Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Supporting Information for

Sustainable CNT-enabled Lithium-ion Battery Manufacturing: Evaluating the Tradeoffs

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This Supporting Information contains:

1. Mathematical equations and notations for input parameters and decision variables of the stochastic goal programming model;
2. Battery life cycle including alternative energy and materials sources;
3. Input data for stochastic goal programming model;
4. Interaction matrix among different criteria and their influence on total production cost; and
5. Response surface plots of production cost and contour maps of the respective response surfaces to the combination of different criteria

Notations for parameters and decision variables in stochastic goal programming model

Notations and parameters used in the model include the following:

g : index of occupational safety level $g \in \{1,2,\dots,4\}$

h : index of material source type, $h \in \{1, 2\}$

i : index of product type, $i \in \{1,2\}$

j : index of energy type, $j \in \{1,2,3\}$

k : index of demand scenarios, $k \in \{1,2,\dots,K\}$

m : index of material type, $m \in \{1,2,\dots,N\}$

p : demand scenario probability

t : index of period, $t \in \{1,2,\dots,T\}$

$w_c^{+/-}$: weights for each criteria c under achievement (+) or over (-) achievement from goals

G_c : goal for criteria c

D_{ikt} : demand for product i in scenario k in period t

C_t^I : inventory cost in period t

C_t^S : shortage cost in period t, assumed to be equal to the unit cost of current battery

C_{mt}^R : cost for purchasing secondary material from type m in period t ($/kg)

C_{jt}^E : cost for purchasing energy from source j in period t ($/kWh)

γ_j : CO_2 avoided when energy source j is preferred to consume (kg/kWh)

δ_m : amount of material type m required to produce lithium-ion battery (g/unit)

μ^Q : lower bound of production volume of battery with CNTs

θ^Q : energy consumed to produce one product (kWh/unit)

θ^C : energy consumed to produce 1 g of MWCNTs

θ_m^R : energy used to produce material type m

$f_{1i}(\bullet)$: function to calculate the cost of producing product type i

$$f_{1i}(Q_{ikt}) = a_1 Q_{ikt}$$

$f_{2g}(\bullet)$: function to calculate the cost of EHS control level g

$$f_{2g}(H_{gkt}, Y_{gkt}) = a_{2g}H_{gkt} + b_{2g}Y_{gkt}$$

$f_{3g}(\bullet)$: function to calculate the energy required to operate the EHS control level g

$$f_{3g}(H_{gkt}, Y_{gkt}) = a_{3g}H_{gkt} + b_{3g}Y_{gkt}$$

$f_{4l}(\bullet)$: function to calculate the cost of capacity expansion – fixed cost

$$f_{4l}\left(\sum_{t=1}^{T-1} X_{kt}\right) = a_{4l}\left(\sum_{t=1}^{T-1} X_{kt}\right) + b_{4l}$$

$f_{5n}(\bullet)$: function to calculate total exposure when there are no EHS control measures

$$f_{5n}(Q_{2kt}, Z_{kt}) = a_{5n}Q_{2kt} + b_{5n}Z_{kt}$$

Decision variables are as follows:

d_{ck}^{+} : under goal G_c for scenario k

d_{ck}^{-} : over goal G_c for scenario k

$(TC)_k$: total cost in scenario k

$(TEU)_k$: total energy use in scenario k

$(TEA)_k$: total CO_2 emission avoided in scenario k

$(TE)_{kt}$: final exposure rate ($\mu g/m^3$ air) in scenario k in period t

$(NMI)_k$: total non-renewable material intensity over product life time in scenario k

ε_{gkt} : final CNT exposure ($\mu g/m^3$ air) for EHS control level g in scenario k in period t

X_{kt} : capacity expansion in scenario k in period t

Q_{ikt} : production volume of product i in scenario k in period t

E_{jkt} : energy type j purchased in scenario k in period t

H_{gkt} : production volume of product 2 (battery with CNTs) produced with EHS control level g in scenario k in period t

R_{hikmt} : amount of material m obtained through source type h (either primary or secondary) for product i in scenario k in period t

I_{ikt} : inventory level for product i in scenario k in period t

S_{ikt} : shortage level for product i in scenario k in period t

$$V_{kl} = \begin{cases} 1 \text{ if total capacity is between } e_l \text{ and } e_{l+1} \text{ in scenario } k \\ 0 \text{ if total capacity is not between } e_l \text{ and } e_{l+1} \text{ in scenario } k \end{cases}$$

C_k^X : capacity expansion cost in scenario k

$Z_{kt} = \begin{cases} 1 \text{ if product 2 is produced in scenario } k \text{ in period } t \\ 0 \text{ if product 2 is not produced in scenario } k \text{ in period } t \end{cases}$

$W_{knt} = \begin{cases} 1 \text{ if production volume of product 2 is between } \varphi_n \text{ and } \varphi_{n+1} \text{ in scenario } k \\ 0 \text{ if production volume of product 2 is not between } \varphi_n \text{ and } \varphi_{n+1} \text{ in scenario } k \end{cases}$

A_{kt} : CNTs exposure concentration ($\mu g/m^3$ air) when no EHS control measures are installed in scenario k in period t

F_g : Fg is a safety factor; it is 1 for g = 1 (no EHS control); it is a positive fraction for g = 2, 3, and 4 (low, medium, and high EHS control); the higher the EHS control level, the smaller the fraction.

$Y_{gkt} = \begin{cases} 1 \text{ if EHS control level } g \text{ is preferred in scenario } k \text{ in period } t \\ 0 \text{ if EHS control level } g \text{ is not preferred in scenario } k \text{ in period } t \end{cases}$

Definition of Goal Programing Model Variables

***Definition total production cost*:**

$$(TC)_k = \left(C_k^X\right) + \left(\sum_{t=2}^{T}\sum_{i=1}^{I}\left(I_{ipt}C_t^I + S_{ipt}C_t^S\right)\right) + \left(\sum_{t=2}^{T}\sum_{i=1}^{I} f_{1i}\left(Q_{ikt}\right)\right) + \left(\sum_{t=2}^{T}\sum_{j=1}^{3} C_{jt}^E E_{jkt}\right) + \left(\sum_{t=2}^{T}\sum_{g=1}^{3} f_{2g}\left(H_{gkt}, Y_{gkt}\right)\right) + \left(\sum_{t=2}^{T}\sum_{i=1}^{I}\sum_{m=1}^{M} C_{mt}^R R_{2ikmt}\right) \qquad \forall k$$

It includes the initial expansion cost, expected inventory and shortage cost, manufacturing cost for each product, renewable energy cost, secondary material cost, and EHS assurance cost for each demand scenario.

Definition of the total non-renewable energy

$$(TEU)_k = \sum_{t=2}^{T} E_{1kt} + \sum_{t=2}^{T} Q_{2kt}\theta^C + \sum_{h=1}^{2}\sum_{i=1}^{I}\sum_{m=1}^{M}\sum_{t=2}^{T} R_{hikmt}\theta_m^R \qquad \forall k$$

It accounts for non-renewable energy consumed for producing batteries, CNTs, and input materials as well as energy used for maintaining EHS controls.

