Supporting Information for

Evaluating the Environmental Impacts of Nano-Enhanced Field Emission Display Using Life Cycle Assessment

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S.1   Process Description of CNT-FED Manufacturing

The manufacturing of a CNT-FED consists of four modules: (1) fabrication of the CNT cathode substrate; (2) fabrication of the phosphor anode substrates; (3) vacuum sealing of the CNT cathode and phosphor anode substrates; and (4) the final assembly of the CNT-FED product. The fabrication of a cathode substrate begins with preparation of a conductive CNT paste, which constitutes the major raw material; the CNTs must be in a highly homogenous and in a uniformly dispersible state. To achieve this, the CNTs must be initially synthesized, purified and dried. The pure CNT powder is then mixed with organic solvents to produce a homogenously dispersed CNT solution, which is ready for application into a conductive paste. The synthesis of CNTs was assumed to be carried out by chemical vapor deposition (CVD) using a C_2H_2 feedstock as the carbon precursor and a bimetallic catalytic system (Ni (20 wt%) & Fe (20 wt%) on Al_2O_3 support (60wt%)) as the substrate for facilitating CNT growth [1]. The synthesis step is followed by treatment of CNTs with a H_2SO_4:HNO_3 acid mixture (3:1 (v/v)) in an ultrasonicator for 6 hours according to the procedure described by Wang et al. [2]. The acid-purified, dry CNT powder is dispersed in an organic solvent, such as isopropanol (IPA), or in plant-derived oil such as terpineol or rapeseed oil. The contents are ultrasonicated to generate a uniformly dispersed CNT solution [3]. If IPA is used as a solvent, the contents are then heated to maximize IPA solvent evaporation (95%) while ensuring the dispersivity of the CNTs in the remaining solvent is not lost. To this CNT solution, designated amounts of glass frit, metal powder, organic binder are added and the mixture is subjected to intense milling in a 3-roll ball mill for 1-2 hours [4]. The metal powder (or metal oxide) enhances the conductivity of the paste [4c]. The glass frit improves cohesion of the CNTs on the substrate after screen printing[4c].

Further, a photosensitive vehicle is added to the above mixture and the milling is continued again for 2-3 hours [4]. However, the use of oils such as rapeseed or terpineol appears to be optional but highly desirable by some in the formulation of the CNT paste [5] but not by all [4a]. Addition of oils such as terpineol or rapeseed oil is to increase stability and dispersibility of CNTs in the solution of CNT paste.

The CNT paste is then screen printed onto an indium tin oxide (ITO) coated glass substrate and subsequently patterned into a predetermined shape using a UV hardening method [4a, 4c]. The patterned CNT-coated glass substrate is then baked at 400-500°C for one hour in a nitrogen rich atmosphere to remove the organic binder from the printed CNT paste [6]. However, the baking process may result in the loss of field emission activity of the CNTs as they tend to bury themselves beneath the organic contents of the paste [4a]. Therefore, the baked CNT-coated glass substrate must be treated with a liquid phase surface treating material comprising of a water soluble organic polymer binder (5-20 wt%) and a metal oxide (3-10 wt%) in water [4a]. This completes the fabrication of the CNT cathode substrate.

The preparation of the anode substrate in Module 2 is a well established process involving deposition of phosphors onto an ITO-coated glass substrate [7]. While many phosphor manufacturing techniques are documented in the open literature, in this study we assumed the use of zinc sulfide (ZnS) phosphors activated with Cu and Ag metals. These production details are provided by Poss [7].

In Module 3, the CNT cathode and phosphor anode substrates are vacuum sealed according to the process given by a US Patent [8] used to seal flat panel displays. Finally, in Module 4, the vacuum sealed CNT-FED is assembled with electronic components such as cables

and printed wiring board (PWB). The entire set-up is encased in a housing to obtain a finished, ready-to-use CNT-FED product.

S.2   Life Cycle Inventory (LCI) of the Metal Catalyst Production Process

A bimetallic system (Ni:Fe:Al_2O_3) catalyst is used in the catalytic chemical vapor deposition (CCVD) reactor to propagate CNT growth. The LCI data is based on the preparation of 1 kg of dry catalyst powder. While the reader can obtain a greater description of metal catalyst preparation from references [1], the method is briefly discussed here. The salts, $NiSO_4$ and $FeSO_4$ along with Al_2O_3 are mixed in DI water and the contents are stirred for one hour at 60°C. The impregnate is then oven dried at 100° C for 12 hrs followed by calcination in a muffle (retort) furnace at 400°C for 4 hrs. After calcination, the contents are ball milled for 60 hrs and reduced under an H_2 atmosphere at 450°C for 3 hrs. The dried metal catalyst powder is now ready to be used as a substrate to propagate CNT growth. A block diagram for production of metal catalyst powder as explained above is shown in Figure 1S.
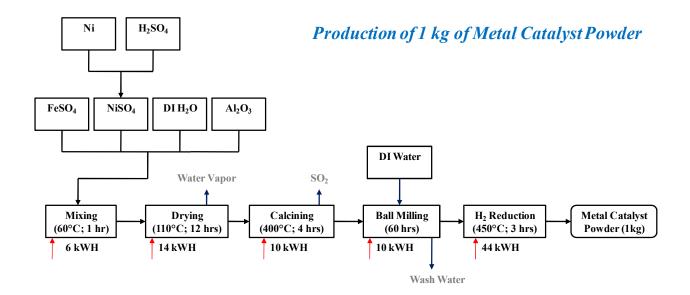

Figure 1S. Block Diagram for Metal Catalyst Powder Production

The LCI data for the production of 1 kg of metal catalyst powder is given in Table 1S.

