Title

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Permalink
https://escholarship.org/uc/item/5hh93790

Journal
Journal of Industrial Ecology, 19(1)

ISSN
1088-1980

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Publication Date
2015-02-01

DOI
10.1111/jiec.12175

The Role of Scale and Technology Maturity in Life Cycle Assessment of Emerging Technologies

A Case Study on Carbon Nanotubes

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Keywords:

carbon nanotubes (CNT)
data maturity
industrial ecology
learning curve
nanotechnology
scaling

Supporting information is available on the *JIE* Web site

Summary

Life cycle assessment (LCA) has been applied for assessing emerging technologies, where large-scale production data are generally lacking. This study introduces a standardized scheme for technology and manufacturing readiness levels to contextualize a technology's development stage. We applied the scheme to a carbon nanotube (CNT) LCA and found that, regardless of synthesis technique, CNT manufacturing will become less energy intensive with increased levels of readiness. We examined the influence of production volume on LCA results using primary data from a commercial CNT manufacturer with approximately 100 grams per day production volume and engineering design of a scaled-up process with 1 tonne per day production capacity. The results show that scaling up could reduce 84% to 94% of its cradle-to-gate impacts, mainly as a result of the recycling of feedstock that becomes economically viable only beyond certain minimum production volume. This study shows that LCAs on emerging technologies based on immature data should be interpreted in conjunction with their technology and manufacturing readiness levels and reinforces the need of standardizing and communicating information on these readiness levels and scale of production in life cycle inventory practices.

Introduction

The need to proactively assess emerging technologies has been acknowledged widely, and life cycle assessment (LCA) has been recognized as a valuable tool to accomplish this task (Klöpffer et al. 2007; Curran 2006). However, when a technology is not mature for mass production, which is often the case with emerging technologies, data are sparsely available and assessments are often based on limited information, such as research publications (Khanna and Bakshi 2009), technology press releases (Khanna et al. 2008), prototypes (Healy et al. 2008), and even patent records (Khanna and Bakshi 2009). Therefore, it is valid to question whether LCA studies on emerging technologies that are based on premature data can adequately represent the environmental impacts of the technologies, after the technologies reach a higher level of maturity or a larger scale of production.

Implications of scaling up of a product or process for manufacturing have been studied in fields such as operations research, economics, and management sciences (Alcorta 1994; Panzar and Willig 1977; Moore 1959; Ferguson 1969). Although less intuitive, the "diseconomies of scale"—where scaling up beyond a certain point has adverse consequences—is also a well-established concept in the literature: An extensive literature

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DOI: 10.1111/jiec.12175

Editor managing review: Stefanie Hellweg

Volume 00, Number 0

review on this topic by Canback and colleagues (2006) indicates that the scale may or may not produce economic benefit, and that the nature of industry will have a role to play. Also, in the LCAs, larger operation scenarios were found to be environmentally efficient when they offered economies of scale for supporting services (Lundin et al. 2000), but proved inefficient when larger scale necessitated more transportation requirements (Bernesson et al. 2004, 2006; Schlich and Fleissner 2004). Thus, there is no unique approach for addressing scaling up, and scaling up may occasionally prove inefficient (Canback et al. 2006; González-Benito and González-Benito 2005).

Among the LCAs on engineered nanomaterials (ENMs), the study by Walser and colleagues (2011) empirically assessed the impact of experience on upscaling from laboratory to pilot plant. Empirical data on plasma polymerization with the silver cosputtering technique producing nanosilver T-shirts at laboratory, and pilot plat scales were available for this study. Their assessment on the commercial-scale production was, however, based on scenarios grounded on engineering estimates, because adequate information on producing nanosilver T-shirts with silver cosputtering technology at the mass scale was not available at the time. In the case of other ENMs, where the commercial production information was also not available, LCAs have simulated scaling up by designing scenarios of process yield enhancements and/or larger scale of production (Khanna et al. 2008; Kushnir and Sandén 2008; Singh et al. 2008). These studies suggest that yield improvement will reduce the environmental impact of ENM manufacturing (Kushnir and Sandén 2008; Singh et al. 2008). This finding is supported by a cost structure study on various synthesis techniques for carbon nanotubes (CNTs), which concluded that, in addition to increased yields, increased working hours could also reduce the production costs (Isaacs et al. 2009). Hence, it appears that the environmental burden of the manufacturing of ENMs could reduce with process maturity, efficiency, and scaling up. However, with the exception of the nanosilver T-shirt study (Walser et al. 2011), the studies leading up to this conclusion are standalone studies of ENMs representing various stages of technological maturity. On this background, the aim of this study is to examine how technological maturity and the scale of production influence the environmental performance of an emerging technology using CNT manufacturing at different scales as an example.