Definition of the total CO_2 emission avoided:

$$\left(TEA\right)_k = \sum_{t=2}^{T}\sum_{j=1}^{2} E_{jkt}\gamma_j \qquad \forall k$$

Definition of the total primary material intensity over product life time:

$$\left(NMI\right)_k = \sum_{t=2}^{T}\sum_{m=1}^{M}\sum_{i=1}^{I}\frac{R_{2ikmt}}{\sigma_i} \qquad \forall k$$

Definition of the total CNT exposure in each scenario:

$$\left(TE\right)_{kt} = \left(\sum_{g=1}^{G}\varepsilon_{gkt}\right) \qquad \forall k;\ \ t = 2,\ldots,T$$

Stochastic Goal Programming Model

The objective function minimizes the weighted deviation from the targets for measures including the total production cost, total non-renewable energy use, CO_2 emissions avoided, primary material intensity, and CNT exposure level.

$$\text{Minimize}\ \left[\sum_{k=1}^{\mu^{T-1}} p_k\left(d_{1k}^{-}w_1^{-} + d_{2k}^{-}w_2^{-} + d_{3k}^{+}w_3^{+} + d_{4k}^{-}w_4^{-}\right)\right] + \left(\sum_{k=1}^{\mu^{T-1}} p_k \sum_{t=2}^{T}\left(d_{5kt}^{-}w_5^{-}\right)\right)$$

The above objective function is subject to the following constraints.

Constraints (1-5) ensure that the total production cost, total non-renewable energy, total CO_2 emission avoided, primary material intensity over product life, and total exposure rate do not deviate from their respective targets by an allowable tolerance limit.

$$(TC)_k - G_1 \le d_{1k}^{-} \qquad \forall k \tag{1}$$

$$(TEU)_k - G_2 \leq d_{2k}^{-} \qquad \forall k \tag{2}$$

$$(TEA)_k - G_3 \geq (-d_{3k}^{+}) \qquad \forall k \tag{3}$$

$$(NMI)_k - G_4 \leq d_{4k}^{-} \qquad \forall k \tag{4}$$

$$(TE)_{kt} - G_5 \leq d_{5kt}^{-} \qquad \forall k;\ t = 2, \ldots, T \tag{5}$$

Constraint (6) ensures that the capacity in each period is equal to or larger than the total production volume in each period.

$$\sum_{i=1}^{2} Q_{ikt} \leq \sum_{\tau=1}^{t-1} X_{kt} \qquad \forall k; \quad t = 2, \ldots, T \tag{6}$$

E_{jkt} is identified as the energy used in the manufacturing facility. Constraint (7) ensures that the total energy required for producing lithium-ion batteries and maintaining EHS control measures when the company produces the lithium-ion battery with CNTs is equal to the summation of all energy types used. The total energy required for maintaining EHS control measures is a function of total production volume of lithium-ion batteries with CNTs (H_{gkt}) and level of EHS control (Y_{gkt}).

$$\sum_{j=1}^{3} E_{jkt} = \sum_{i=1}^{2} Q_{ikt}\theta^{Q} + \left(\sum_{g=1}^{3} f_3\big(H_{gkt}, Y_{gkt}\big)\right) \qquad \forall k;\ t = 2, \ldots, T \tag{7}$$

It is assumed that the lithium-ion battery company has a preference for using both primary/virgin and secondary material types. Therefore, Constraint (8) ensures that the total weight of the materials used to produce the batteries is equal to the summation of both material types (primary/virgin or secondary) purchased.

$$\sum_{h=1}^{2} R_{hikmt} = Q_{ikt}\delta_m \qquad \forall i, k, m; \quad t = 2, \ldots, T \tag{8}$$

Constraints (9-10) calculate inventory and shortage values in period *t*. Constraint (9-10) ensures that either inventory or shortage is zero in each period. From period 3 and onwards, the previous period's inventory is also taken into account to calculate the current period's inventory or shortage. When company cannot meet the demand in period *t*, it is assumed that the company loses revenue due to not meeting the demand.

$$I_{ik2} - S_{ik2} = Q_{ik2} - D_{ik2} \qquad \forall i, k \tag{9}$$

$$I_{ikt} - S_{ikt} = Q_{ikt} - D_{ikt} + I_{ik(t-1)} \qquad \forall i, k;\ t = 3, \dots, T \tag{10}$$

According to the previous study on economic analysis of lithium-ion battery production[6], the association between capacity expansion volume and expansion cost is exponential. Cost per expansion volume is higher when the company prefers to increase the capacity in lower amounts as compared to when the company prefers to increase the capacity in higher volumes. The exponential function was linearized (converted to 3 linear functions) to use in the linear stochastic goal programming model. Based on the capacity expansion volume, the model picks one of the linear function to calculate the expansion cost. Constraints (11-14) calculate the expansion costs. If the final capacity in period *T* is between e_l and e_{l+1}, then V_{kl} is equal to 1, and the expansion cost is calculated by using the fitted equation $f_{4l}(\sum_{t=1}^{T-1} X_{kt})$; otherwise V_{kl} is equal to 0 to indicate that the final capacity has no limits.

$$\sum_{t=1}^{T-1} X_{kt} \le e_{l+1} + M(1 - V_{kl}) \qquad \forall k;\ l = 1, \dots, L-1 \tag{11}$$

$$\sum_{t=1}^{T-1} X_{kt} \ge e_l - M(1 - V_{kl}) \qquad \forall k;\ l = 1, \dots, L-1 \tag{12}$$

$$\sum_{l=1}^{L} V_{kl} = 1 \qquad \forall k;\ l = 1, \dots, L-1 \tag{13}$$

$$C_k^X \geq \left[f_{4l} \left(\sum_{t=1}^{T-1} X_{kt} \right) \right] - M(1 - V_{kl}) \qquad \forall k;\ l = 1, \dots, L-1 \tag{14}$$

Constraint (15) enforces a lower limit on the production volume if the company decides to produce lithium-ion batteries with CNTs.

$$Q_{2t} \geq \ \mu^Q(Z_{kt}) \qquad \forall k;\ \ t = 2, \dots, T \tag{15}$$

CNT exposure level is a function of production volume and workspace volume. As the production volume increases the workspace volume increases exponentially. Therefore, the association between CNT lithium-ion battery production volume and CNT exposure level is exponential. CNTs exposure per production volume is higher when the company prefers to produce CNT lithium-ion batteries in low volume as compared to when the company prefers to produce them in high volume . Constraints (16-20) calculate the exposure levels when the company produces CNT-enabled lithium-ion batteries. The exposure concentration without EHS controls (A_{kt}) is calculated based on the production volume (Q_{2kt}) of lithium-ion batteries with CNTs.

