure 3. (a) Main effects plot: Slopes indicate how the total cost changes with each factor's different values; demand scenario probabilities show the highest impact on total cost. (b) Interaction effect plot: Slopes indicate the effect of factor pairs on total cost; the interaction of demand scenario and technology evolution probabilities has highest impact on total cost.

probabilities sets are used in each level. A full factorial design of experiments is considered for studying the main and interaction effects of the factors on total cost. A three-level design with five factors has 243 possible treatments (combinations). The MSP model was run for each treatment, and the results were analyzed using MINITAB software. The main and interaction plots for total cost are shown in Figure 3. In Figure 3a, it is clear that demand scenario probabilities have a larger effect on the total cost than the other factors. If the demand increases by a high percentage in the future, then the total production cost will increase significantly due to the fixed capacity and high occupational safety cost assumptions. The second factor that has a significant effect on the total cost is the technological evolution factor. If a fast technological evolution is more likely to occur in the future, then the total production cost will decrease. Regulation and facility size also influence total cost, but not as significantly as the demand and technology evolution factors. The expansion budget limit does not have a significant effect on total cost due to capacity expansion restrictions based on regulations and facility size.

The interaction effect graph in Figure 3b shows the effect of factor pairs on total cost. As shown in Figure 3b, the interaction between demand and technology has a large effect on the total production cost than other pairs of factors. The response surface graph in Figure 4 shows the effect of the technology evolution and demand scenario probabilities on total cost.

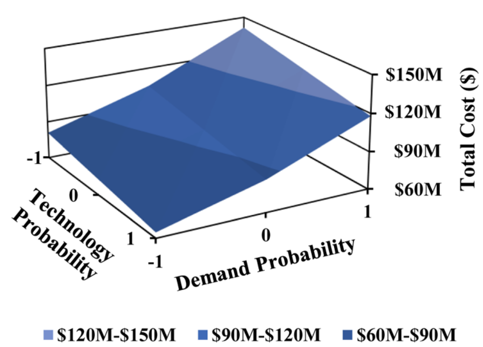


Figure 4. Surface graph (interaction graph) shows the effect of the technology evolution and demand scenario probabilities on total cost. Rapid technology evolution decreases the total cost in the future, whereas higher demand in the future would increase total costs significantly.

When a low percentage of increased demand and fast technological evolution are observed, the total production cost decreases, whereas the total production cost is expected to increase when demand grows by high percentage and technological evolution happens slowly in the future. Because the model is run for fixed facility size and mandatory strict regulations are assumed, capacity expansion is not allowed after a certain production volume. This is the reason that shortage values increase with a high percentage of increased CNT demand.

■ CONCLUSION

Interest in advanced manufacturing is swelling in the United States, Europe, and Asia. With new nanomanufacturing processes under development, funding from government and industry consortia will not only introduce technology disruptions but will also invigorate market demand for nanomaterials and nanoenabled products. The expansion optimization models developed and presented are timely and can be valuable for companies using various nanomanufacturing processes.

Capacity expansion planning in nanomanufacturing can be challenging for decision makers due to uncertainties in demand, changes in technology, and occupational safety regulations. The model presented in this paper would be helpful for companies in the nanomanufacturing industry to make decisions under unknown conditions. For instance, when rapid technology evolution is expected to happen or when regulation is expected to become more stringent, the model recommends no expansion with larger process lines in the first period and instead recommends postponing until new technologies are available that have higher production rates with lower CNTs releases into the work environment. When higher consumption, less stringent regulation, and slow technology evolution are expected in the future, an expansion with larger process lines in the first period is recommended. The model recommends the timing for expansion as well as expansion quantities for each technology. In addition to expansion planning, results from the model also offer visions for production planning and occupational safety management decisions. As a result, the model provides insights to decision makers in the nanomanufacturing industry regarding expansion strategies, production planning decisions, and occupational safety management decisions for various scenarios depending on the input parameters.

The MSP model created in this work serves as a decision support tool to help manufacturers improve planning for capacity expansion in markets with large uncertainties in technology and the regulatory environment. A disadvantage of the MSP model is the long run times; the number of scenarios increases exponentially with the planning periods. However, by using the MSP model, nanomanufacturing producers can compare capacity expansion strategies to minimize company expenditures and revenue losses due to demand fluctuations. The model also helps manufacturers to manage occupational exposures within the regulatory exposure limits.

Results from these models are already finding application in industry. Moving forward and working with companies, the model will be modified to optimize the facility size in order to remove the capacity expansion restrictions due to the predetermined fixed capacity and occupational safety regulations. Therefore, facility size will also be determined with consideration of a future increased demand, technological evolution, and regulation scenarios. The model can be also extended by including additional sustainable manufacturing indicators/metrics such as water intensity, energy intensity, and greenhouse gas intensity for carbon nanotube production processes. Consequently, the model will be useful for decisions on new facility development and expansion.

■ ASSOCIATED CONTENT

Ⓢ Supporting Information

Detailed explanation of Monte Carlo simulation model, output of the simulation model, input data for multistage stochastic programming model, results for MSP model, and input data for design of experiment analysis. This material is available free of charge via the Internet at http://pubs.acs.org.

■ AUTHOR INFORMATION

Corresponding Author

*E-mail: j.isaacs@neu.edu. Telephone: 617-373-3989. Fax 617-373-2981.

Notes

The authors declare no competing financial interest.

■ ACKNOWLEDGMENTS

We thank A. Busnaina, M. Eckelman, A. Hakimian, and other members of the NSF-funded Nanoscale Science and Engineering Center for High-rate Nanomanufacturing (EEC-0832785) and C. Bosso, W. Walker, and other members of the Nanotechnology and Society Research Group (SES-0609078). This work was supported by National Science Foundation Scalable Nanomanufacturing Awards CMMI-1120329 and EEC-0832785.

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