Monitoring the carbon footprint (R-NMR Task 2.5)

of Remote NMR (R-NMR):
Moving NMR infrastructures to remote access capabilities

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Introduction

Description of work: In task 2.5, we will select a set of tools for the calculation of carbon footprint that are suitable to cover the range of impacts caused by the operation of NMR infrastructures. All partners will adopt a common approach to the calculation of the footprint of their users' travel. In addition, we will look into tools that can capture the footprint of equipment usage. The results of these analyses will be communicated to the relevant stakeholders.

Virtually all our activities leave a carbon footprint and NMR is no different. Some activities are directly related to burning fossil fuels. These include transport (sea, air, road and, to an extent, rail) and heating (excluding heat pumps). However, most NMR related activities are dependent on electricity and here the carbon footprint is closely tied to the type of power generation plants used in a specific country. Countries with many hydro, nuclear and renewable power generating plants will generate a smaller carbon footprint per unit of electric power. On the other hand, countries with mostly coal or gas powered plants will leave a much larger carbon footprint. When considering EU member states, the difference can be on the order of a hundredfold (Figure 1). The EU-27 average of 275 g CO_2e equivalents per kWh will be used in all calculations.

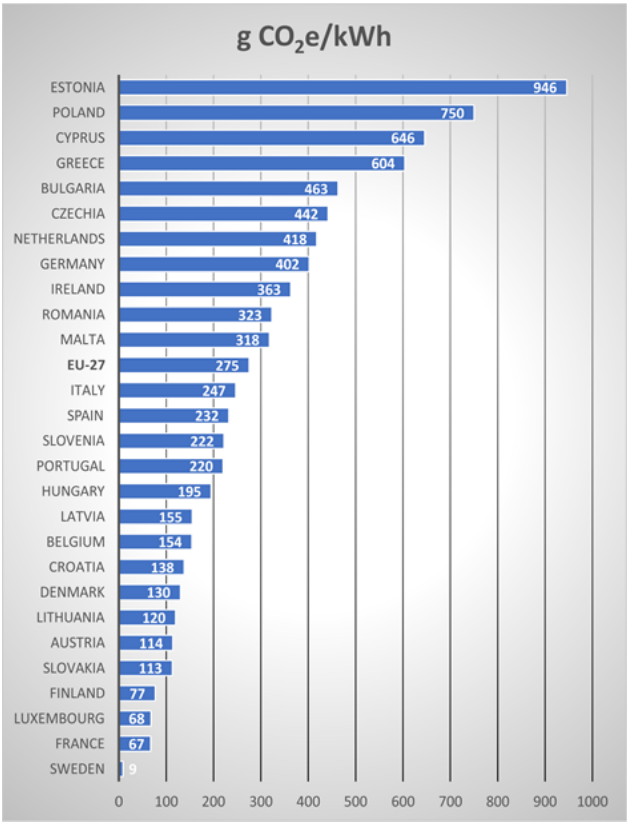

Figure 1 - CO_2 equivalents per kWh of electricity produced in different member states (Source: EEA). For completeness, the value for the UK is 269 CO_2 equivalents per kWh.

In the sections that follow, the carbon footprint of various aspects of the operation of an NMR facility will be discussed. These include: transport of people and of samples, the electricity consumption associated with various hardware components of NMR spectrometers, air conditioning of NMR facilities, liquid helium, and liquid nitrogen.

Transport

Personnel (scientists):

Travelling is a carbon intensive activity, especially when air travel is involved. When work cannot be done remotely or samples cannot easily be shipped, travelling scientists can estimate their carbon footprint using an air or train travel calculator:

ICAO - International Civil Aviation Organization
https://www.icao.int/environmental-protection/Carbonoffset/

Rail Europe
https://www.raileurope.com/

Air travel produces considerably (an order of magnitude) more carbon emissions compared to rail travel. However, over large distances or some destinations travelling over land (even within continental Europe) can take days and flying is the only reasonable option. On the other hand, where high-speed (direct) rail connections exist between destinations flying should be avoided.

Example 1: Paris to Ljubljana is a 2 hour flight compared to an 18 hour train trip one-way. Prices of air and train tickets on this route are comparable. However, flying releases around 140 kg CO_2e, while the train produces less than 10 kg CO_2e.