Table 1S. LCI Data for Metal Catalyst Powder Production

Inputs	
Materials/Energy	**Quantity**
Ni	210 g
Dilute H_2SO_4	351 g
Al_2O_3	630 g
$FeSO_4$	571 g
DI Water	12 kg
Total Energy	84 kWh
Outputs (Emissions, Discharges & Wastes Generated)	
SO_2	300 mg
Water Vapor	10 kg
Wash Water	2 kg

The above LCI data for the metal catalyst production is supported by the following calculations/assumptions:

a) The modules for Ni, $FeSO_4$, Al_2O_3 and DI water are available in the Ecoinvent database [9], whereas dilute H_2SO_4 was provided by ERG [10].

b) The amount of metal catalyst to be produced is 1.05 kg (assuming 5% material lost during processing). The weights of individual components: Ni, Fe and Al_2O_3 in the metal catalyst system was calculated according to the specified composition (20:20:60)% by weight.

c) $NiSO_4$ is used as the precursor for Ni and is prepared by adding Ni pellets to dilute H_2SO_4. The corresponding stoichometric equation for preparation of $NiSO_4$ is given as

$$Ni + H_2SO_4 ======= NiSO_4 + H_2$$

d) $FeSO_4$ is used as the precursor for Fe and is calculated according to stoichometric equation

$$Fe + H_2SO_4 ======= FeSO_4 + H_2$$

e) DI water consumption was assumed to be 12 liters of which 10 liters are used for mixing $NiSO_4$, $FeSO_4$ and Al_2O_3 and 2 liters for washing the ball mills after milling the metal catalyst powder.

f) Energy estimation was performed using data from equipment specification sheets. This resulted in 6 kWh for mixing based on using a PM 40 mixer from Thermo Electron Corporation [11] plus 14 kWh for drying based on a lab gravity oven from Engineered Production Systems [12] plus 10 kWh for calcination based on a K114 model furnace from Kendro Laboratory Products [13] plus 10 kWh for milling of metal catalyst powder assuming the final catalyst median powder diameter is 80 nm [10] plus 44 kWh for the H_2 reduction based on Model G 1200 CAMCo furnace [14].

g) Due to heating the sulfate bearing metal salts, there is a possibility that SO_2 gas is emitted during the calcination process. While no direct information is available to confirm this, we calculated the amount of SO_2 released for 1 kg of powder calcined based on SO_2 release data provided by the cement industry (~ 0.2-0.3 kg SO_2/1 ton cement) (powder based industry) [15].

S.3   LCI of CNT Synthesis in CCVD Reactor

The dry, metal catalyst powder as prepared above is then loaded into a CCVD unit and heated to (800-900°C) for 30 minutes in N_2 atmosphere to activate the catalytic sites. Heating is continued in the presence of an H_2 and N_2 gas mixture for one hour. Then, C_2H_2 used as a carbon source, is introduced into the reactor, along with H_2 and N_2, where the ratio of the three gases mixture is $20(C_2H_2):20(H_2):60(N_2)$% by volume, and with a reaction time of 30 min. Additional details of the CNT synthesis process can be obtained

from Liu et. al. [1b]. A block diagram for production of 1 kg of CNTs synthesized in a CCVD reactor system is shown in Figure 2S.
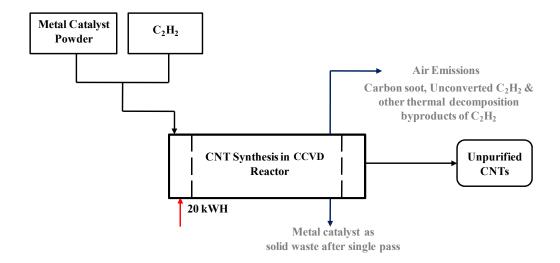
Production of 1 kg of Unpurified CNTs

Figure 2S. Block Diagram for Production of Carbon Nanotubes Using CCVD Reactor

The LCI data for the production of 1 kg of unpurified CNTs is given in Table 2S.

