THE UNIVERSITY of EDINBURGH
School of Chemistry

UKMRM, London

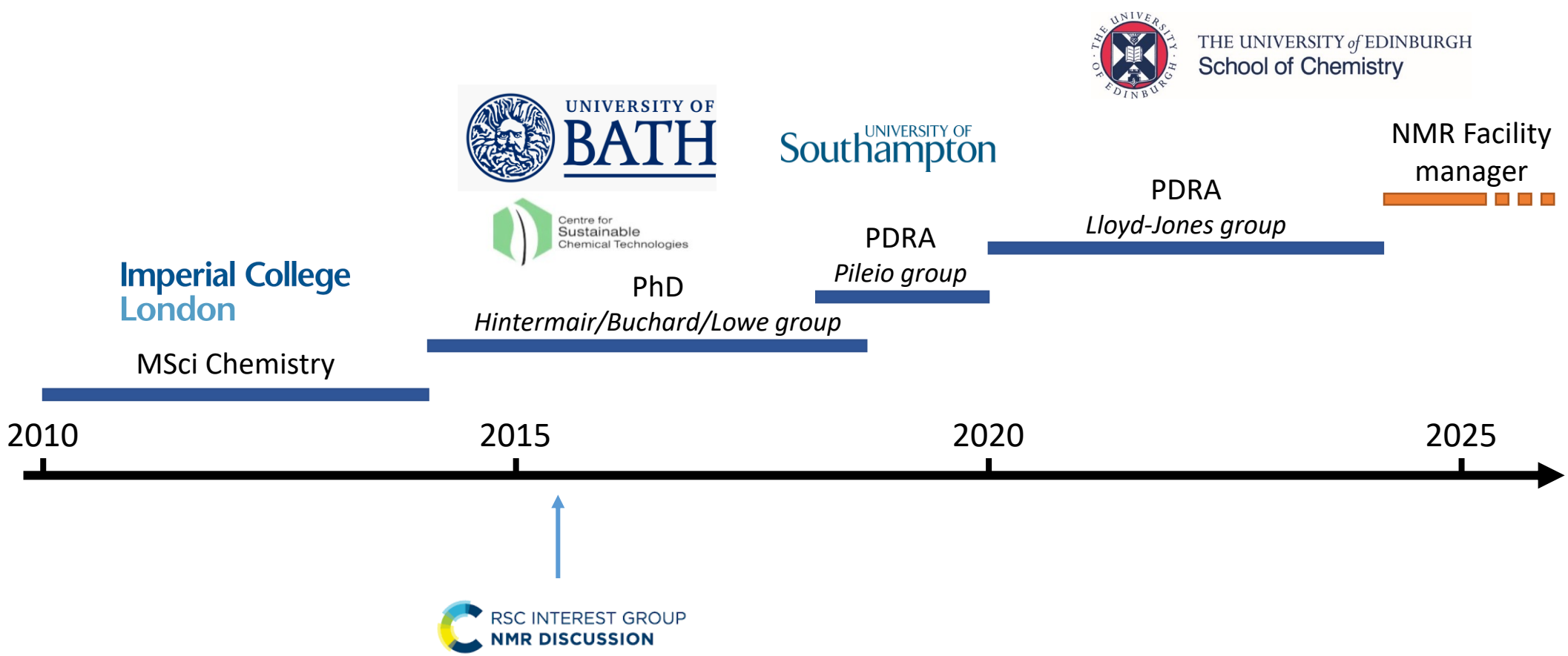
16th June 2025

# Perspectives of a new NMR facility manager

**Dr Andrew Hall**

NMR facility manager

# Background


THE UNIVERSITY of EDINBURGH
School of Chemistry
UNIVERSITY OF BATH
Centre for Sustainable Chemical Technologies
UNIVERSITY OF Southampton
THE UNIVERSITY of EDINBURGH
School of Chemistry
NMR Facility manager
PDRA
Lloyd-Jones group
PDRA
Pileio group
PhD
Hintermair/Buchard/Lowe group
Imperial College London
MSci Chemistry
2010
2015
2020
2025
RSC INTEREST GROUP
NMR DISCUSSION