$$Q_{2kt} \leq \varphi_{n+1} Z_{kt} + M(1 - W_{knt}) \qquad \forall k;\ \ n = 1, .., N-1;\ \ t = 2, \dots, T \tag{16}$$

$$Q_{2kt} \geq \varphi_n Z_{kt} - M(1 - W_{knt}) \qquad \forall k;\ \ n = 1, .., N-1;\ \ t = 2, \dots, T \tag{17}$$

$$\sum_{n=1}^{N} W_{knt} = 1 \qquad \forall k;\ \ n = 1, \dots, N-1;\ \ t = 2, \dots, T \tag{18}$$

$$A_{kt} \geq [f_{5n}(Q_{2kt}, Z_{kt})] - M(1 - W_{knt}) \quad \forall k;\; n = 1, .., N-1;\; t = 2, \dots, T \tag{19}$$

$$A_{kt} \leq [f_{5n}(Q_{2kt}, Z_{kt})] \quad \forall k;\; n = 1, .., N-1;\; t = 2, \dots, T \tag{20}$$

Constraint (21) ensures that only one EHS control level exists when the company produces lithium-ion batteries with CNTs.

$$\sum_{g=1}^{G} Y_{gkt} = Z_{kt} \quad \forall k;\; t = 2, \dots, T \tag{21}$$

Constraint (22) ensures that the EHS control level is not lowered. For example, if $Y_{2k2} = 1$, then either Y_{2k3} or Y_{3k3} must be 1 in period 3.

$$\sum_{g}^{G} Y_{gk(t+1)} \geq Y_{gkt} \quad \forall k, g;\; t = 2, \dots, T-1 \tag{22}$$

Constraint (23-24) calculates the final exposure when EHS control level g exists in the company.

$$\varepsilon_{gkt} \geq A_{kt} F_g - M\left(1 - Y_{gkt}\right) \quad \forall k;\; t = 2, \dots, T \tag{23}$$

$$\left(\varepsilon_{gkt}\right) \leq \mathrm{A}_{kt}\, \mathrm{F}_g \quad \forall k; \forall g;\; t = 2, \dots, T \tag{24}$$

In order to calculate the EHS cost, production volume of batteries with CNTs for each EHS control level g needs to be calculated. In each period, the model picks only one EHS control level (Constraint 21). Constraint (25-27) ensures that the company use EHS control level that caters to the production volume of batteries with CNTs. Constraint (25-27) calculates the production volume of batteries with CNTs when EHS control level g exists in the company.

$$H_{gkt} \geq Q_{2kt} - M\left(1 - Y_{gkt}\right) \quad \forall g, k;\; t = 2, \dots, T \tag{25}$$

$$H_{gkt} \leq Q_{2kt} + M\left(1 - Y_{gkt}\right) \quad \forall g, k;\; t = 2, \dots, T \tag{26}$$

$$H_{gkt} \le MY_{gkt} \qquad \forall g,k;\ t = 2,\ldots,T \tag{27}$$

Constraints (28-31) set the binary variables.

$$V_{kl} \in \{0,1\} \qquad \forall k,l \tag{28}$$

$$W_{knt} \in \{0,1\} \qquad \forall k;\ \ n = 1,..,N-1;\ \ t = 2,\ldots,T \tag{29}$$

$$Y_{gkt} \in \{0,1\} \qquad \forall g,k;\ \ t = 2,\ldots,T \tag{30}$$

$$Z_{kt} \in \{0,1\} \qquad \forall\ k;\ \ t = 2,\ldots,T \tag{31}$$

Constraint (32) ensures that all the variables are non-negative.

$$A_{kt}, E_{jkt}, H_{gkt}, I_{ikt}, R_{hikmt}, Q_{ikt}, S_{ikt}, \varepsilon_{gkt}, X_{kt} \ge 0 \qquad \forall g,h,i,j,k;\ \ t = 2,\ldots,T \tag{32}$$

Constraint (33) declares the integer variables.

$$E_{jkt}, H_{gkt}, I_{ikt}, R_{hikmt}, Q_{ikt}, S_{ikt}, X_{kt} \in Z \qquad \forall g,h,i,j,k;\ \ t = 2,\ldots,T \tag{33}$$

In addition to the above listed constraints, non-anticipativity constraints are included. For the three periods and nine hypothetical demand scenarios considered for validation of this model (see Figure 1a), twelve non-anticipativity constraints (34-45) ensure that all of the demand scenarios with a common history have the same decisions up to the current time.

$$A_{12} = A_{22} = A_{32}; A_{42} = A_{52} = A_{62}; A_{72} = A_{82} = A_{92} \tag{34}$$

$$E_{j12} = E_{j22} = E_{j32}; E_{j42} = E_{j52} = E_{j62}; E_{j72} = E_{j82} = E_{j92} \qquad \forall j \tag{35}$$

$$H_{g12} = H_{g22} = H_{g32}; H_{g42} = H_{g52} = H_{g62}; H_{g72} = H_{g82} = H_{g92} \qquad \forall g \tag{36}$$

$$I_{i12} = I_{i22} = I_{i32}; I_{i42} = I_{i52} = I_{i62}; I_{i72} = I_{i82} = I_{i92} \qquad \forall i \tag{37}$$

$$R_{h1m2} = R_{h2m2} = R_{h3m2}; R_{h4m2} = R_{h5m2} = R_{h6m2}; R_{h7m2} = R_{h8m2} = R_{h9m2} \qquad \forall h,m \tag{38}$$

$$Q_{i12} = Q_{i22} = Q_{i32}; Q_{i42} = Q_{i52} = Q_{i62}; Q_{i72} = Q_{i82} = Q_{i92} \qquad \forall i \tag{39}$$

$$S_{i12} = S_{i22} = S_{i32}; S_{i42} = S_{i52} = S_{i62}; S_{i72} = S_{i82} = S_{i92} \qquad \forall i \tag{40}$$

$$W_{1n2} = W_{2n2} = W_{3n2}; W_{4n2} = W_{5n2} = W_{6n2}; W_{7n2} = W_{8n2} = W_{9n2} \qquad n = 1,\ldots,N-1 \tag{41}$$

$$X_{12} = X_{22} = X_{32}; X_{42} = X_{52} = X_{62}; X_{72} = X_{82} = X_{92} \tag{42}$$

$$Y_{g12} = Y_{g22} = Y_{g32}; Y_{g42} = Y_{g52} = Y_{g62}; Y_{g72} = Y_{g82} = Y_{g92} \qquad \forall g \tag{43}$$

$$Z_{12} = Z_{22} = Z_{32}; Z_{42} = Z_{52} = Z_{62}; Z_{72} = Z_{82} = Z_{92} \tag{44}$$

$$\varepsilon_{12} = \varepsilon_{22} = \varepsilon_{32}; \varepsilon_{42} = \varepsilon_{52} = \varepsilon_{62}; \varepsilon_{72} = \varepsilon_{82} = \varepsilon_{92} \tag{45}$$