Example 2: Paris to Marseille is a 1.5 hour flight compared to a 3.5 hour train ride. Transfers to and from the airport as well as waiting at check-in makes the travel time comparable. So is the price. Flying releases around 90 kg CO_2e, while the train accounts for less than 5 kg CO_2e.

Cargo (sample shipment):

Shipping samples is again least environmentally friendly when using air freight. Shipping stable samples at ambient temperature can be done with standard parcel delivery methods with a negligible carbon footprint. On the other hand, sensitive samples are usually shipped on dry ice with parcel sizes between 0.1 and 0.2 m^3 weighing between 10 and 20 kg. Furthermore, most of the parcel weight is frozen CO_2, which should be added directly to the carbon footprint.

The carbon footprint of shipping larger packages with samples can be estimated using an online calculator. However, most web calculators deal with tonnes of cargo or standard shipping container units, which are not suitable for NMR samples weighing a few grams or kilograms. DHL offers a web-based calculator where the carbon footprint of smaller parcels can be estimated.

https://www.dhl-carboncalculator.com/

The calculator is based on the EN 16258 standard, which establishes a common methodology for the calculation and declaration of energy consumption and greenhouse gas emissions related to any transport service.

A summary of carbon emissions associated with different modes of sample transport is presented in Table 1.

Transport mode	**Emissions (g CO_2e / tonne·km)**
Road	62
Rail	22
Short sea	16
Intermodal road/rail	26
Intermodal road/short sea	21
Deep-sea container	8
Air-freight	602

Table 1 – Emissions associated with different modes of transport. (Source: McKinnon et al., Measuring and Managing CO_2 *Emissions of European Chemical Transport, Heriot-Watt University, 2011).*

Electricity

A typical modern solution-state NMR spectrometer equipped with a cryo-probe has a number of components including the NMR console, the PC and display screen, an air cooler (BCU) for temperature control of the sample, a cryo-cooling unit, a helium compressor and a water chiller. The typical power consumption associated with each of these components is summarized in Table 2.

System Component	Power consumption (kW)
NMR console (NEO OneBay)	1.3
PC and display	0.2
Air cooler (BCU)	0.6
Cryo cooling unit	0.5
Helium compressor	7.5
Water chiller	3.6

Table 2 – Summary of power consumption associated with NMR spectrometer components (Source: Bruker Site planning guide).

In total that is 13.7 kW of continuous power draw and 120 MWh in a year. Using the EU-27 average this produces 33 tonnes of CO_2e per year. Interestingly, most of the power draw is associated with components related to the cryo-probe (Cryo cooling unit, helium compressor and water chiller). An NMR spectrometer with a room temperature probe would draw only 2.1 kW and produce 5 tonnes of CO_2e. Spectrometers optimised for solids also do not require these 'cryo' components. However, they do use higher power amplifiers and a typical solids console will draw an additional 1.7 kW.

Superconducting magnets do not draw electrical power during their operation. However, pumped (2K) magnets do require constant operation of vacuum pumps, which use on average 0.5 kW and thus produce 1.2 tonnes of CO_2e per year.

Modern fluorescent or even LED lighting is relatively efficient. Nevertheless, lighting can be turned off, while the spectrometer is operated remotely for a modest energy saving. Modern PCs, which control the spectrometer, use between 150 and 200 W and need to be turned on at all times.

Air conditioning

Boards in NMR consoles are particularly sensitive to temperature and require a constant flow of cool air. Rooms where consoles are located need tight temperature regulation (cooling). Therefore, air conditioning units run continuously. However, cooling power requirements can vary considerably depending on room size and configuration as well as the climate and season.

On the other hand, if the magnet is not in the same room as the consoles, the magnet room may not need as tight temperature regulation. The same goes for some auxiliary components.

The room where the operator sits can also be cooled less, especially when the spectrometer is operated remotely. Nevertheless, it will be assumed that all electrical power used by different components of NMR systems is converted to heat, which needs to be removed. A typical modern air conditioning unit has a seasonal energy efficiency ratio of around 6 (W/W), which means that an additional ⅙ of the carbon footprint caused by usage of electricity is produced due to heat removal.