This article is structured as follows: First, the concepts of technology and manufacturing readiness and their respective scales leading to industrial-scale production are introduced. Then, several peer-reviewed LCAs on engineered nanomaterials are assessed with regard to their technology and manufacturing maturity levels with a focus on CNT studies. Next, a case study on single-wall carbon nanotubes (SWCNTs) based on data from a CNT manufacturer on two scales of production is presented, ending with the *Discussion* as the last section of the article.

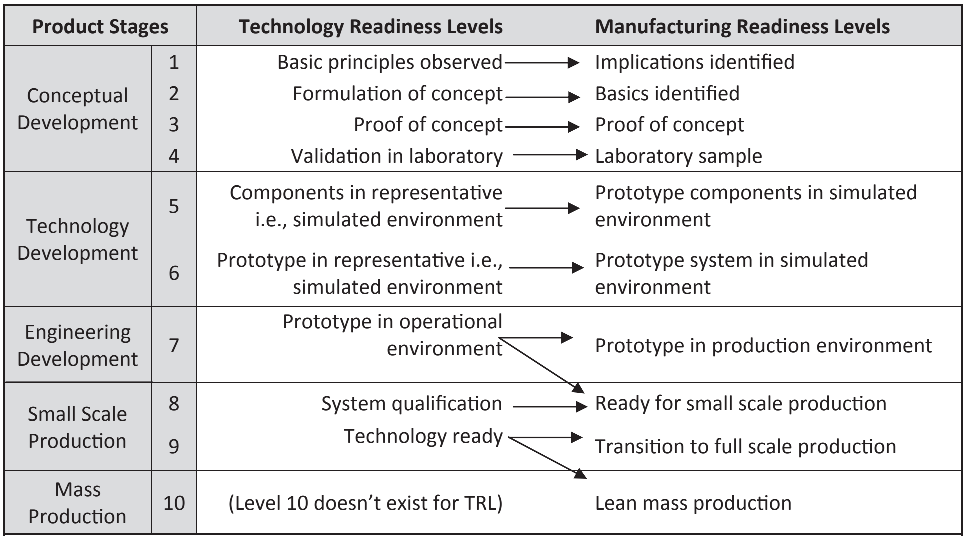
Technology and Manufacturing Readiness Levels

Currently, there are no internationally accepted standards for describing the stage of technology development in LCA. Therefore in this section, we are introducing technology and manufacturing readiness from other established literature. The concept of technology readiness was first addressed by the National Aeronautics and Space Administration (NASA) during the 1960s (Hicks et al. 2009) and was later formalized, also by NASA, into technology readiness levels (TRLs) to provide a systematic measurement system to assess the maturity of a particular technology as well as to conduct a consistent comparison of maturity between different technologies (Mankins 1995). Readiness of technology, however, implies functional readiness, but not manufacturing readiness (Hicks et al. 2009). The latter concept is captured in the manufacturing readiness levels (MRLs) as measured by some U.S. government agencies, including the Department of Defense (DoD) and the National Renewable Energy Laboratory, to assess not just the maturity of a given technology, but also that of components or subsystems from a manufacturing perspective.

Appendix A from the DoD's Deskbook (DoD 2012) on MRL lists extensive criteria to connect TRLs to MRLs. We provide our condensed version of these criteria in figure 1. Levels of manufacturing maturity assume certain corresponding readiness levels of technology. It is important to understand MRLs in relation to corresponding TRLs. For example, some studies (Kushnir and Sandén 2008; Singh et al. 2008) assess the environmental impacts of CNT synthesis at mass production scenario (i.e., at MRL around 9 or 10). In order for MRL to be at 9 to 10, the TRL needs to be at a minimum of 9, as indicated in figure 1. However, in reality, the data available for these studies can be around the TRL 6 to 7 range (Kushnir and Sandén 2008; Singh et al. 2008), which needs to be supplemented with yield and efficiency assumptions to simulate scenarios with MRLs 9 or 10.

Survey Results: Readiness Levels in the Life Cycle Assessments of Engineered Nanomaterials

We examined several peer-reviewed LCAs on ENMs (Bauer et al. 2008; Grubb and Bakshi 2011; Healy et al. 2008; Khanna and Bakshi 2009; Khanna et al. 2008; Köhler et al. 2009; Kushnir and Sandén 2008; Lloyd and Lave 2003; Meyer et al. 2010; Sengül and Theis 2011; Singh et al. 2008; Walser et al. 2011) to assess the readiness level of the technologies at the time of their LCA. The levels were assessed according to the sources of data used; whether the data were supported by a laboratory experiment performed recently or a few years ago, or whether they were based on patent information or taken from publicly available literature by the research groups and manufacturers, and so on, was taken into consideration. The readiness level