Battery life cycle including alternative energy and materials sources

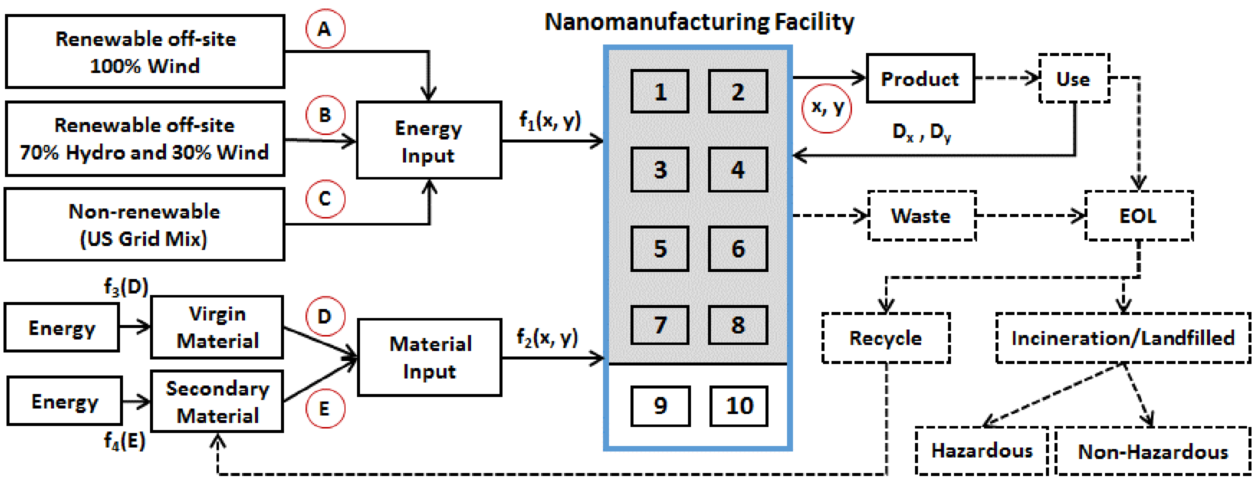


Figure S1: Sustainable manufacturing indicators/metrics (renewable proportion of energy consumed, CO2 emission avoided and recycled content of material input) considered in the study; dashed lines indicate processes outside the scope of this study. ABCDE represent the quantities of the respective flows, with x and y as the products (traditional and CNT-enabled batteries), and D_x and D_y are the demand for each, respectively. The nanomanufacturing facility shows 6 existing fabrication lines with expansion capacity for two additional lines in this case. The cost functions, $f_i(\bullet)$, are explained in the nomenclature above.

Input data for stochastic goal programming model

Table S1 Data pertaining to conventional and CNT-enabled lithium-ion batteries

Model Parameter related to Lithium-ion Batteries	**Value**
Number of cylindrical cells per module [6]	6
Battery weight [6]	0.41 kg
Variable costs [6]	Raw material cost, labor cost, and energy cost
Variable cost for conventional a lithium-ion battery [6]	$18 per battery
Variable cost for a CNT-enabled lithium-ion battery [6]	$22 per battery
Energy to produce a conventional lithium-ion battery [6]	4.39 kWh per battery
Energy to produce a CNT-enabled lithium-ion battery [6]	4.39 kWh per battery
Energy required to produce 1 g of CNTs [7]	0.052 kWh
Shortage cost for a conventional lithium-ion battery [6]	$32 per battery
Shortage cost for a CNT-enabled lithium-ion battery [6]	$45 per battery
Inventory cost	Assumed negligible
Scope of the stochastic goal programming model	3 periods and 9 demand scenarios

Table S2 Carbon emissions and purchase cost for each energy types

Energy Type	**Carbon Emission (kg CO_2/Kwh)**	**Purchase Cost*** ($/Kwh)**
US Grid Mix	0.76*	0.15
100% Wind	0.012**	0.188
30% Wind and 70% Hydro	0.021**	0.174

* ecoinvent: TRACI [1]
** International Panel on Climate Change [2]
*** Based on National Grid electric utility rates [3]

Table S3 **Energy data for producing primary and secondary materials and price data for purchasing primary and secondary materials**

	Energy* (KWh/kg)		**Purchase Cost ($/kg)**	
	Primary	**Secondary**	**Primary**	**Secondary*** **
Lithium	126	31.5	68**	34-136
Nickel	54	13.5	11.11**	5.5-22.22
Cobalt	36	9	31**	15.5-62
Aluminum	55	13.7	1.62**	0.81-3.24
Copper	17	4.2	5.03**	9.50-10.06

* Source: ecoinvent 2.2 [4]

** Source: London Metal Exchange [5]

*** For the base case and Cases A and B, the secondary materials cost is assumed to be the half of the cost of primary materials; for Cases A* and B*, secondary materials are assumed unavailable; and for sensitivity analyses, the secondary material cost is varied from half to twice the primary material cost.

Interaction matrix among different criteria and their influence on total production cost