Table 2S. LCI Data for Production of Unpurified CNTs

Materials/Energy	Quantity
Metal Catalyst powder	3.6075 kg
C_2H_2	4.44 kg
H_2	0.57 kg
N_2	39.10 kg
Total Energy	20 kWh
Outputs (Emissions, Discharges & Wastes Generated)	
Solid catalyst waste after single pass	2.331 kg
Unconverted C_2H_2	25.2 g
Particulate Matter (PM2.5)	48.56 g
Cumulative Volatile Organic Chemicals (VOCs)	48.70 mg
Naphthalene	43.21 µg
Acenaphthylene	1.36 µg
Acenaphthene	0.43 µg
Phenanthrene	0.86 µg
Fluorene	0.43 µg
Anthracene	0.13 µg

Fluoroanthene	0.21 µg
Pyrene	0.27 µg

The above LCI data for CNT synthesis is supported by the following calculations/assumptions:

a) LCI data for the metal catalyst powder was obtained from the data for stage 1 described previously. The LCI data for C_2H_2, H_2, and N_2 are available in the Ecoinvent database [9]. For air emissions, C_2H_2, VOCs and PAH entries are available in the "air emissions" category of the Ecoinvent database. However for VOCs, the value obtained is a cumulative value, whereas for individual chemicals (e.g. naphthalene, anthracene etc) they are entered for PAHs.

b) We assumed the CNT synthesis is performed in a CCVD reactor provided by First Nano, a division of CVD Equipment Corporation, NY, USA. First Nano has a wide range of advanced turnkey type thermal catalytic CVD systems, which are built on a modular platform (i.e. it houses key process components in one unit), fully automated and is equipped with exhaust gas handling system as well. For the production units operating to synthesize CNTs for end product applications such as CNT-FEDs, it is customary to adapt these advanced CVD systems. So, our LCI data is based on the assumption the modular CVD and accompanying exhaust gas treatment system (scrubbing) provided by First Nano, and more specifically their Easy Tube ™ 2000 CVD system [16], is used for CNT synthesis.

c) The quantity of energy consumed for CNT synthesis is based on an equipment rating provided for the Easy Tube™ 2000 CVD system [16] which closely matches with the data

given by Kushnir et al. [17] for 1 kg of CNTs synthesized in a fluidized bed CVD (only process heating considered).

d) Carbon deposition yield (CDY) and synthesis reaction yield (SRY) are assumed to be 30% for each [1a, 5a]. The CDY is the ratio of ((mass of carbon deposited)/(mass of catalyst fed in dry form)*100), whereas the SRY is ratio of ((mass of carbon deposited)/(mass of carbon fed into the system)*100). Thus the amount of metal catalyst powder needed to synthesize 1 kg of CNTs is 3.33 kg, (1 kg/ 0.3), whereas the C_2H_2 needed is 3.6075 kg ((1/0.3)*(26/24)) respectively.

e) The quantities of the H_2 and N_2 inputs are calculated based on the processing conditions described by Liu et al. [1b]. The paper describes 100% N_2 being introduced into the system followed by a 20:80% by volume ratio of $H_2:N_2$ for one hour. This is followed by the introduction of a three-gas mixture ($H_2:C_2H_2:N_2$) being fed into the system in a ratio of 20:20:60% by volume. The ratio of volume percentage for the three gases is then converted to a mass basis, resulting in a mass percentage ratio of $H_2(2\%):C_2H_2(25\%):N_2(73\%)$. Thus during synthesis, the amount of C_2H_2 fed into the system is 3.6075 kg (based on the SRY as calculated above). Additionally, the amounts of H_2 and N_2 fed into the system are 0.2886 and 10.53 kg, respectively. During catalyst preheating, the amount of N_2 used is 14.43 kg, whereas during H_2 reduction, the amounts of H_2 and N_2 fed are 0.29 and 14.14 kg, respectively. Thus, the total amount of H_2, C_2H_2 and N_2 gases consumed during the entire process (i.e. inclusive preheating, H_2 reduction and synthesis steps) are 0.5786, 3.6075, and 39.1 kg, respectively.

f) The catalyst was assumed to be used only for one pass and after the CNT synthesis is completed; the left over catalyst powder is disposed of as a solid hazardous waste.

g) The unreacted C_2H_2, along with its thermal decomposition products such as benzene, toluene, and but-1-en-3-yne, etc. [18] vented from CCVD are sent to an exhaust gas system for the Easy Tube ™ 2000, where scrubbing is performed to retain these toxic gases. The release of toxic byproducts such as VOCs and PAHs is a serious issue when using hydrocarbon feedstocks for CNT synthesis [19]. By employing an advanced CVD systems equipped with built-in scrubber systems, the release of toxic exhaust gases into the atmosphere can be contained effectively. For C_2H_2, 70% of the gas appears in the effluent (since SRY is 30%) and leaves the reactor unreacted. This value is in close agreement with the effluent C_2H_2 concentration reported by Schmitt et al. [18] after a synthesis time of 30 min. Thus, 70% of 3.6075 kg = 2.5252 kg of C_2H_2 will leave the reactor and be sent to the exhaust system, where exhaust gas treatment efficiency was assumed to be 99%. Thus, the amount of unconverted C_2H_2 vented to the atmosphere is 25.25 grams.