# Expectations

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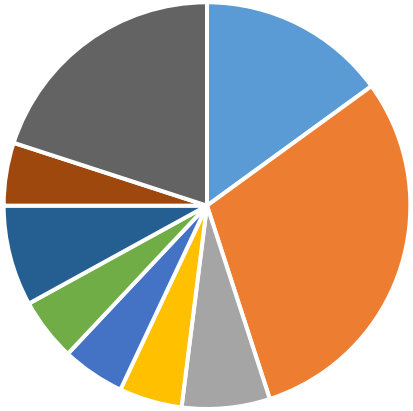
## Job description

- Maintain spectrometers
- Training and helping users
- Lab management
- Grant applications & papers
- Industrial work
- Data and IT management
- Budgeting

## Reality



- Maintain spectrometers
- Training and helping users
- Lab management
- Grant applications & papers
- Industrial work
- Data and IT management
- Budgeting
- Procurement
- Helium recovery

# New skills

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- Solid-state NMR
- Biological NMR
- Edinburgh manager programme
- 2K magnet system
- Helium recovery

**+ LOTS of on-the-job training**

# Challenges

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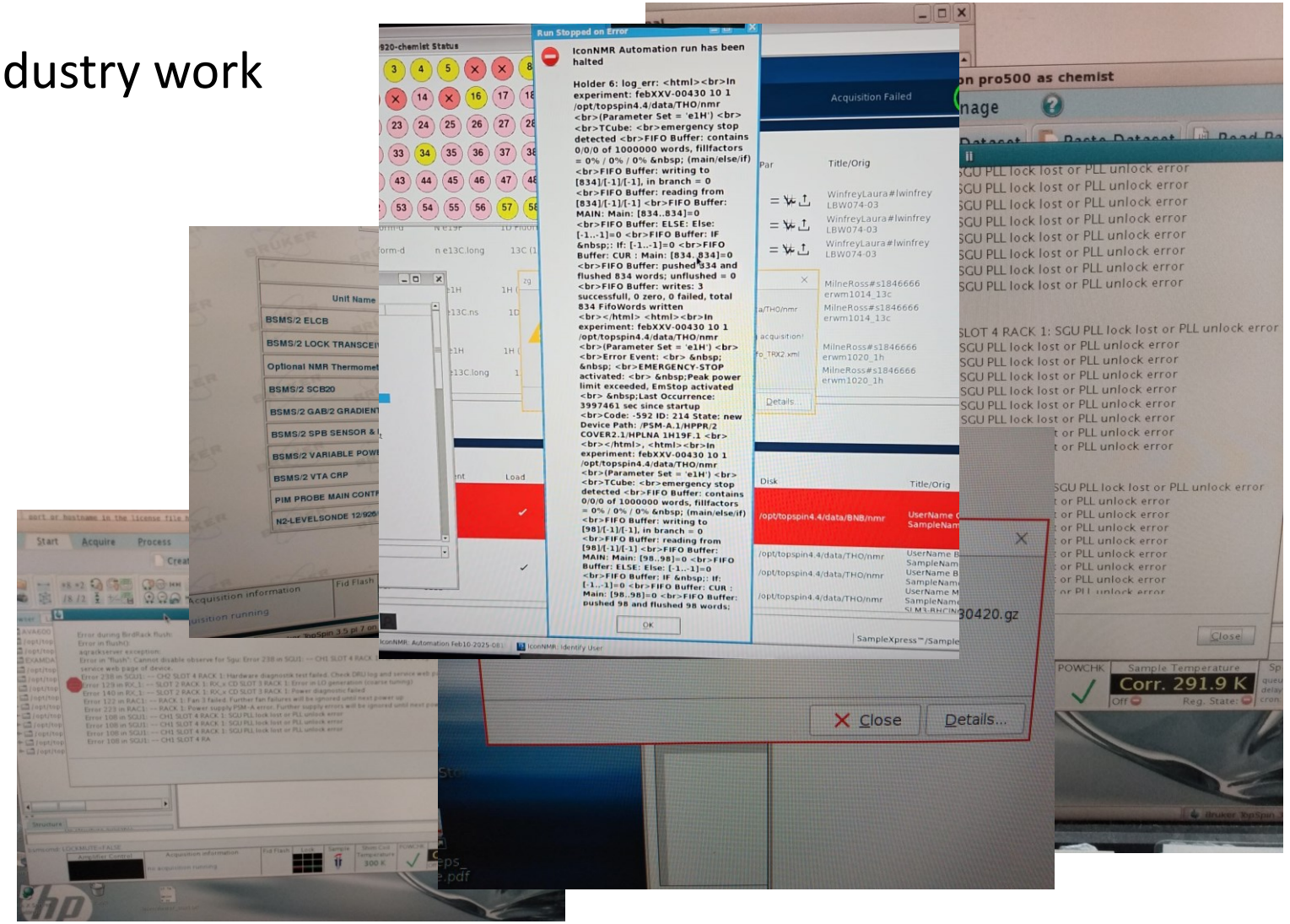
- Quoting for grants and industry work
- Budget management
- Finding time for research
- Aging computer systems