Product Stages		Technology Readiness Levels		Manufacturing Readiness Levels
Conceptual Development	1	Basic principles observed	→	Implications identified
	2	Formulation of concept	→	Basics identified
	3	Proof of concept	→	Proof of concept
	4	Validation in laboratory	→	Laboratory sample
Technology Development	5	Components in representative i.e., simulated environment	→	Prototype components in simulated environment
	6	Prototype in representative i.e., simulated environment	→	Prototype system in simulated environment
Engineering Development	7	Prototype in operational environment	→	Prototype in production environment
Small Scale Production	8	System qualification	→	Ready for small scale production
	9	Technology ready	→	Transition to full scale production
Mass Production	10	(Level 10 doesn't exist for TRL)		Lean mass production

Figure 1 Relationship between technology readiness level (TRL) and manufacturing readiness level based on the U.S. Department of Defense Deskbook. Source of data: *DoD*2012

assignments and respective data source information are presented in table S1-1 in the supporting information available on the Journal's website. Our survey indicates that the TRLs of the studies range from 5 to 9, with most being around levels 7 to 8. This indicates that most LCAs were based on data that were technologically in the range from prototype to preproduction sampling, and that manufacturing readiness of these processes had not reached the maturity for mass production at the time of the assessment.

An LCA better represents the environmental performance of full-scale production only when it is performed on a fully mature process (i.e., when at MRL 10). However, waiting for the manufacturing maturity of emerging technologies to be at level 9 or 10 would defeat the purpose of conducting early assessments to proactively identify potential environmental concerns. Hence, it is valuable to understand how indicative and applicable early assessments are when they are based on immature data, and how the results may change when the technology becomes mature. This question will be explored next in the context of production energy requirements for CNTs, because their energy-intensive manufacturing has been highlighted in the literature (Gutowski et al. 2010; Healy et al. 2008; Khanna et al. 2008; Singh et al. 2008).

Readiness Levels and Energy Estimates of Carbon Nanotube Manufacturing

Several LCA studies on CNTs (table S1-1 in the supporting information on the Web) have estimated the energy requirements for CNT synthesis. A compilation of these CNT studies along with two additional engineering studies (Bronikowski et al. 2001; Nikolaev et al. 1999) on CNT manufacturing is provided in table S1-2 in the supporting information on the Web. As illustrated in figure 2, estimates on energy consumption for CNT manufacturing for three different synthesis methods (chemical vapor deposition [CVD], high-pressure carbon monoxide conversion [HiPco], and arc discharge [Arc]) generally decrease progressively as the process matures from laboratory scale (MRL around 6) to small production scale (MRL around 7 to 8) to a mass production scenario (MRL around 10). As the CNT manufacturing becomes more mature from prototype or small-scale production to industrial-scale production, a reduction of approximately two to three orders of magnitude in manufacturing energy intensity can be expected.

With adequate data, the trend observed with TRLs and MRLs can be captured and validated quantitatively with more-established methodologies, such as those employed by learning curve (LC) analysis. To illustrate this, an assessment akin to that of LCs, but based only on limited data points on production energy requirements with the CVD method (four from the literature and two provided by the case study in the next section) and market forecast on production capacity, is provided in supporting information S1 on the Web.

Because of the limited availability of CNT production studies with adequate details, a separate TRL-MRL trend analysis for specific types of CNTs (single-wall, multi-wall, or fiber), feedstock (methane, carbon monoxide [CO], and so on), or even production energy boundaries is currently not possible. Available studies were therefore aggregated based on fabrication technologies used in order to gauge the overall trend. Though some of these LCAs address two different scales, none of them provides production energy requirement at both scales. Moreover, none of them is based on data from a commercial plant. This gap can be partially addressed with a case study on one single product line with two different scales. These data points are provided by a cradle-to-gate study on SWCNTs in the next section. This case study allows an observation on the same process as it ramps up from small-scale to industrial-scale production. Moreover, it is based on the real-life data from a commercial manufacturer of SWCNTs and has thus allowed environmental