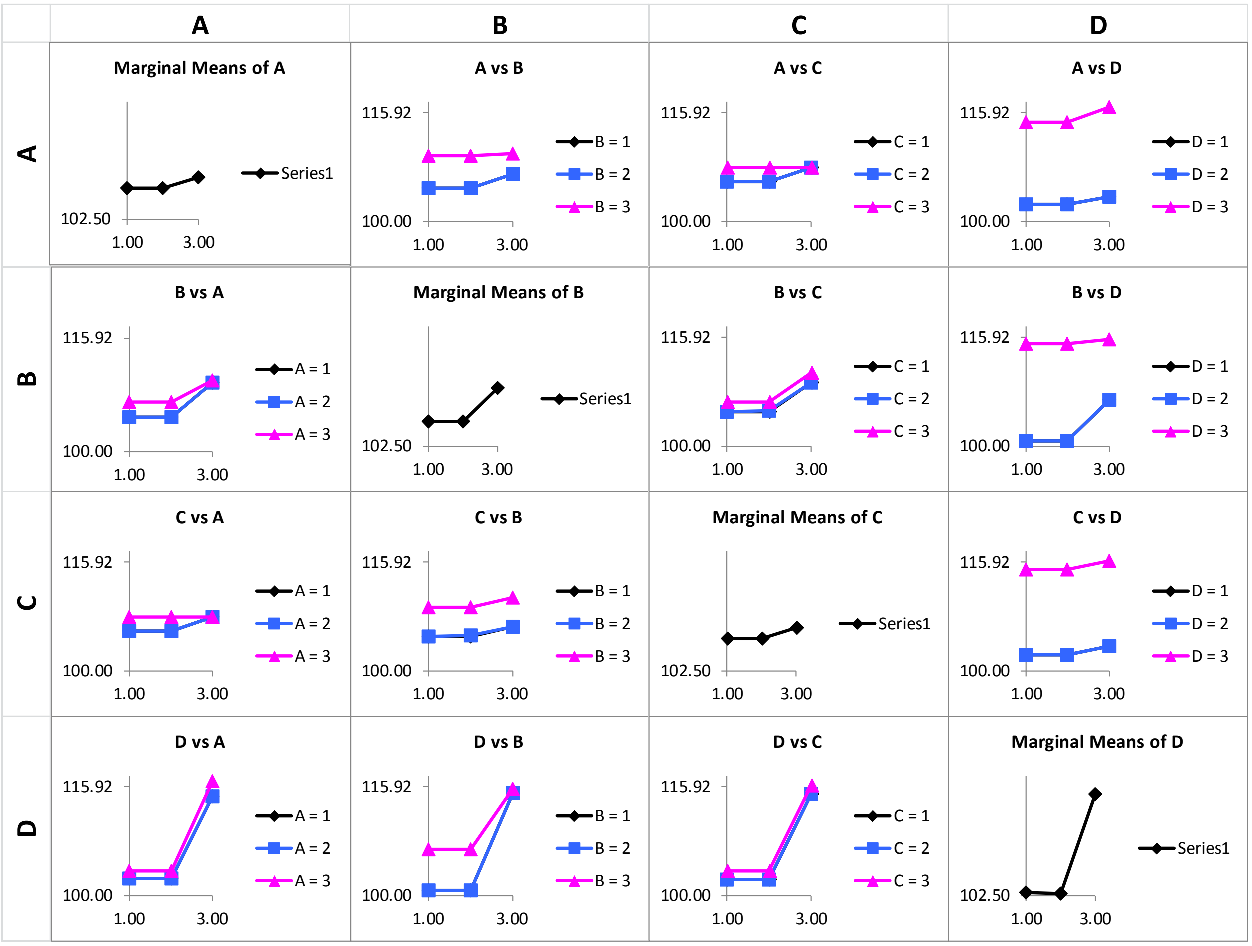


Figure S2: illustrates a pairwise comparison of the impact on total production cost among all the criteria by assigning low, medium and high priority to one of the criterions. A, B, C and D indicate non-renewable energy used, CO_2 emission avoided, primary materials intensity and CNT exposure level, respectively. In each pair, intersected lines illustrate high interaction and significant impact on total production cost, while parallel lines indicate no interaction among the compared pair which means no significant impact on total production cost.

Response surface plots of production cost and contour maps of the respective response surfaces to the combination of different criteria

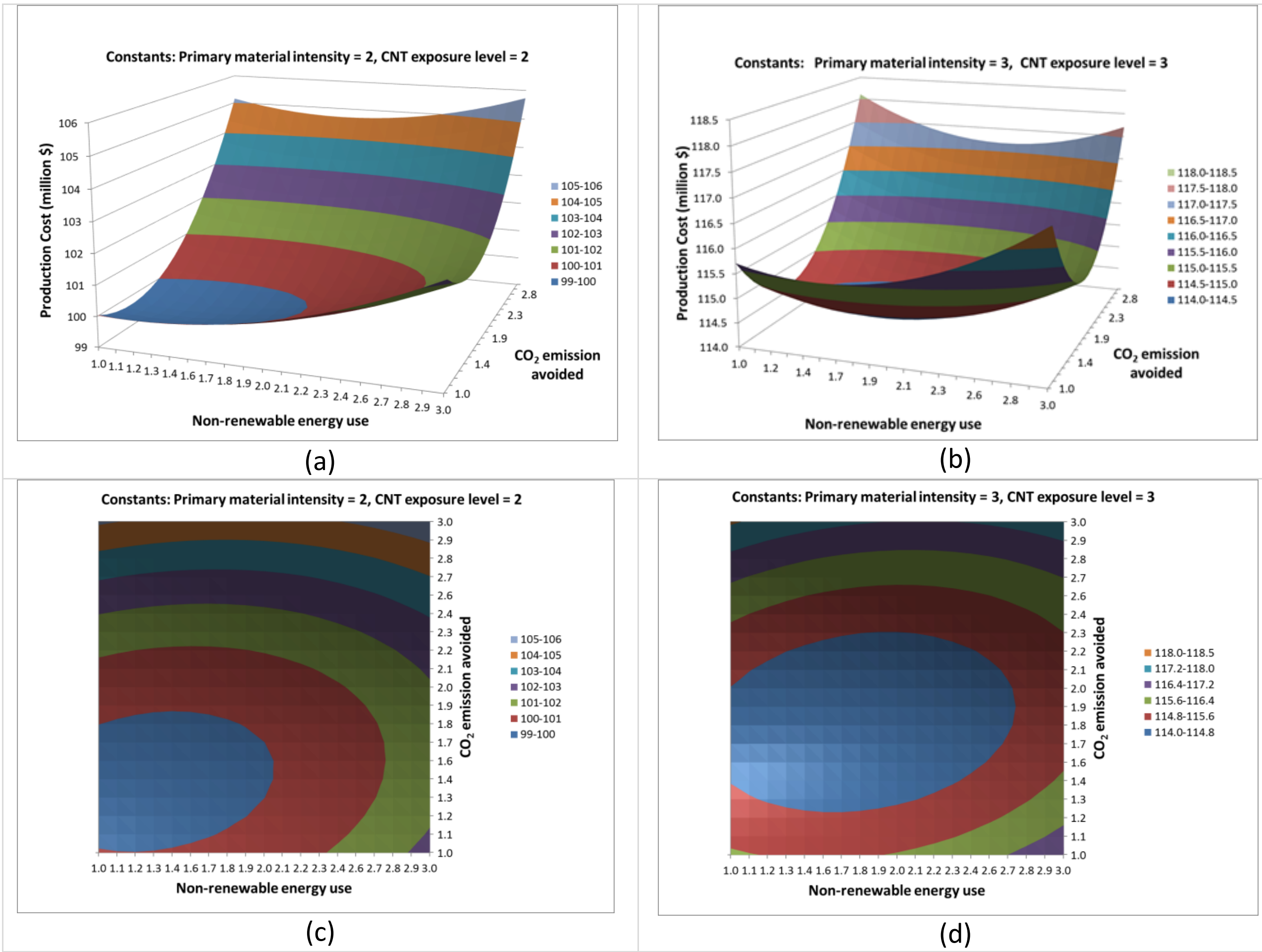


Figure S3: S3a and S3b indicate total production cost response surface plots for low to high priority of non-renewable energy used and CO_2 emission avoided when medium and high priorities are considered for primary material intensity and CNT exposure level, respectively. Figure S3c and S3d illustrate total production cost contour maps for non-renewable energy used and CO_2 emission avoided when medium and high priorities are considered for primary material intensity and CNT exposure level, respectively.