h) The amount of H_2 and N_2 released into the atmosphere was assumed to be negligible.

i) The amount of particulate matter (carbon soot) released was assumed to be 48.56 grams per kg of CNTs synthesized. This value is based on a personal communication with a carbon nanoparticle manufacturing company (confidential).

j) <u>VOC and PAH Emission Assumptions:</u> Plata et al. [19] reported that different types of VOCs and PAHs are released in the effluent when C_2H_4 is used as a carbon precursor to synthesize CNTs. Further, Plata mentions the VOC and PAH emissions are an order of magnitude less for C_2H_2 used as a carbon feedstock than for those released when C_2H_4 is used as a feedstock [20]. Our emission values for VOCs and various PAHs are based on data reported by Plata et al. [19] for C_2H_4 feedstock. but the final emissions for VOCs and PAHs (Table S2) are ten times less than the reported data for C_2H_4 feedstock,

k) <u>VOC Calculation Based on Plata's Data</u>: According to Plata et al. [19], the concentration of VOCs for 70 SCCM (standard cubic centimeters per minute) of entering C_2H_4 gas (at 1040°C) ranges from 17.6 ppmv (1,3-cyclopentadiene) to 17,000 ppmv (methane). Thus, for 70 SCCM of C_2H_4, a cumulative value of 20,000 ppmv was assumed.

The value from ppmv to mg/m^3 can be converted according to following formula:

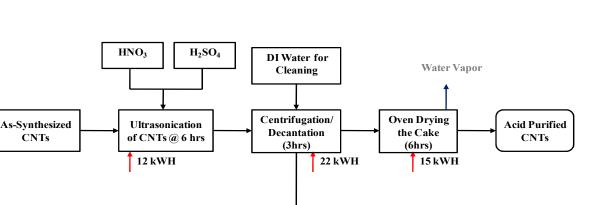$$mg/m^3 = (ppmv)*(12.187)*(MW)/(273 + T) \qquad (1)$$

Where ppmv = concentration of gas component; 12.187 = conversion factor; MW = molecular weight of the component; and T = temperature in °C [21].

Based on the above formula, the cumulative VOC value of 20,000 ppmv is equivalent to 2,970 mg/m^3; since methane is a major VOC constituent (17,000 ppmv), the molecular weight of methane is used in Equation 1. On the other hand, 70 SCCM = 0.07 SLPM (standard liters per minute) of C_2H_4 and 330 SCCM = 0.33 SLPM of H_2 is fed into the reactor for 30 minutes. Thus for 30 minutes, the total volume of the gas mixture feed is 12 liters (0.012 m^3). Therefore, the mass of cumulative VOCs released will be (2970 mg/m^3)*(0.012) = 35.64 mg. Now, 70 SCCM of C_2H_4 = 0.088 g/min; thus for 30 minutes, the amount of hydrocarbon (C_2H_4) fed into system is 2.64 g. Therefore, for 2.64 g of C_2H_4, the cumulative VOC release will be 35.64 mg. But as assumed earlier, when C_2H_2 is used as a feedstock instead of C_2H_4, the amount of VOC release would be ten times less which means for 2.64 g of C_2H_2, the cumulative VOC release will be 3.564 mg. Further, when exhaust controls are applied with 99% efficiency, the amount of VOCs vented to the atmosphere is 0.03567 mg = 35.64 µg. Assuming a linear relationship between C_2H_2 use and VOC release, 3.6075 kg of C_2H_2 usage will result in 48.70 mg of VOCs released.

l) <u>PAH Calculations Based on Plata's Data</u>: Plata et al. [19] reported the amounts of various PAHs released per gram of C_2H_4 used as carbon feedstock, by assuming these amounts to be 10 times less when C_2H_2 is used. Further, when exhaust gas treatment controls are applied, the PAH emission quantities must be further reduced by 99%. Thus, the final emissions of various PAHs to the atmosphere when 3.6075 kg of C_2H_2 is used as feedstock are: 43.21 μg of naphthalene; 1.36 μg of acenaphthylene; 0.43 μg of acenaphthene; 0.86 μg of fluorene; 0.43 μg of phenanthrene; 0.13 μg of anthracene; 0.21 μg of fluoroanthrene; and 0.27 μg of pyrene respectively.

S.4 LCI of CNT Acid Purification Step

The as-synthesized CNTs obtained above are then purified in an ultrasonicator by washing in a mixture of concentrated HNO_3 and H_2SO_4 in a ratio of 3:1 by volume [2]. The ultrasonication step is succeeded by centrifugation/decantation, followed by oven drying of the cake to obtain the acid purified CNTs in a dry form. A diagram for the CNT acid purification step is shown in Figure 3S.

Production of 1 kg of Acid Purified CNTs

Figure 3S. Block Diagram for Acid Purification of Carbon Nanotubes

The LCI data for the CNT acid purification step is given in Table 3S.