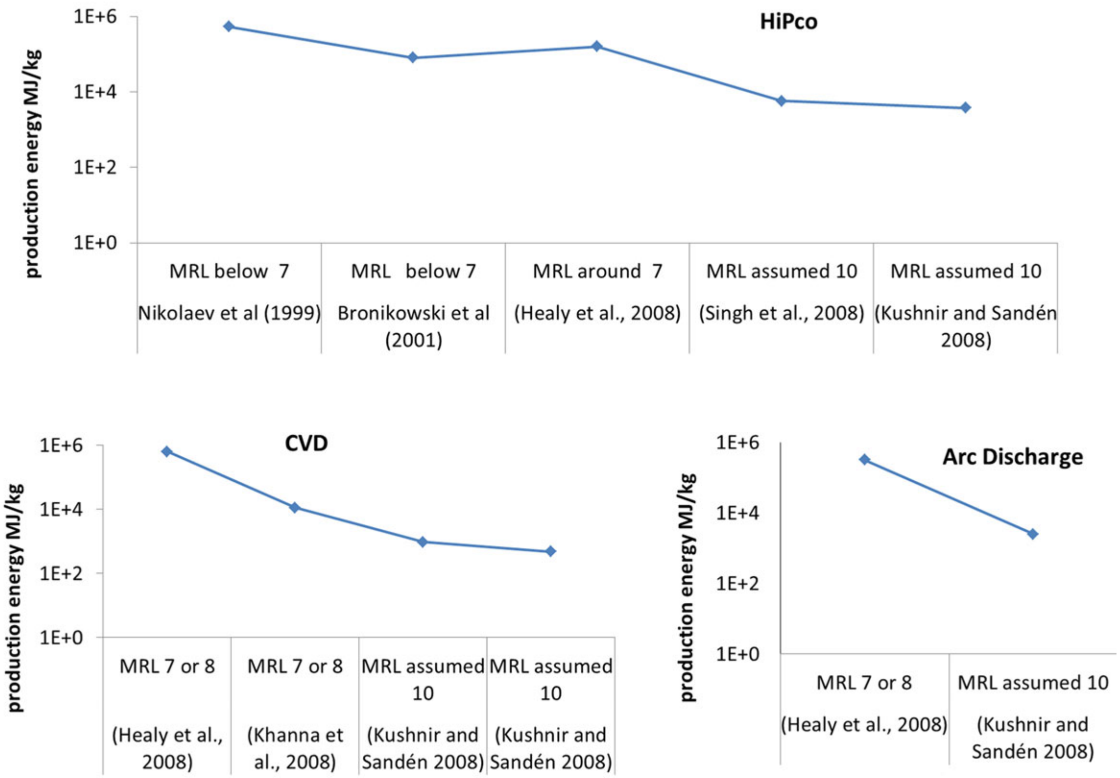


Figure 2 Decrease in energy requirement for carbon nanotube synthesis is observed with increased level of manufacturing readiness for high-pressure carbon monoxide conversion (HiPco), chemical vapor deposition (CVD), and arc discharge (Arc) manufacturing. MRL = manufacturing readiness level; MJ/kg = megajoules per kilogram.

assessment on CNT manufacturing at two different scales in a more realistic and consistent setting.

Case Study: Cradle-to-Gate Assessment of Single-Wall Carbon Nanotubes

Based on a commercial CNT plant, we conducted a cradle-to-gate environmental assessment on the SWCNTs synthesized with a catalytic method called CoMoCAT®, which stands to represent the cobalt-molybdenum (Co-Mo) catalytic method. As the first step, the current small-scale production rate of approximately 100 grams (g) of SWCNT per day was examined.

As described in the literature (Monzon et al. 2008; Kitiyanan et al. 2000), the CoMoCAT process is based on a Co-Mo catalyst that enables SWCNT growth. Here, SWCNTs are grown by the decomposition of CO into carbon (C) and carbon dioxide (CO_2) at 700 to 950°C and pressure that typically ranges from 1 to 10 atmospheric pressure. Figure S1-2 and the *SWCNT Manufacturing with CoMoCAT Process* section in supporting information S1 on the Web provide additional processing details, including the life cycle inventory (LCI), and a schematic for the CoMoCAT SWCNT synthesis method.

The aim of this case study was to perform a cradle-to-gate assessment on the small-scale CoMoCAT SWCNT manufacturing process as well as on a mass production scenario. Because SWCNTs manufactured by both processes are intended for the same applications, and are expected to have similar technical performance, the reference flow for both cradle-to-gate assessments is 1 kilogram (kg) of SWCNT with tube diameter (0.9 ± 0.2 nanometers), aspect ratio (1,000), C content (90% by weight), and (7,6) chirality for more than 50% of tubes. SWCNTs of this type are currently primarily used in flexible electronics and displays, where they can be deposited in thin films (De Volder et al. 2013).

