Article

Synthesis of carbon nanotubes via liquid injection chemical vapour deposition as a vector for the chemical recycling of waste composite carbon sources

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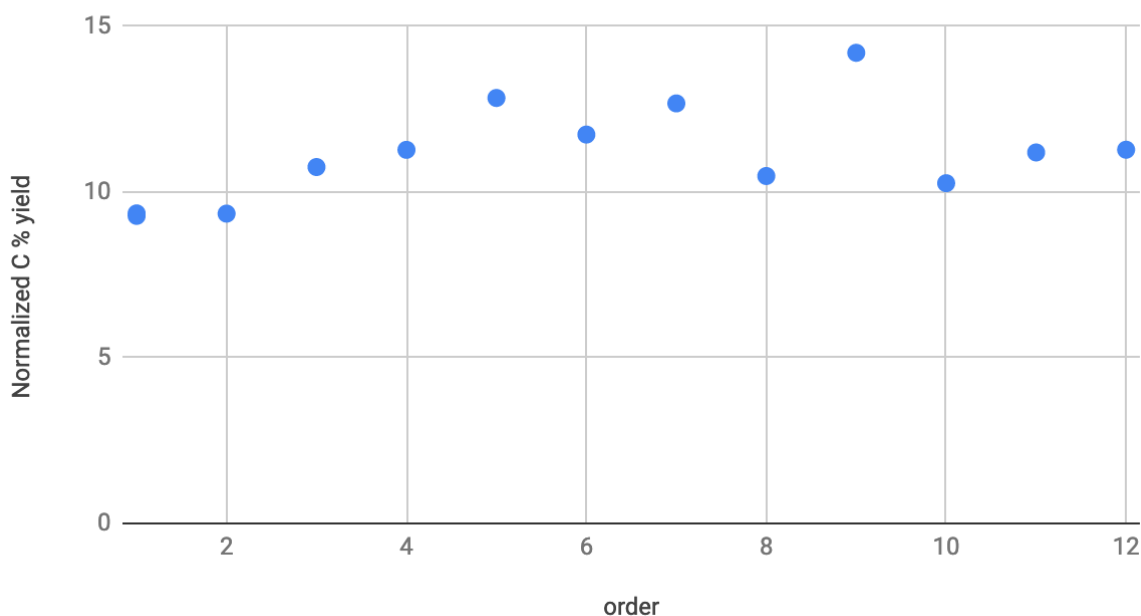**Supplementary information.**

Figure 1. MWCNT yield versus order of the reaction.

Comment: Seasoned veterans growing carbon nanotubes are aware that ageing of the quartz tube, wherein the quartz two becomes black or the quartz tube develops a carbon layer through subsequent growth, can improve Carbon Nanotube growth through the process of carbothermic reduction. We note that in between each reaction, no cleaning or no chemical cleaning of the quartz tube was done. So, all the reactions were carried out on an aged quartz tube, and because of this, we carried out the reactions in a randomised order to avoid any to mitigate cumulative positive results that compound as the ageing continues. So the positive results we're seeing in terms of yield, we believe are to do with the actual concentration of polystyrene content and not from the cumulative use, or aging of the furnace.
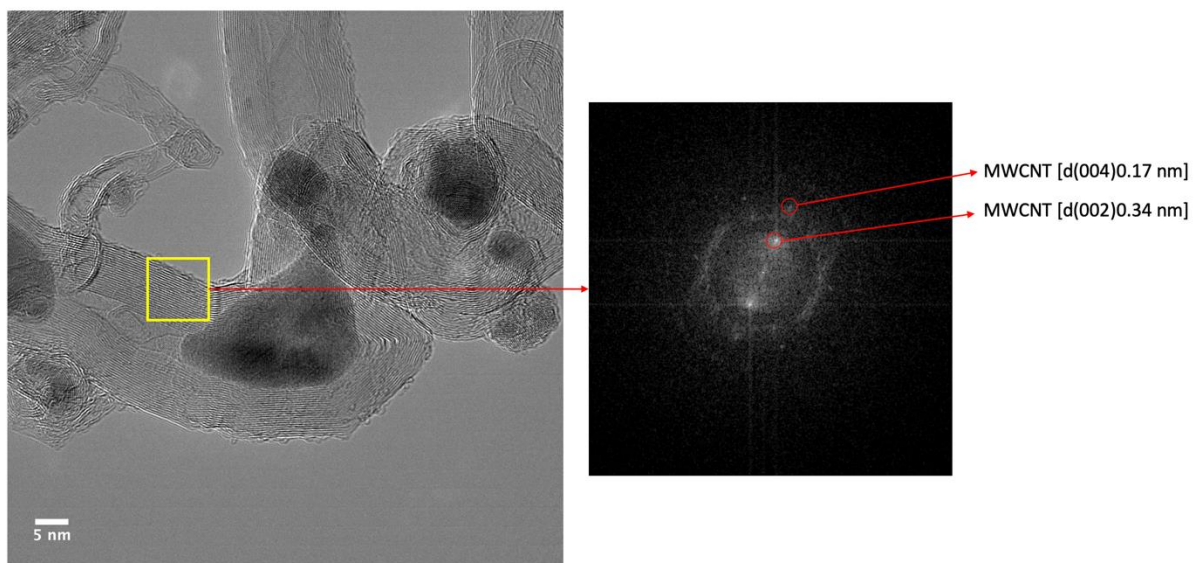
FFT of the MWCNT