Table 3S. LCI Data for CNT Purification

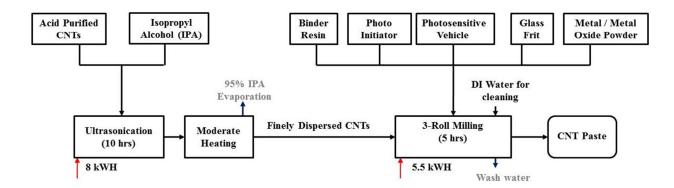| Materials/Energy	Quantity
As synthesized CNTs	1.11 kg
Concentrated HNO_3 (68%)	38.621 kg
Concentrated H_2SO_4 (98%)	153.18 kg
DI Water	544 kg
Total Energy	49 kWh
Outputs (Emissions, Discharges & Wastes Generated)	
Water vapor emission to air	10 kg
Wash water effluent to wastewater treatment plant	736 kg

The above LCI data for the CNT acid purification step is supported by following calculations/ assumptions:

a) The LCI data for acid purified CNTs is obtained from stage 2, whereas the LCI data for concentrated HNO_3 and H_2SO_4 plus DI water are available in Ecoinvent [9].

b) Consumption of acids was calculated based on the assumption that 37.5 mL of H_2SO_4 and 12.5 mL of HNO_3 (total 50 mL) are mixed and used to wash 500 mg of CNTs [2]. Assuming a 90% purification yield, the acid consumption was calculated to be 111 liters, where the quantity of H_2SO_4 is 83.25 liters and HNO_3 is 27.75 liters, respectively

c) The energy consumption for the ultrasonication step was calculated based on an ultrasonic processor UIP 2000 hd with a 2000 W rating and an upper range processing liquid capacity of 0.5 m^3 supplied by Hielscher Ultrasonics GMBH [22]. The energy consumption of centrifugation/decantation was based upon the equipment specification sheet supplied by Rousselet Inc, from France [23]. Energy consumed in the oven drying step was based on the power ratings provided on the data sheet provided by Cole Parmer for one gravity convection oven dryer unit.

d) The decanted acid is removed from the centrifuge and collected in a waste container. Subsequently, the cake (wet CNT powder) was assumed to be rinsed twice with DI water, where the amount of DI water used for each wash is double (222 liters) the amount of acid used. Finally, after transferring the cake to the oven dryer unit, the centrifuge was assumed to be rinsed with 100 liters of DI water. Thus, the amount of DI water consumed, for this step, is 544 liters per batch.

e) The decanted acid solution and wash water are collected in a waste container and is sent to a wastewater treatment plant without further pretreatment.

f) The residual water associated with the CNT cake is removed as water vapor (~ 10 kg) in the oven drying step.

S.5   LCI of Conductive CNT Paste Preparation

A simplified process description for the CNT paste was previously provided in S.1. A block diagram for preparation of CNT paste is shown in Figure 4S.

Figure 4S. Block Diagram for Preparation of Carbon Nanotube Conductive Paste (for Baseline Case (Scenario 0)

The LCI data for CNT paste preparation step is step is given in Table 4S.

Table 4S. LCI Data for Carbon Nanotube Conductive Paste Preparation

Materials/Energy	Inputs				
	Quantity				
	Scenario 0 (IPA & Ag Powder)	Scenario 1 (IPA & Zn Powder)	Scenario 2 (Rapeseed Oil & Ag Powder)	Scenario 3 (IPA & TiO_2	Scenario 4 (Rapeseed Oil & TiO_2
Acid Purified CNTs	30 g	30 g	15 g	15 g	5 g
Isopropyl Alcohol (IPA) for CNT Dispersion	7.074 kg (9 Liters)	7.074 kg (9Liters)	Not Used	3.537 kg (4.5 Liters)	Not Used
Rapeseed Oil for CNT Dispersion	Not Used	Not Used	150 g	Not Used	50 g
Organic Binder (Epoxy Resin)	39 g	39 g	44 g	39 g	49 g
Photosensitive Vehicle (Methyl Acrylate)	20 g	20 g	35 g	25 g	30 g
Photo Initiator (Anthraquinone)	1 g	1 g	1 g	1 g	1 g
Glass Frit	5 g	5 g	Not Used	5 g	Not Used
Metal Powder	Ag powder 5 g	Zn Powder 5 g	Ag Powder 5 g	Not Used	Not Used
Metal Oxide Powder	Not Used	Not Used	Not Used	TiO_2 15 g	TiO_2 15 g
DI Water	5 kg	5 kg	5 kg	5 kg	5 kg
Total Energy	14.5 kWh	14.5 kWh	14.5 kWh	14.5 kWh	14.5 kWh
Outputs (Emissions, Discharges & Wastes Generated)					
IPA Solvent Emission to Air	36 g	36 g	None	18 g	None
Wash water effluent to wastewater treatment plant	5 kg	5 kg	5 kg	5 kg	5 kg

The above LCI data for the CNT paste formation step is supported by the following calculations/ assumptions:

a) The LCI data module for acid-purified CNTs was obtained as described above in S4, whereas all other LCI data modules are available in the US Life Cycle Inventory Database (USLCI) [24] or the Ecoinvent [9] database, with preference given to the former; where data were not available, the latter was used.