As illustrated in figure 3, the manufacturing process is within the system boundaries of this assessment. Using available LCI databases (Suh 2005, 2010; Ecoinvent 2010), these boundaries are extended to include the upstream processes whose outputs serve as inputs to SWCNT manufacturing. Some services, such as maintenance of machinery, are excluded because their impacts were considered negligible. Also, this process may release trace amounts of Co and Mo compounds by wastewater. Because the manufacturer treats wastewater to meet applicable regulations, it is assumed that dissolved metals in the treated wastewater discharged from the manufacturer are below the maximum permitted contaminant levels, and that SWCNTs released by wastewater during production are at low parts per billion levels. However, because this information could not be independently validated, it was not considered in this analysis, which focused more on energy consumption and material resource impacts. The potential adverse environmental and health effects of CNTs upon exposure may differ according to

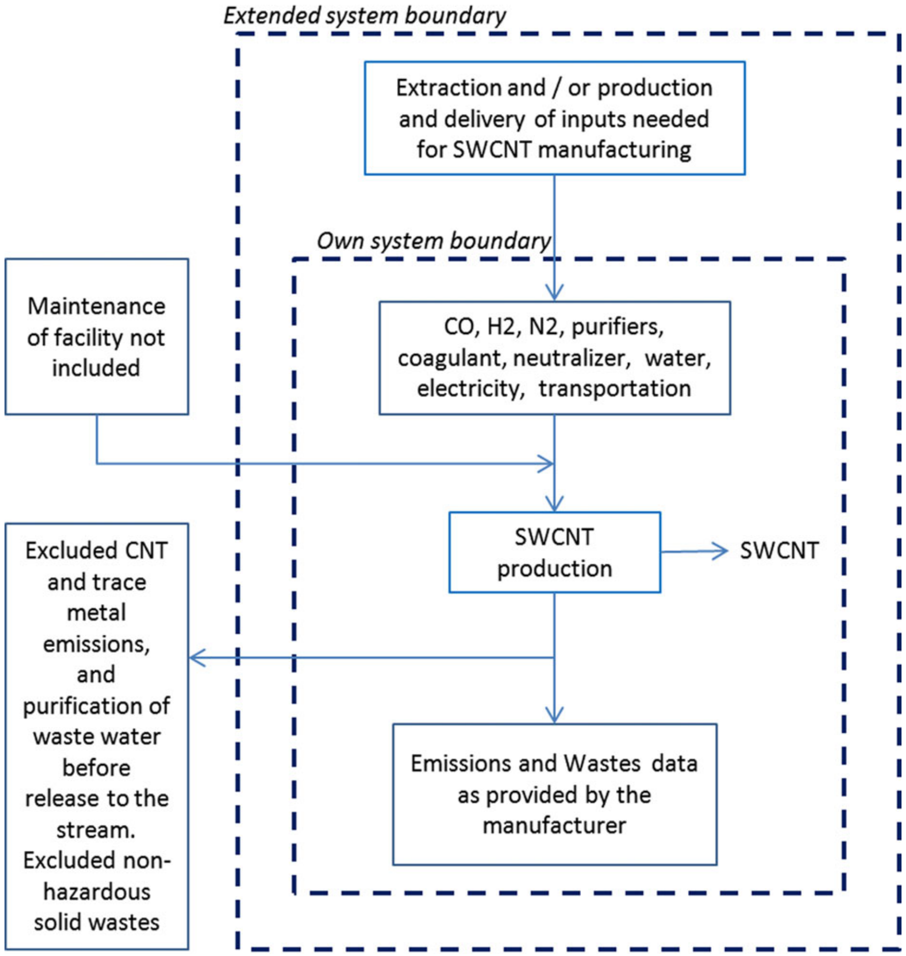


Figure 3 System boundaries of the cradle-to-gate assessment of single-wall carbon nanotubes (SWCNTs). CNT = carbon nanotubes; CO = carbon monoxide; H_2 = hydrogen; N_2 = nitrogen gas.

the specific situation (Colvin 2003; Stone et al. 2010). Interested readers are directed to the risk assessments literature on CNTs for more on the toxicity and environmental health and safety potential of CNTs (Shvedova et al. 2003; Maynard et al. 2004; Lam et al. 2006; Pacurari et al. 2010; Lee et al. 2010).

SWCNTs are the only output of this production process, and there are no coproducts generated at any stage. Hence, there is no multifunctionality in the current small scale as well as in the modified scaled-up process. Moreover, the manufacturing setup is exclusively used for the SWCNT manufacturing process. The manufacturer provided data on the material and energy inputs as well as on the direct emissions, and these are accounted for in the assessment.

The manufacturer has been planning on a scaling up of the current 100 g/day production to the levels of tonne per day and has gone through a detailed process design and engineering estimates for the scaled-up operation. The scaled-up process employs a refined nanotube harvesting method to release the SWCNTs from the supported catalyst and subsequently recycle the catalyst, which becomes economically viable as a result of the increased volume of feedstock and catalyst uses. Recycling of gases (CO and liquid hydrogen [H_2]) and catalyst not only reduces the use of feedstock and catalyst, but also minimizes purification and waste treatment operations. By doing so, the new design is expected to reduce unit cost by as much as tenfold. However, significant investments in new machinery will be necessary to implement these modifications for scaled-up manufacturing (table S1-3 in the supporting information on the Web).