Liquid helium

Helium (He) is found as a trace gas in natural gas wells and regenerates very slowly as a by-product of uranium decay. While all natural gas deposits contain some helium it is often not separated and sold commercially. Currently the only significant suppliers are the United States, Algeria and Qatar. Therefore, helium needs to be shipped to Europe from overseas.

Newly extracted helium is normally liquified on site (overseas) and then transported by sea and road to a filling plant in Europe. The final leg to individual NMR facilities is by road. However, compared to the high carbon footprint of He liquefaction transport carbon footprint is negligible even if importing from the USA. Nevertheless, small scale helium liquefiers are available and relatively pure captured helium gas can be reliquefied on site, which eliminates any carbon emissions related to long distance transport. Around 10-20% of helium gas is lost during the process. Considerable amounts of helium are also lost with handling when transferring the liquid gas to smaller containers and finally into the NMR magnet.

Once helium is vented into the atmosphere it is uneconomical to recover and slowly diffuses into space. Current estimates suggest helium supplies on Earth will be depleted within a century. Some sort of helium recovery is therefore necessary for its long-term use as a cryogenic gas. Unfortunately, helium recycling is not widely used. This is mostly related to the additional cost of capture and/or liquefaction equipment as well as the high energy demand and consequently the carbon footprint.

Efficiency of a helium liquefaction plant depends amongst other things on the percentage of helium in the natural gas mixture (Figure 2). It is very costly to exploit wells with less than 3% helium and the carbon footprint is consequently also very large. The optimistic value of 200 kWh/kmol can be converted to 50 kWh/kg He or 6.25 kWh/L He for liquefaction alone. Using the EU-27 average CO_2 equivalents per kWh of electricity this corresponds to more than 1.7 kg CO_2 equivalents per 1 L of liquid helium. This does not include the carbon footprint and other environmental impacts related to exploiting a natural gas well. However, these can be eliminated if helium is captured on site from magnet boil off. Helium capture equipment is readily available and does not produce a large carbon footprint since at this stage the gas is only compressed into storage cylinders ready for transport to the liquefaction plant.

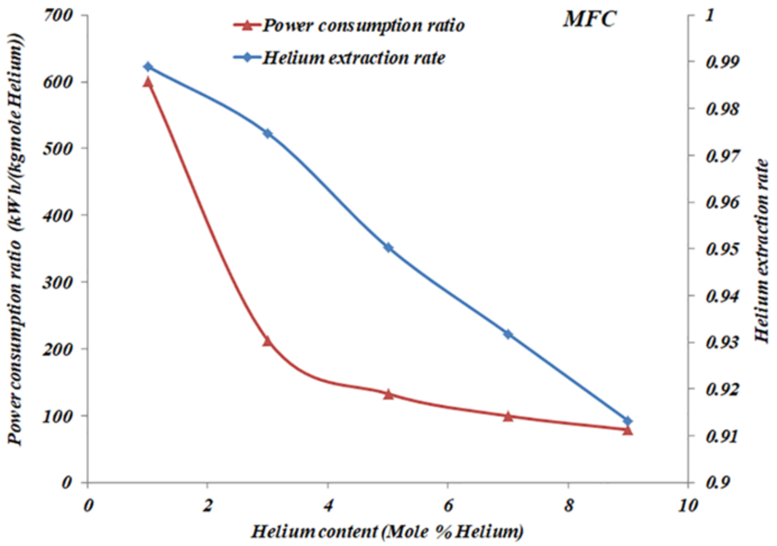

Figure 2 - Power consumption and extraction rates for different fractions of He in natural gas wells. (Source: Zaitsev et al., Int. J. Energy Res. 2020.)