b) Dispersion of acid purified CNTs in IPA is performed according to a procedure described by Mao et al. (US Patent 7,040,948 B2)[25] According to this procedure, 1g of acid-purified CNTs requires 300 mL IPA.

c) The total weight of CNT paste composition is fixed as 100 g for baseline as well as other alternate scenarios considered.

d) The CNT paste composition for scenario 0 was based on a US Patent (7,648,424 B2) [4a]. According to Jin et al. [4a], the CNT paste composition (used for baseline scenario in our study) is comprised of 1-30% wt of finely dispersed CNTs; 30-60% mixture of organic binder and an organic vehicle; 0.1-20% of frit; and 0.1 -20% metal powder (e.g. Ag, Al, Zn, Cu or Ni). Specifically, the CNT composition used was: 30% finely dispersed CNTs; 40% organic binder (epoxy resin) and 20% photosensitive organic vehicle (methyl methacrylate monomer); 5% frit and 5% Ag metal powder. The CNT paste composition used in scenario 1 (for contribution analysis) is same as scenario 0 except that Zn powder is used in place of Ag powder.

e) The energy consumption for ultrasonication was calculated to be 8 kW based on the assumption that 80W of a 59 kHz lab model ultrasonicator is used for the dispersion [2]. For heating the solution on a laboratory-sized heater, approximately 1 kW of energy is used whereas the energy consumption for a 3-roll milling operation was estimated to be 5.5 kW based on an equipment data specification sheet provided by EXAKT [26]. Energy consumption for ultrasonication and 3-roll mill was obtained from equipment data specification sheets.

f) After milling, 5 liters (5 kg) of DI water are used for cleaning the mills and correspondingly 5 kg of rinse water are released. This water was assumed to be sent to a wastewater treatment plant for treatment

g) It was assumed that 95% of the IPA solvent evaporates during the heating step. Additionally, it was assumed proper controls are applied to capture the evaporated IPA solvent with an efficiency of 99%.

h) LCI data for CNT paste composition in scenarios 2 and 4 is obtained from US Patent (2008/0004380 A1).[5b] According to this patent the CNT paste composition can contain anywhere from 0.01-15wt% CNTs; 1-70% binder resin; 1-70% photosensitive vehicle; 5-60% metal oxide powder (e.g. SiO_2, TiO_2, ZrO, SnO); and remaining percentage of a solvent (e.g., rapeseed oil or terpineol) maintain CNT dispersion).

i) IPA solvent is replaced with Rapeseed oil in scenario 2 and is used for dispersing CNTs. It can be noted that the viscosity of rapeseed oil is 160 cP as against IPA solvent (2.86 cP). Therefore, the former is used in less proportion in CNT paste composition.

j) In scenario 3, the CNT paste composition is exactly identical to scenario 0 except that Ag powder is replaced with TiO_2. The CNT paste composition for scenario 3 is obtained from US Patent (7,648, 424, B2) [5b]

k) In scenario 4, IPA solvent is replaced by Rapeseed oil and Ag powder is replaced by TiO_2.

S.6   LCI of Conductive CNT Cathode Substrate Fabrication

A simplified process description of screen printing of CNT paste onto a glass substrate is given in S.1. A block diagram for preparation of the CNT cathode substrate is shown in Figure 5S.
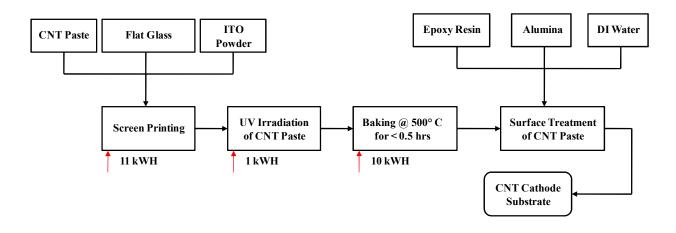
Figure 5S. Block Diagram for Fabrication of a CNT Cathode Substrate

The LCI data for the CNT cathode substrate production step is step is given in Table 5S.

Table 5S. LCI Data for CNT Cathode Substrate Production

Inputs	
Materials/Energy	**Quantity**
As synthesized CNTs (Baseline Scenario)	100 g
Flat glass Cr coated	608.59 g
ITO Powder	0.5 g
Epoxy Resin	200 g
DI Water	700 g
Alumina	100 g
Total Energy	3.6 kWh

The above LCI data for the CNT cathode substrate fabrication step is supported by the following calculations/assumptions:

a) The LCI data module for the CNT paste (100g) was obtained from stage 4 above (baseline scenario). The LCI data for Cr-coated flat glass, ITO powder, epoxy resin, and DI water are available in Ecoinvent [9], whereas alumina data are available in the USLCI database [24].

b) Energy consumption for the screen printing was based on specification data obtained from the LS-34 TV screen printer model from the Marubeni American Corporation [27]; for the UV irradiation step, energy was based on a lamp power density of 20 mW/cm^2 [28]; and for the baking step from equipment data specification sheets [12].