Because the manufacturer and first-tier input suppliers are based in the United States, the characterization factors provided by the U.S. Environmental Protection Agency (US EPA)-developed Tool for the Reduction and Assessment of Chemical and Other Environmental Impacts (TRACI) (Bare 2002) were used to assess the environmental impacts assessed under this case study. Also, the Comprehensive Environmental Data Archive (CEDA) (Suh 2005, 2010) was used to assess the contribution of the additional manufacturing machinery through a hybrid approach (Suh et al. 2004; Suh 2004).

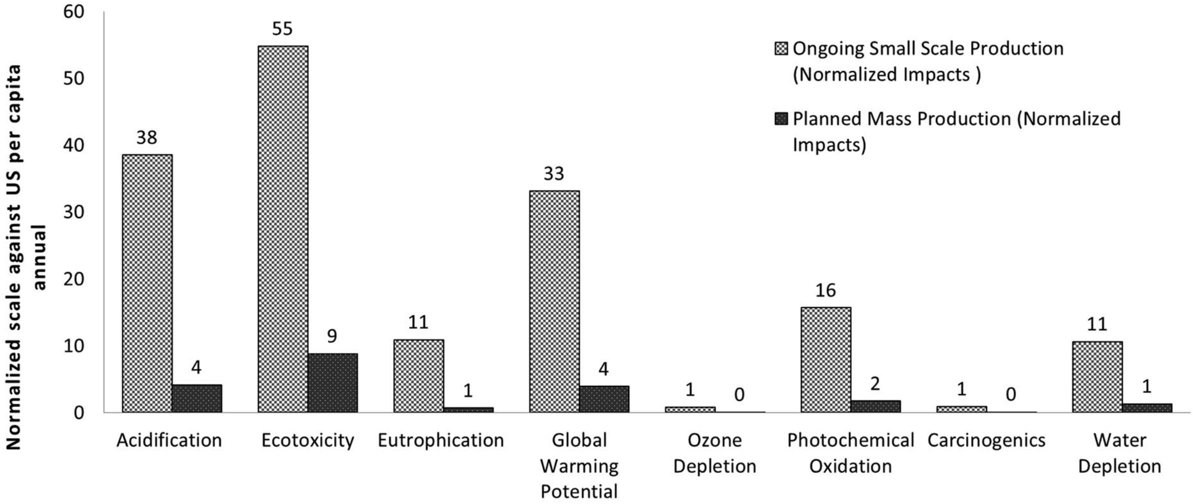


Figure 4 Significant reductions in the cradle-to-gate environmental impacts as the single-wall carbon nanotube manufacturing process scales up from small to mass production. Occupational exposure, toxicity of dissolved metals, or carbon nanotube in treated wastewater as well as potential impacts during use or disposal phases are not considered.

Case Study Results

Figure 4 provides a comparison between normalized impacts resulting from the current small-scale production and the proposed industrial-scale production. The normalization is with reference to the corresponding U.S. annual per capita impact levels (Kim et al. 2012). As figure 4 indicates, significant reductions in all environmental impacts can be expected with the scaling up of the SWCNT manufacturing process. More details on the quantification of the impact categories are provided in tables S1-4 and S1-5 in the supporting information on the Web.

This trend of decreasing environmental burden with increased manufacturing readiness is also applicable to the production energy requirements for SWCNT production. The small-scale process for SWCNT production by CoMoCAT indicates a production (catalysis, synthesis, purification, and drying) energy requirement of 7.8E + 04 megajoules per kilogram (MJ/kg) and a planned ramped-up process to industrial scale indicates an energy requirement of 1.0E + 04 MJ/kg. These two data points are also in agreement with the trend of a decreasing production energy requirement with increasing MRL observed in our analysis of previous studies, as illustrated in figure 2.

The manufacturer expects minimal changes in direct emissions and releases on a mass equivalent basis as the process scales up from small to mass scale. This indicates that the reductions in indirect environmental impacts are mostly the result of recycling of inputs that are consumed in the subsequent synthesis cycle. Because of the reduced need for virgin inputs, the inputs that dominate various environmental impacts will differ between the two MRLs. For example, as illustrated in figure 5a, CO is the most impactful input across the board for the current small-scale manufacturing, but as the process is scaled up (figure 5b), nitrogen gas (N_2) becomes more or at least equally impactful as CO. It is important to note these changes in the relative contributions of inputs in the given impact categories, especially when further reductions in the environmental impact are planned after the manufacturing process scales up. More detailed contribution analysis for individual impact categories is provided in table S1-5 and figure S1-3 in the supporting information on the Web.