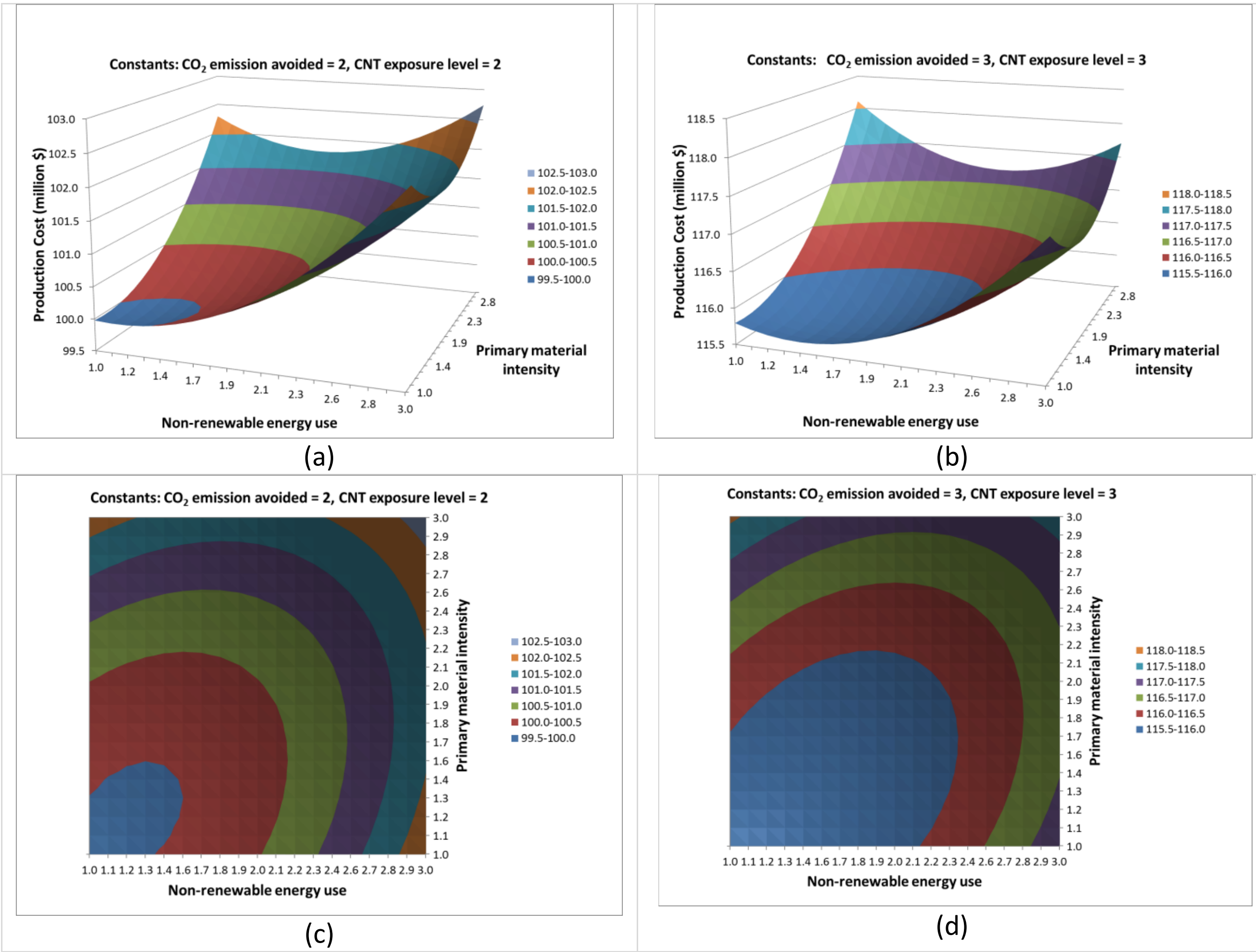


Figure S4: S4a and S4b indicate total production cost response surface plots for low to high priority of non-renewable energy used and primary material intensity when medium and high priorities are considered for CO_2 emission avoided and CNT exposure level, respectively. Figure S4c and S4d illustrate total production cost contour maps for non-renewable energy used and primary material intensity when medium and high priorities are considered for CO_2 emission avoided and CNT exposure level, respectively.

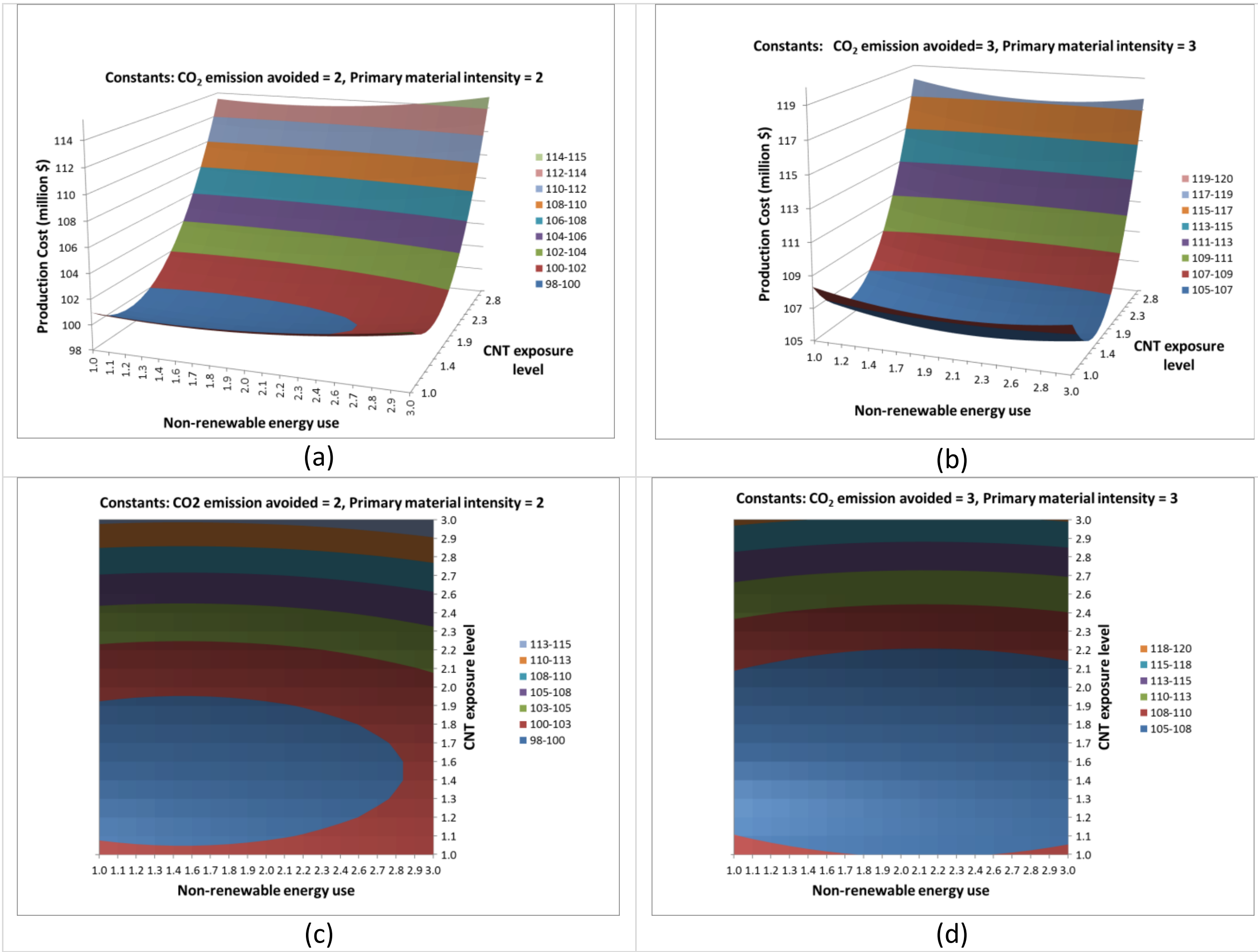
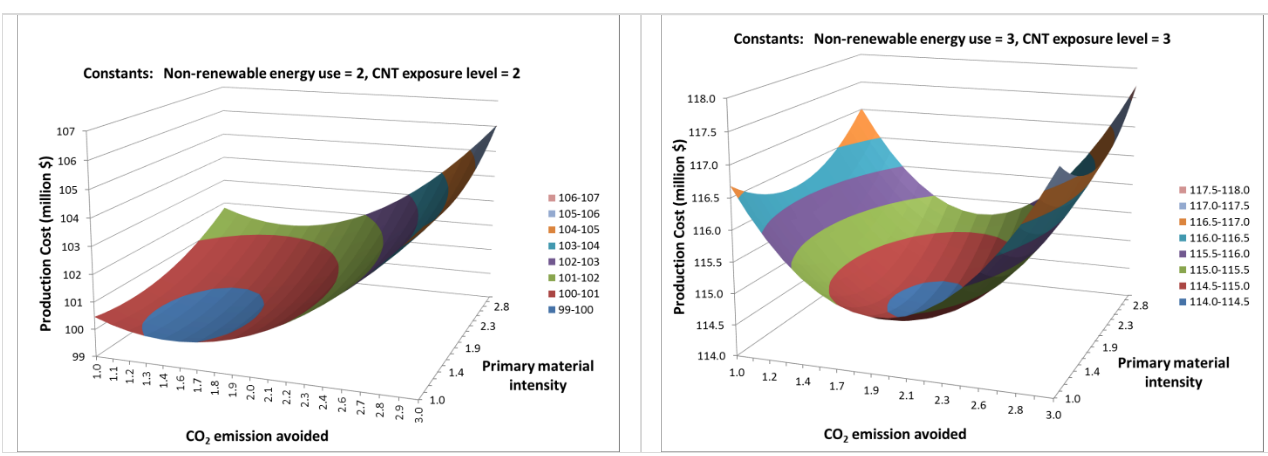