c) The amount calculated was based on assuming the glass has a density of 2.63 g/cm^3 [29] and a thickness of 2.8 mm. , it was assumed the viewing area for a CNT-FED is similar to that of a LCD display, as considered in a USEPA study [30] (122 inch^2 = 787.095 cm^2). Thus, the volume of the glass is (787.09 cm^2)*(0.28 cm) 220.38 cm^3. Based on the density of glass, the mass of glass used was assumed to be 2.63 (g/cm^3)*(220.38 cm^3) = 579.61 g. Assuming 5% more glass is needed to account for processing losses, the total mass of glass used was 608.59 g

d) The quantity of glass was assumed to be same as 15-inch LCD panel [30]. Further, 5% more glass was assumed in order to compensate while processing the glass substrate.

e) The module for sputtering ITO onto the glass substrate is available in Ecoinvent [9].

The materials used in the surface treatment of baked, CNT cathode substrates were based on the description provided by Jin et al. [4a]

S.7   LCI of Phosphor Anode Substrate Fabrication

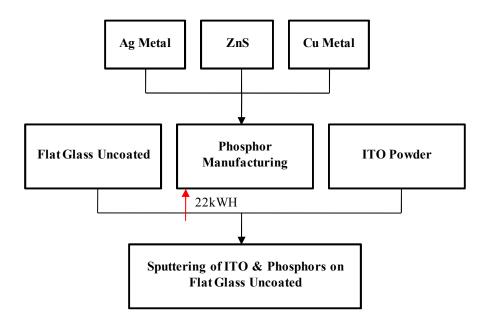A block diagram for the preparation of a phosphor anode substrate is shown in Figure 6S.

Figure 6S. Block Diagram for Fabrication of a Phosphor Anode Substrate

The LCI data for phosphor anode substrate fabrication step is given in Table 6S.

Table 6S. LCI Data for Phosphor Anode Substrate Fabrication

Inputs	
Materials/Energy	**Quantity**
ZnS	18.8 g
Cu	6.3 mg
Concentrated H_2SO_4 (for formation of $CuSO_4$)	20.38 mg
Ag	22.86 mg
Concentrated HNO_3(for formation of $AgNO_3$)	13.35 mg
NaCl	1.11 g
Flat glass uncoated	608.5 g
ITO Powder	0.5 g
Total Energy	7.5 kWh

The above LCI data for the CNT cathode substrate fabrication step is supported by the following calculations/assumptions:

a) The materials and energy used in zinc sulfide phosphor manufacturing are based on US patent literature (USP 3,657, 142) [7]. The patent states $ZnS:NaCl:CuSO_4:AgNO_3$ are in the quantity of 2724:56:0.083:1.56 (PBW) parts by weight, respectively. Furthermore, the total amount of phosphor needed was assumed to be similar to the quantity needed for a

15-inch CRT desktop display which is 20 grams. Thus, the amounts of individual chemicals in 20 grams are 18.8 g of ZnS, 1.11 g of NaCl, 16.6 mg of $CuSO_4$ and 36 mg $AgNO_3$. However, since the modules for $CuSO_4$ and $AgNO_3$ are not available in the Ecoinvent database, the amounts of Cu and concentrated H_2SO_4 needed to form $CuSO_4$ and the amounts of Ag and concentrated HNO_3 needed to form $AgNO_3$ were estimated based on respective stoichiometric equations.

b) The amount of glass substrate was assumed to be similar to the amount of glass used in the CNT cathode substrate preparation.

c) The amount of ITO powder coated on the glass substrate was based on the quantity used for LCD panels [30].

d) Energy consumption for phosphor manufacturing was based on the description given in a US Patent (3,657,142) [7]. Additionally, the phosphors are heated in a muffle (retort) furnace for 3 hours at 900-1300°C.

S.8   LCI Data for Vacuum Sealing CNT Cathode and Phosphor Anode Substrates

A block diagram for the vacuum sealing step is shown in Figure 7S.
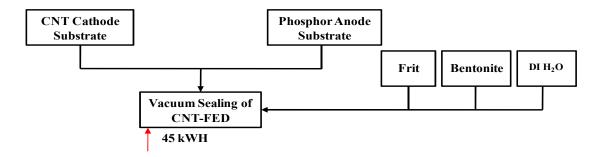
Vacuum Sealing of One CNT-FED Substrate

Figure 7S. Block Diagram for Vacuum Sealing Operation of CNT-FED

The LCI data for Phosphor anode fabrication step is given in Table 7S.