Uncertainty and Sensitivity Analysis

Process data for this study were provided by the manufacturer. The data were single-point values and without any uncertainty information. Hence, the standard procedure for uncertainty quantification developed by Ecoinvent (Frischknecht et al. 2004) is employed in this study to estimate the parameter uncertainties at the process level. This method is based on the introduction of pedigree matrix in the LCA literature by Wiedema and Wesnæs (1996). Because most of the data were based on direct measurements, came from the production unit that produced the version of SWCNT under study, and were less than 6 months old, all the input and output data points indicate a high level of pedigree for the current process. The 95% interval of geometric standard deviation (i.e., $SD_g95\%$) for the data for both the processes falls in the range from 1 to around 2. The detailed pedigree matrices and calculations for the current and proposed scaled-up process are provided in supporting information S1 on the Web (tables S1-6 and S1-7). Readers are directed to the Ecoinvent (Frischknecht et al. 2004; Ecoinvent 2010) and CEDA literature (Suh 2010) for the discussion on the uncertainties associated with those databases.

The anticipated reductions upon scaling up are conditional on the scaled-up production closely following the modified (i.e., scaled-up) synthesis protocol. Because the scaling up is still at a planning stage, there may be some variance upon its realization. This possibility of variation and the lack of visibility to the

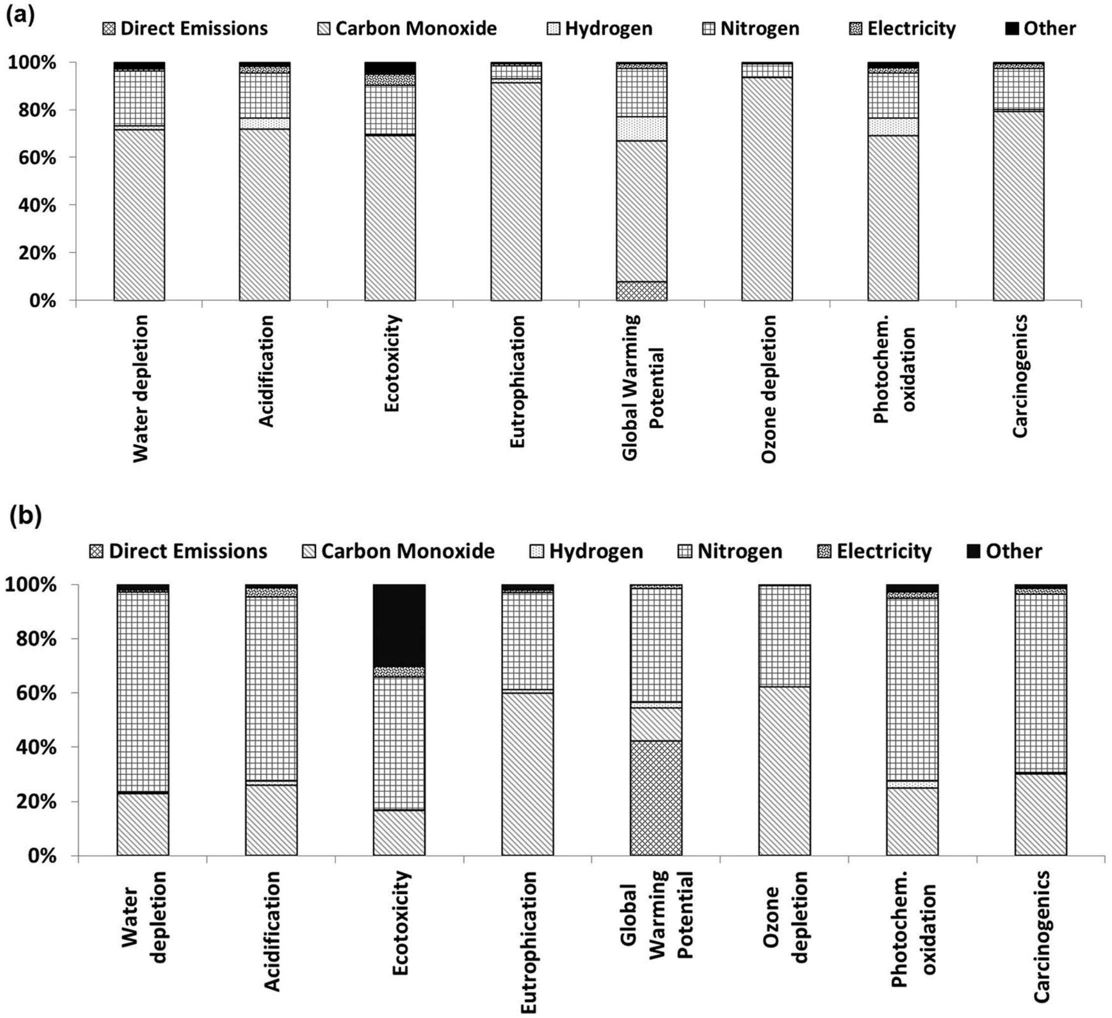


Figure 5 (a) Contribution of various inputs to the environmental impact categories based on the current small-scale process of single-wall carbon nanotube production. (b) Contribution from various inputs to the environmental categories based on the process for the planned production rampup to the industrial scale of manufacturing of single-wall carbon nanotubes.