# New spectrometer

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- Funding from UoE for new 400 MHz solid/liquid spectrometer
- Upgrading existing 300 MHz solids
- Procurement ongoing
  - slow process!

# Helium liquefier

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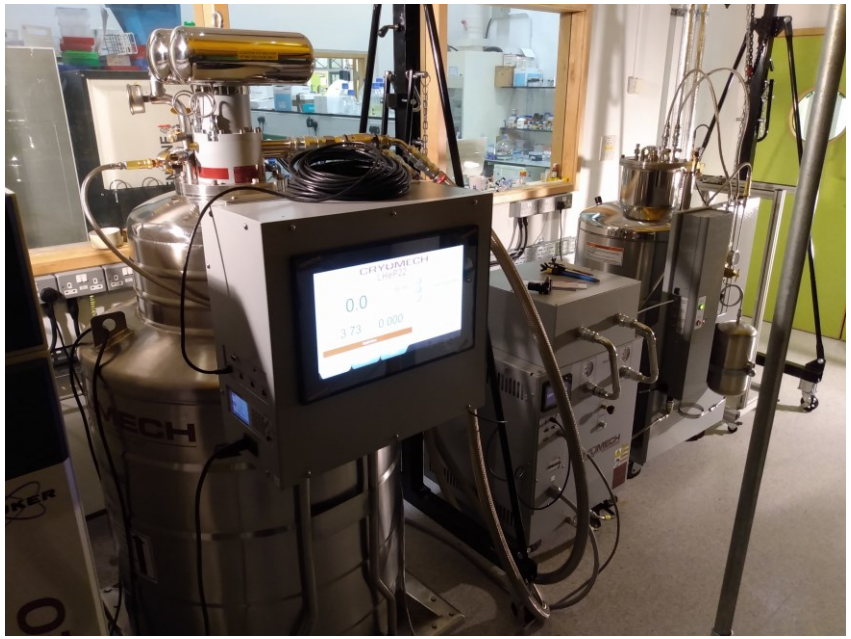




Bluefors LHeP22, 250 L capacity

- 26 L/day
- 14 days to fill Dewar
- ~£3.25 /L
- Estimated 438 gCO2e/L
- Payback time = 3 years