Figure S5: S5a and S5b indicate total production cost response surface plots for low to high priority of non-renewable energy used and CNT exposure level when medium and high priorities are considered for CO_2 emission avoided and primary material intensity, respectively. Figure S5c and S5d illustrate total production cost contour maps for non-renewable energy used and CNT exposure level when medium and high priorities are considered for CO_2 emission avoided and primary material intensity, respectively.



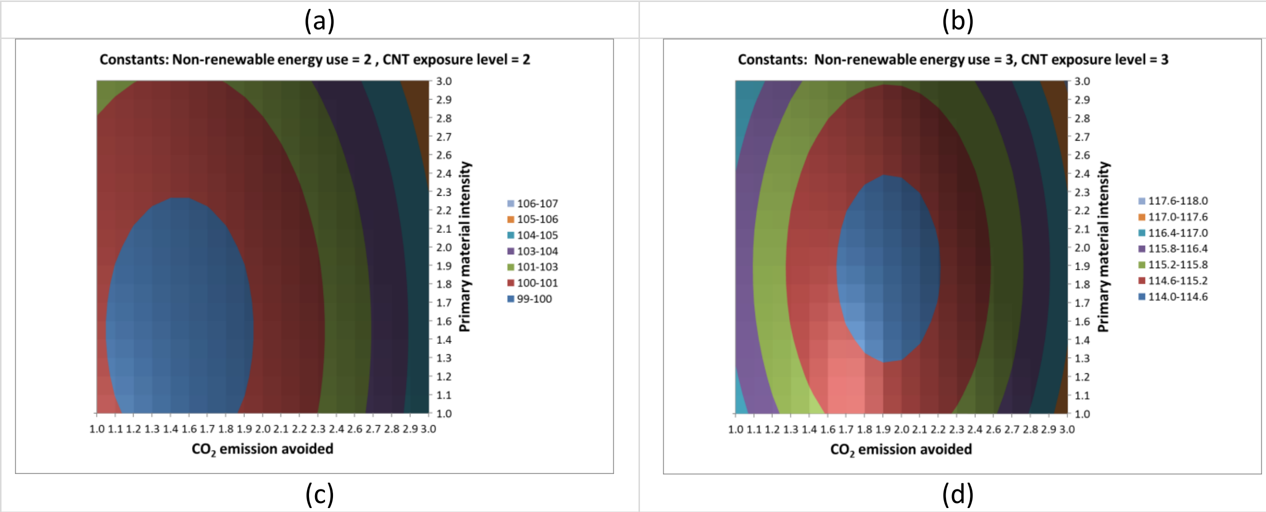
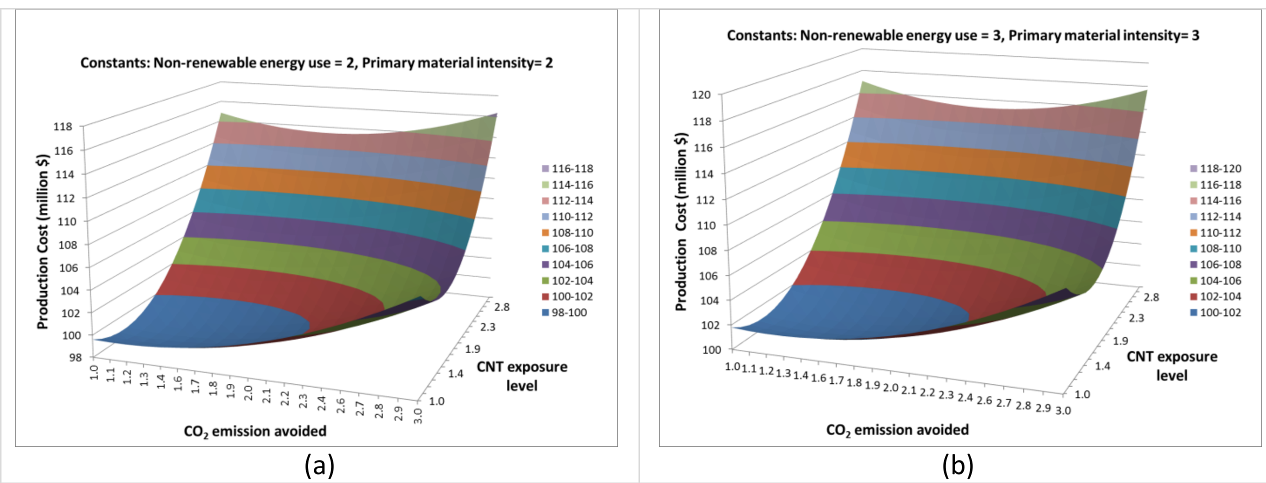
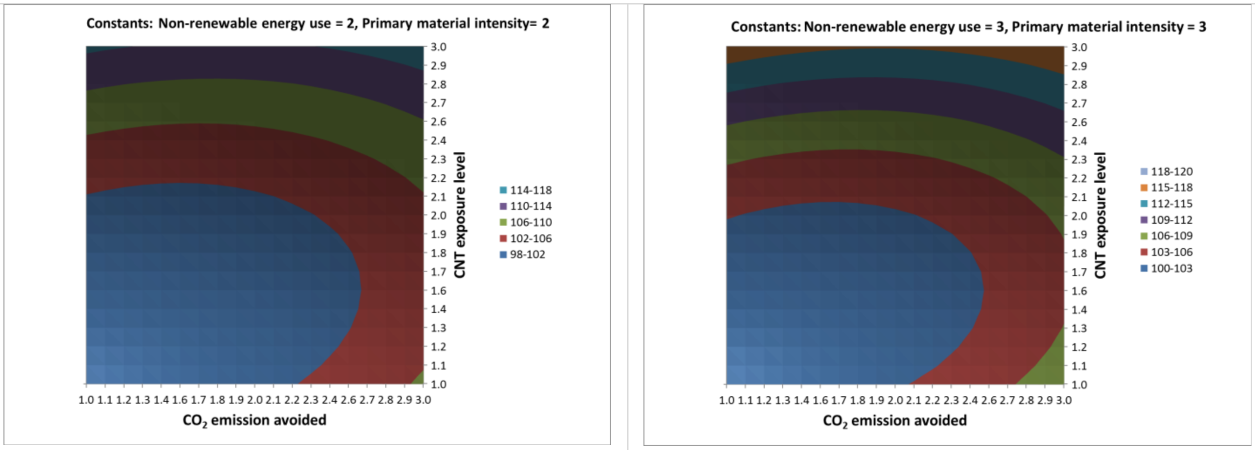