assumptions and model behind manufacturer's scaled-up scenario make it important to examine the effects of the deviation from the baseline scenario. This was done for the global warming (GW) where its sensitivity for various input scenarios was evaluated by increasing the quantities of its four most impactful inputs (i.e., CO, H_2, N_2, and electricity), as revealed by the contribution analysis. As figure S1-4 in the supporting information on the Web indicates, even for the most conservative scenario, where we consider that all four inputs increase five times compared to their quantities anticipated by the baseline scenario, the resulting indirect GW was estimated to be approximately 4.4E + 05 kg carbon dioxide equivalents CO_2-eq (i.e., over a 40% reduction from 7.5E + 05 kg CO_2-eq of the current manufacturing process).

Further, an assessment on the additional manufacturing equipment requirements for mass production was conducted based on the CEDA database (Suh 2005, 2010) for various production scenarios. The GW contribution of the additional asset requirements, even for the most conservative scenario, was found to be approximately 350 kg CO_2-eq, which is negligible, compared to the global warming potential of small- or mass-scale production. More details on the additional asset requirements are available in figure S1-5 in the supporting information on the Web.

Discussion

Our literature review indicates that generally the LCAs of ENM are conducted when the technology is mature enough only to produce prototypes with the intended functionality, and when its manufacturing readiness, at best, is at a small-scale production level. Our case study on SWCNTs found that the readiness levels may influence the environmental assessment of a product, in that the environmental burden per unit output is likely to reduce with the increased technology and manufacturing maturity levels.

This study indicates that 84% to 94% reduction in the cradle-to-gate environmental impacts may be expected after CNT manufacturing ramps up from small- (TRL and MRL around 7 to 8) to large-scale (MRL 9 to 10) production. It also shows that relative contributions of inputs toward specific impact categories may also change when the technology and manufacturing processes mature. This is on account of various efficiency measures, such as reuse and recycling during each SWCNT synthesis cycle, becoming feasible only beyond a certain production volume.

The analysis with readiness levels illustrate that whereas an early LCA study can provide an initial baseline, an assessment with more-detailed manufacturing process data can indicate a more representative magnitude of environmental impacts as the technology matures. In the absence of such data, it might be useful to broadly assess the technology's readiness levels. Hence, we recommend a careful interpretation of early LCA studies on emerging technologies that are, of necessity, based on the information derived from bench, pilot, or small-scale operations. The magnitude of environmental impacts of emerging technologies at their mass production scale can be significantly smaller than a linear extrapolation of early LCAs may suggest. When adequate data become available, an LC-like approach may be implemented to further assess the nonlinear effects of scaling up as briefly illustrated in supporting information S1 on the Web.

In general, LCA calculations are made at the level of a functional unit, and therefore the information on the technology maturity and scale of production is not readily available in LCA results. Our study suggests that processes at a different technology maturity and scale of production can create a material difference in their environmental performances, and making such information available to LCA practitioners is of significant importance in properly interpreting an LCA result. In particular, our case study shows that most of the reductions in environmental impacts are achieved in the larger-scale production through improving raw material efficiency achieved by efficiency measures, such as reusing and recycling raw materials. LCAs based on information from small-scale operations are recommended to test the case of higher materials efficiency in larger-scale production.

Recent LCA data exchange formats, such as ecoSpold v2 (Ecoinvent 2010) and the International Reference Life Cycle Data System (ILCD) Handbook (EC-JRC-IES 2010), included new metadata or comment fields on annual production volume. The relevance of scale information was also highlighted in a recent international effort to provide guidance on LCI database development (UNEP 2011). For the majority of the unit process data currently used by LCA practitioners, however, such fields are yet to be populated. Our study confirms the importance of providing such information, especially for emerging technologies for LCA practitioners to properly interpret life cycle information.

Acknowledgments

This work was supported by the National Science Foundation (NSF) and the US EPA under Cooperative Agreement Number DBI-0830117. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the NSF or US EPA. This work has not been subjected to US EPA review, and no official endorsement should be inferred.

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