Table 7S. LCI Data for Phosphor Anode Fabrication

Inputs	
Materials/Energy	**Quantity**
CNT Cathode Substrate	709 g
Phosphor Anode Substrate	629 g
Frit	98 g
Bentonite	2 g
DI Water	150 g
Total Energy	45 kWh

The above LCI data for the vacuum sealing of CNT-FED is supported by the following calculations/assumptions.

a) The LCI data modules for the CNT cathode substrate and phosphor anode were obtained from stages 5 & 6 respectively. The chemicals, including energy consumption, for the vacuum sealing were obtained from a US patent (6,554,672 B2) data [8]

S.9 LCI Data for Complete Assembly of CNT-FED Device

A block diagram for complete assembly of a CNT-FED device is shown in Figure 8S.
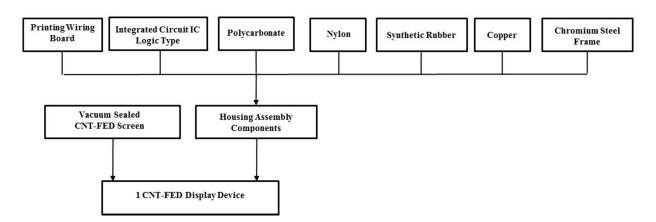

Figure 8S. Block Diagram for Complete Assembly of one CNT-FED Product

The LCI data for the complete assembly of CNT-FED device is given in Table 8S.

Table 8S. LCI for CNT-FED Device Assembly

Inputs	
Materials/Energy	**Quantity**
Vacuum sealed CNT-FED	1438 g
Chromium Steel	177.20 g
Copper at regional storage	4.8422 g
Printed wiring board	68.415 g
Integrated Circuit IC Logic Type	12.80 g
Polycarbonate	500 g
Nylon 6	9.8406 g
Synthetic Rubber	6.3261 g

The above LCI data for the complete assembly of a CNT-FED device is supported by the following calculations/assumptions:

a) The LCI data for the vacuum sealed CNT-FED is obtained from S.8.

b) The amounts of cable, steel, printed circuit board, and polymer materials were assumed to be same as that for an LCD desktop panel [30].

S.10   Contribution of Environmental Impacts of CNT Paste Formulation toward Fabrication of CNT Cathode Substrate

In Figure 9S, the cradle-to-gate impact assessment results for CNT cathode substrate fabrication (Module 1) are set at 100%, as represented by the black bars. Module 1 includes CNT paste formulation as well as screen printing, UV irradiation, and baking and surface treatment of the CNT cathode substrate. The white bars represent the normalized cradle-to-gate impact assessment results for CNT paste formulation only (a step within Module 1). CNT paste formulation is responsible for 95-98% of the overall total impact resulting from the CNT cathode substrate fabrication step. The remaining steps combined contribute 2-5% of the impacts.
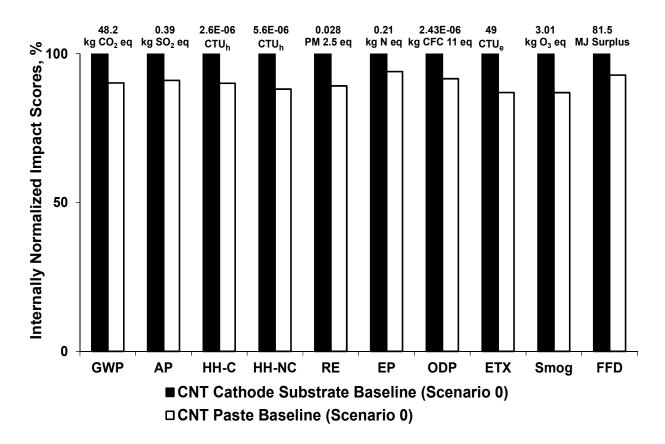
Figure 9S. Contribution of CNT Paste Preparation (Baseline Scenario) Impacts toward CNT Cathode Fabrication Step

S.11   Cradle-to-Gate Life Cycle Impact Assessment Results for four different CNT Paste Formulation Scenarios

The cradle-to-gate life cycle impact assessment results for the four different CNT paste preparation methods (one baseline scenario and three alternate scenarios used for sensitivity analysis) are given in Figure 10S.
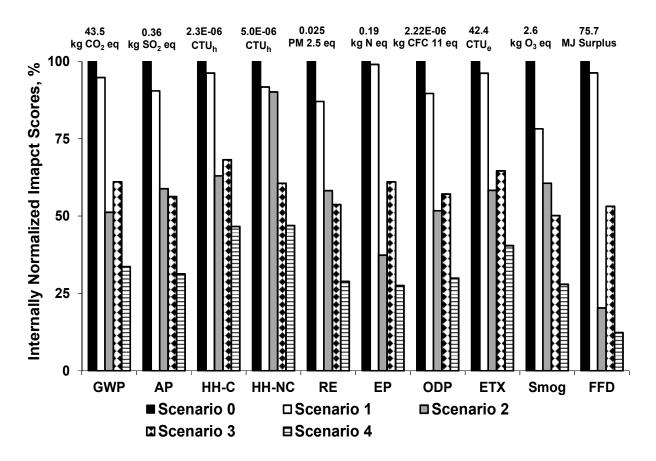
Figure 10S. Comparison of Impact Assessment Results for Four Different CNT Paste Formulation Scenarios

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