MWCNT [d(004)0.17 nm]

MWCNT [d(002)0.34 nm]

Figure SI2: FFT of HRTEM images.

FFT of local area

0.20 nm
0.22 nm

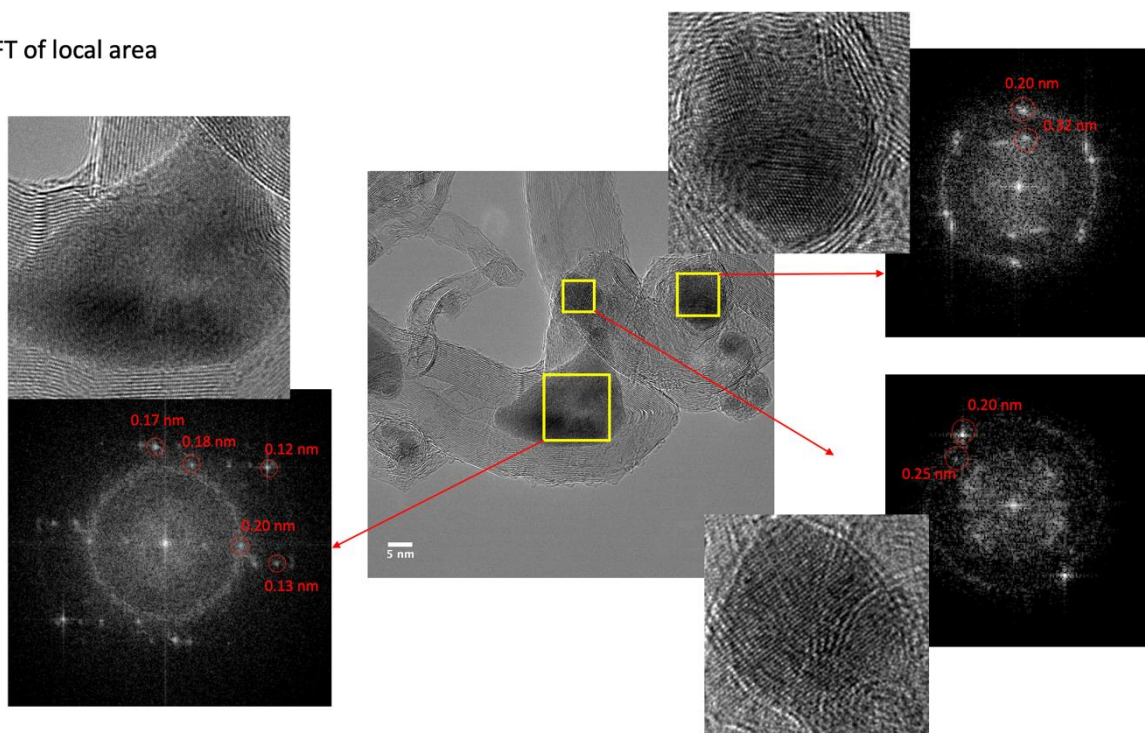0.17 nm
0.18 nm
0.12 nm
0.20 nm
0.13 nm

0.20 nm
0.25 nm

Figure SI3: FFT of HRTEM images.
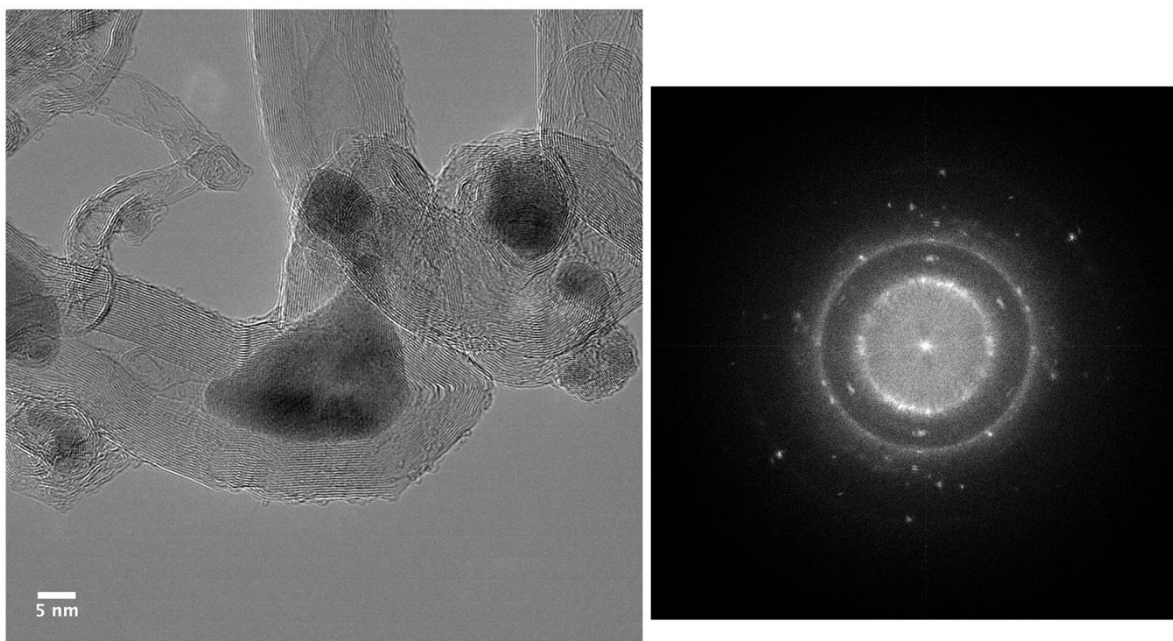
FFT of the whole image