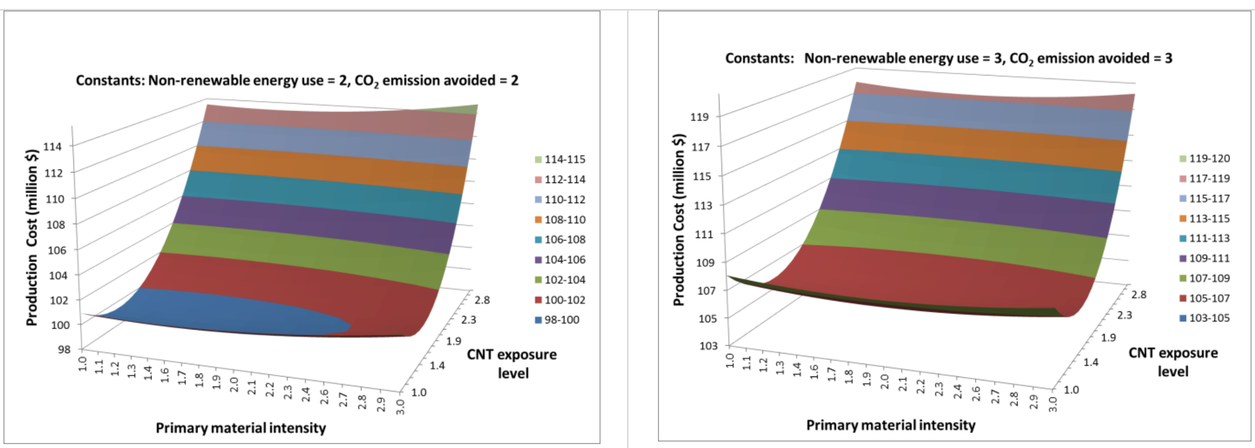
Figure S6: S6a and S6b indicate total production cost response surface plots for low to high priority of CO_2 emission avoided and primary material intensity when medium and high priorities are considered for non-renewable energy used and CNT exposure level, respectively. Figure S6c and S6d illustrate total production cost contour maps for CO_2 emission avoided and primary material intensity when medium and high priorities are considered for non-renewable energy used and CNT exposure level, respectively.



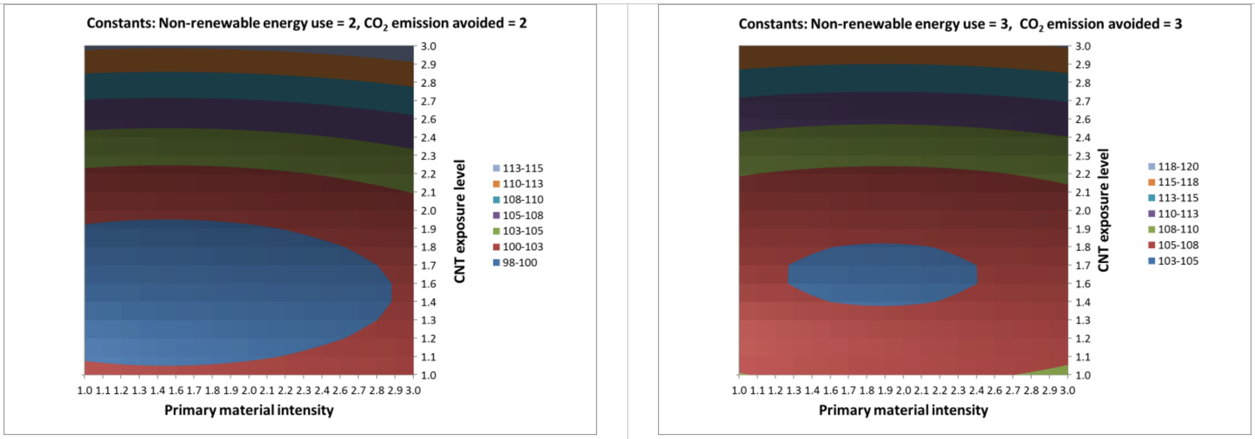


(c) (d)

Figure S7: S7a and S7b indicate total production cost response surface plots for low to high priority of CO_2 emission avoided and CNT exposure level when medium and high priorities are considered for non-renewable energy used and primary material intensity, respectively. Figure S7c and S7d illustrate total production cost contour maps for CO_2 emission avoided and CNT exposure level when medium and high priorities are considered for non-renewable energy used and primary material intensity, respectively.



(a) (b)



(c) (d)

Figure S8: S8a and S8b indicate total production cost response surface plots for low to high priority of primary material intensity and CNT exposure level when medium and high priorities are considered for non-renewable energy used and CO_2 emission avoided, respectively. Figure S8c and S8d illustrate total production cost contour maps for primary material intensity and CNT exposure level when medium and high priorities are considered for non-renewable energy used and CO_2 emission avoided, respectively.

References

1. Ecoinvent Center, ecoinvent Version 2. http://www.ecoinvent.org/database/ecoinvent-version-2/reports-on-ecoinvent-2/reports-on-ecoinvent-2.html, last access August 2016.

2. International Panel on Climate Change (IPCC) Annex III—technology-specific cost and performance parameters. http://www.ipcc.ch/report/ar5/wg3/, last access August 2016.

3. National Grid GreenUp Providers, http://www.nationalgridus.com/masselectric/home/energychoice/4_greenup_provider.asp, last access August 2016.

4. Granta Design, in *CES EDUPACK*, Cambridge, UK, Cambridge, UK, 2015.

5. London Metal Exchange, https://www.lme.com, last access August 2016.

6. Hakimian, A.; Kamarthi, S.; Erbis, S.; Abraham, K. M.; Cullinane, T. P.; Isaacs, J. A., Economic Analysis of CNT Lithium-Ion Battery Manufacturing. *Environmental Science: Nano* 2015, *2*, 463-476, DOI: 10.1039/c5en00078e.

7. Kushnir, D.; Sandén, B. A., Energy Requirements of Carbon Nanoparticle Production. *Journal of Industrial Ecology* 2008**,** *12* (3), 360-375.