Magnet	**Helium consumption**		**Liquefaction cost**	**CO2 emissions**
	(ml / h)	**(L / year)**	**(MWh / year)**	**(kg CO_2e / year)**
400 MHz	13	114	0.7	196
500 MHz	13	114	0.7	196
600 MHz	16	140	0.9	241
700 MHz	26	228	1.4	392
800 MHz	47	412	2.6	708
1.0 GHz (2K)	< 250	< 2190	< 13.7	< 3765
1.2 GHz (2K)	< 250	< 2190	< 13.7	< 3765

Table 3 - Helium consumption of modern (current generation) NMR magnets

Due to scarcity of and recent price increases for liquid helium, manufacturers are trying to decrease helium consumption of NMR magnets. Modern lower field conventional 4K superconducting magnets consume relatively small volumes of liquid helium (Tables 3, 4 and 5). On the other hand, the highest field NMR spectrometers (1.0 and 1.2 GHz) use pumped 2K superconducting magnets. These use evaporative cooling to maintain superconductivity of coil and joint material at high magnetic fields. Since this is achieved by a pumping process, which actively removes helium from the upper bath, helium consumption greatly increases. Advances in NMR magnet design allow the latest generation of 800 MHz magnets to switch from a pumped 2K to a conventional 4K magnet design greatly reducing its helium consumption (Table 5).

Magnet	**Helium consumption**		**Liquefaction cost**	**CO2 emissions**
600 MHz	**(ml / h)**	**(L / year)**	**(MWh / year)**	**(kg CO_2e / year)**
early gen.	40	350	2,2	602
last gen.	26	228	1,4	392
current gen.	16	140	0,9	241

Table 4 - Helium consumption of different generations of 600 MHz NMR magnets.

Magnet	**Helium consumption**		**Liquefaction cost**	**CO2 emissions**
800 MHz	**(ml / h)**	**(L / year)**	**(MWh / year)**	**(kg CO_2e / year)**
last gen. (2K)	140	1226	7,7	2108
current gen. (4K)	47	412	2,6	708

Table 5 - Helium consumption of different generations of 800 MHz NMR magnets.

Liquid nitrogen

In contrast to helium, nitrogen is the major component of Earth's atmosphere and can be liquified anywhere on the planet. This eliminates long distance transport of the liquified gas (LN2). However, nitrogen liquefaction is still moderately energy demanding. A typical plant can liquefy nitrogen with an energy cost of 0.5 kWh/L LN2, which corresponds to 0.14 kg CO_2 equivalents per 1 L of LN2. A modern 600 MHz NMR magnet will use around 2600 L of LN2 per year, which corresponds to 364 kg CO_2e. On the other hand, an early generation pumped 800 MHz magnet uses around 7800 L of LN2, which is responsible for 1092 kg CO_2e per year.

Nitrogen gas can be also recycled on site via an accessory nitrogen liquefier, which greatly reduces the number of nitrogen refills each year. This also reduces the need to transport LN2 over large distances. If the NMR system is already equipped with a cryo platform (for a cryo-probe) the nitrogen liquefier simply uses the extra cooling capacity of the cryo platform.

Summary

It is evident that (by far) the largest sources of carbon emissions are the power-hungry components related to cryoprobe operation. However, cryoprobes offer a huge advantage in sensitivity and have become the norm for biomolecular NMR. Since most of the carbon footprint is a consequence of electrical power generation the total carbon footprint of an NMR system can depend dramatically on the country where the spectrometer is operated or even the source of electricity purchased by the institution where the spectrometer is located.

With older NMR systems using pumped magnets large quantities of cryogenic gases are also a considerable source of carbon emissions. Upgrading to a non-pumped magnet can save a few tonnes of CO_2e per year. Even smaller systems (600 MHz or less) can benefit greatly from a magnet upgrade and cut the usage of cryogenic gases in half. However, there is a considerable financial cost associated with the purchase of a new magnet. Currently all magnets offering gigahertz field strengths still require pumping and are (environmentally) more expensive to run. A summary of the carbon footprint associated with some typical spectrometer configurations is shown in Table 6. This information will be useful to NMR facilities in their calculation of the carbon footprint associated with operation of their NMR spectrometers.

Tonnes of CO_2e per year	**current gen. 600 MHz (4K, RT probe)**	**current gen. 600 MHz (4K, cryoprobe)**	**early gen. 800 MHz (2K, cryoprobe)**
Electricity	5.1	33.0	34.2
Air conditioning	0.9	5.5	5.7
He	0.2	0.2	2.1
LN2	0.4	0.4	1.1
Total	**6.6**	**39.1**	**45.1**

Table 6 - Carbon footprint breakdown for some typical spectrometer configurations.