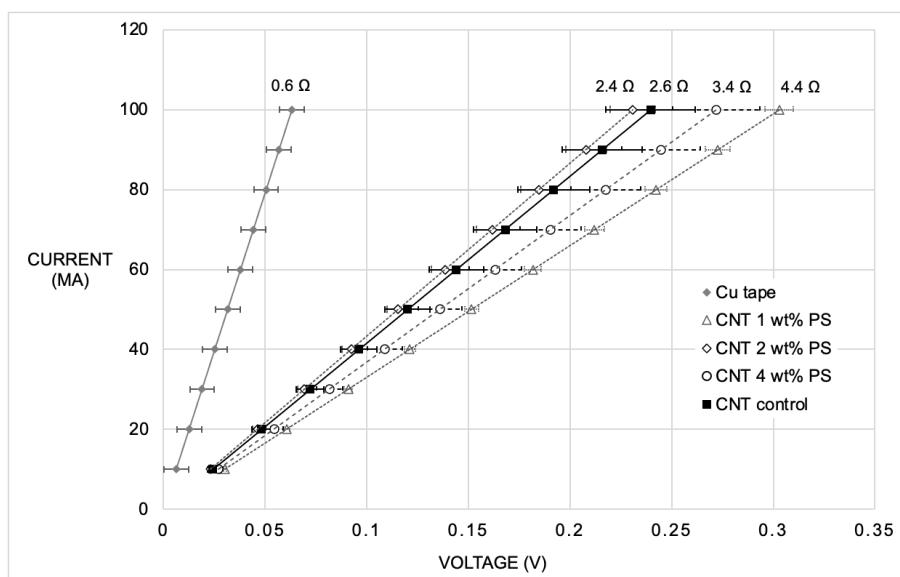**Figure SI4: FFT of whole HRTEM image.**

Figure SI5: Voltage drop date for CNT films

Figure SI6: Picture of the CNT Ethernet Cable

Discussion on potential environmental impacts of CNT manufacturing

- This is what it is written in the Simapro Database Manual about normalization.

"Many methods allow the impact category indicator results to be compared by a reference (or normal) value. This mean that the impact category is divided by the reference. A commonly used reference is the average yearly environmental load in a country or continent, divided by the number of inhabitants. However, the reference may be chosen freely. You could also choose the environmental load of lighting a 60W bulb for one hour, 100 km of transport by car or 1 liter of milk. This can be useful to communicate the results to non LCA experts, as you benchmark your own LCA against something everybody can imagine. In SimaPro, there are often alternative normalization sets available. After normalization the impact category indicators all have the same unit, which makes it easier to compare them. Normalization can be applied on both characterization and damage assessment results. PLEASE NOTE: SimaPro does not divide by the reference value (N), but multiplies by the inverse. If you edit or add a normalization value in a method, you must therefore enter the inverted value (1/N)."

Link to the Database Manual: [DatabaseManualMethods.pdf (simapro.com)](DatabaseManualMethods.pdf)

- Here are some examples of the use of normalised results in the literature.

    - Healy, Meagan L., Lindsay J. Dahlben, and Jacqueline A. Isaacs. "Environmental assessment of single-walled carbon nanotube processes." *Journal of Industrial Ecology* 12.3 (2008): 376-393.

    - Griffiths, O. Glyn, et al. "Identifying the largest environmental life cycle impacts during carbon nanotube synthesis via chemical vapour deposition." *Journal of cleaner production* 42 (2013): 180-189.

    - Heidari, Ava, and Habibollah Younesi. "Synthesis, characterization and life cycle assessment of carbon nanospheres from waste tires pyrolysis over ferrocene catalyst." *Journal of Environmental Chemical Engineering* 8.2 (2020): 103669.

    - Gavankar, Sheetal, Sangwon Suh, and Arturo A. Keller. "The role of scale and technology maturity in life cycle assessment of emerging technologies: a case study on carbon nanotubes." *Journal of Industrial Ecology* 19.1 (2015): 51-60.

- **Discussion on Fossil CO_2 eq and CO_2 uptake**

The only information shared in the Simapro Database Manual about the method used for the CO_2 emissions calculations are the following ones (Method: IPCC 2013 GWP 100a).

"IPCC 2013 is an update of the method IPCC 2007 developed by the International Panel on Climate Change. This method lists the climate change factors of IPCC with a timeframe of 20 and 100 years. 6.4.1 Characterization IPCC characterization factors for the direct (except CH4) global warming potential of air emissions. They are:

• not including indirect formation of dinitrogen monoxide from nitrogen emissions.

• not accounting for radiative forcing due to emissions of NOx, water, sulphate, etc. in the lower stratosphere + upper troposphere.

• not considering the range of indirect effects given by IPCC.

• not including CO_2 formation from CO emissions"

Moreover, they say that "Fossil based carbon" correspond to carbon originating from fossil fuels and "Carbon uptake" correspond to the CO_2 that is stored in plants and trees as they grow.

In our case, most of the CO_2 absorption comes from energy consumption. As the Simapro database does not share much information in this area, it can only be assumed that this uptake is due to the fact that the UK uses incinerators as an energy resource in part. Thus, the reuse of household waste is taken into account in the LCA and appears as CO_2 uptake.

- **Discussion on CO₂ eq emissions of an airplane calculations**

Here is the list of all the assumptions that I made to calculate the CO_2 emissions of an airplane during its use.

- The weight of copper wire in a plane is equal to 1 519.6 kg. This weight has been determined using the document "Aircraft Electrical Wire" [1] from the company Tyco Electronics. The paper state that the cables, model 55PC, used in Boeing 747 aircraft since 1992, weight 4.5 lbs per 1,000 ft length.

  So $141\ miles\ =\ 744{,}480\ ft$

  $\to 4.5 * \frac{744{,}480}{1000} = 3{,}350.16\ lbs \to \sim \mathbf{1519.6\ kg}$, this results in a weight saving of 1163.44 kg.

- The weight of CNTs has been determined by dividing the weight of copper wire by the copper density (8.96 g/cm³) and then multiplicated by the CNTs density (2.1 g/cm³) [Lu et al. *"Determination of carbon nanotube density by gradient sedimentation"*] [2].

  So, $1519.6 * \frac{2.1}{8.96} = \mathbf{356.16\ kg}$

- A Boeing 747-400 fly during its lifespan for approximately 100 000 hours (Here are some websites with information on the life span of the Boeing 747-400: <u>Average Life Expectancy Of A Boeing 747 - Airliners.net</u>, <u>A 747 Aircraft Owned By Idiot Investors Recently Arrived In St Vincent. - Asberth News Network (annsvg.com)</u>, <u>The Commercial Aircraft With The Highest Hours And Flight Cycles - Simple Flying</u>) at an average speed of approximately 900 km/h. The value of the average speed of the Boeing has been determined from various information found online. On specialized aircraft websites, it is stated that a Boeing 747-400 flies at a maximum speed of about 930 to 940 km/h and a long range cruise speed of 907km/h (here are some examples of aircraft websites: <u>1989 - 2010 Boeing 747-400 | Top Speed</u>, <u>Boeing 747-400 - Price, Specs, Photo Gallery, History - Aero Corner</u>, <u>Airliners.net</u>). Taking into account the take-off and landing phases, I have made the assumption that the aircraft should fly at an average speed of 900 km/h.

- A Boeing 747-400 have an average of 20 000 compression and decompression cycles (<u>A 747 Aircraft Owned By Idiot Investors Recently Arrived In St Vincent. - Asberth News Network (annsvg.com)</u>).

- Using the latest data, I was able to determine that the average length of a Boeing 747-400 flights is 4 500 km. Multiplying the lifetime by the average speed of the aircraft and dividing by the average number of compression and decompression cycles gives the average flight length of a Boeing 747-400.

  So, $\frac{100\,000 \times 900}{20\,000} = \mathbf{4\,500\ km}$

- An empty Boeing 747-400 has a mass of 183.5 tons, a tank capacity of 217 000 litres and a travel range of 13 500 km (<u>Boeing 747-400 - Price, Specs, Photo Gallery, History - Aero Corner</u>, <u>Boeing 747 Specs: Weight, Length, Range, Wingspan & More (knaviation.net)</u>). With all this information I was able to determine the weight of the plane before it took off for a 4500km flight. By dividing the maximum tank capacity by the maximum travel range

and then multiplying by the average length of a flight I get the volume of kerosene needed to complete a flight.

So, $\frac{217\,000 \times 4\,500}{13\,500} \approx$ **72 300 L**, knowing that the density of kerosene is 0.8 g/cm³,

-> $72\,300 \times 0.8 = $ **57 840 kg**, adding this mass to the empty mass of the aircraft gives,

-> $183\,500 + 57\,840 = $ **241 340 kg** which represents the average weight of a Boeing 747-400 before take-off for a 4500 km flight.

- Knowing now the average mass of the aircraft with copper wires, we can determine its mass with CNT wires.
  So, 241 340 - 1163.44 $\approx$ **240 180. kg**

- Knowing now the average weight of the aircraft and the distance travelled during its lifetime, it is possible to calculate the tonne-kilometre (tkm) that needs to be fed into the Simapro software to calculate the CO_2 emissions.
  So, $241.34 \times 100\,000 \times 900 = $ **21 720 600 000 tkm** for a plane with copper
  And $240.18 \times 100\,000 \times 900 = $ **21 616 200 000 tkm** for a plane with CNTs.

- In order to verify the results obtained with Simapro, I tried to find out how much CO_2 was emitted by burning 1 kg of kerosene. According to the website Combustion of Fuels - Carbon Dioxide Emission (engineeringtoolbox.com), 1 kg of kerosene emits 3 kg of CO_2 into the air. Knowing that to travel 13,500 km a Boeing 747-400 needs about 217 000 L of kerosene we can deduce 217 000/13 500 = 16.07 kg of kerosene is required to cover 1 km (I found in the literature that 1 km consumes on average 12.63 kg of kerosene). As mentioned earlier, a Boeing 747-400 will travel approximately 90 000 000 km during its lifetime.
  So this gives us,
  $90\,000\,000 \times 16.07 \times 3 \approx 4\,338\,900\,000 \; kg \; of \; CO2 \; or$ **4 338.9 $kton \; of \; CO2$**

  Or by using the data found online: $90\,000\,000 \times 12.63 \times 3 \approx$ **3 410.1 $kton \; of \; CO2$**

  Knowing that the CO_2 emissions found in the simulation were in the orders of magnitude of **4 500 kton of CO_2 eq (to which just CO_2 contributed 4 450 kton).**

Reference:

[1] Cinibulk, W. , 2001, Aircraft Electrical Wire, Wire Manufacturers Perspective, Tyco Electronics (Raychem), visited on: aircraft_electrical_wire.pdf (mitrecaasd.org)

[2] Lu, Q., Keskar, G., Ciocan, R., Rao, R., Mathur, R. B., Rao, A. M., & Larcom, L. L. (2006). Determination of carbon nanotube density by gradient sedimentation. *The Journal of Physical* Chemistry B, 110(48), 24371-24376.