# Helium liquefier

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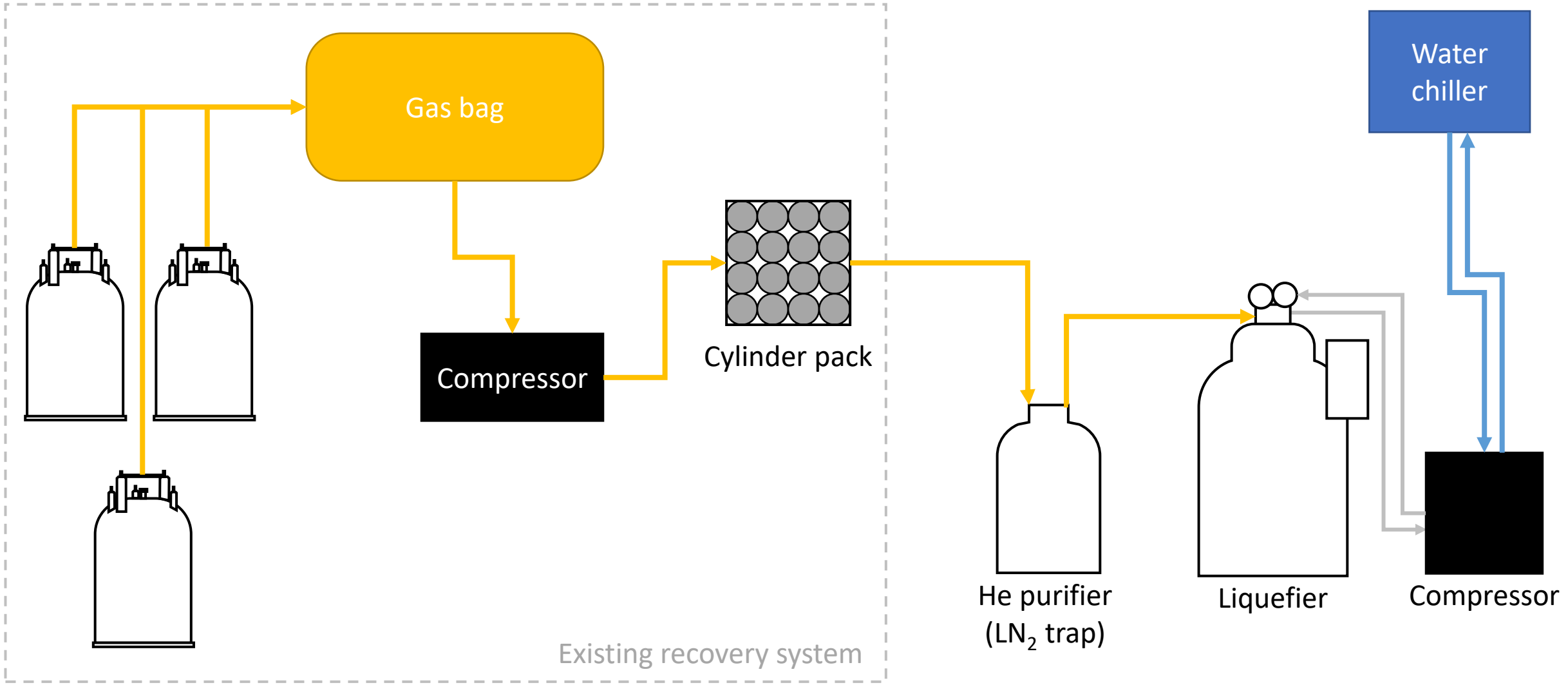

# Helium liquefier

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- Bluefors (Cryomech) LHeP22 liquefier
  - 26 L/day capacity (nominally 22 L/day)
  - 250 L Dewar
  - 14 days to fill Dewar (incl. cool down)
  - 250 L liquid = 190 $m^3$ gas (21 cylinders at 200 bar)
  - Weekly boil-off = 36 $m^3$ (5x 4K magnets, 1x 2K magnet, 2x MS magnets)
  - Boil-off during refills = 35 - 40 $m^3$
  - **Liquefier run two weeks per month**

- Helium gas purifier
  - $LN_2$ trap
  - Regenerated once a month
  - >99.99% purity

# Helium liquefier

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- Financial
  - Total system cost ~£250k (not including gas recovery system)
  - Annual helium consumption = 3000 L
  - Annual helium cost = £80k
  - **Pay-back time = 3 years**
- Energy
  - Liquefier = 12A @ 3-phase 400V = 6.65 kW[(1)]
  - Water chiller
    - Pump = 1.5A @ 3-phase 400V = 0.83 kW[(1)]
    - Compressor (~50% duty cycle) = 6.4A @ 3-phase 400V = 1.8 kW[(1)]
  - Total = 9.3 kW
  - Approximately 12.5 kWh/Litre, **~£3.25 /Litre**
  - Average 35 $gCO_2e$/kWh[(2)] = **438 $gCO_2e$/Litre** [619 $gCO_2e$/Litre for commercially purchased liquid][(3)]

1) Active power, power factor (estimated) = 0.8
2) Scotland electricity generation 2022, https://www.gov.scot/publications/energy-statistics-for-scotland-q1-2024/pages/electricity-generation-emissions/
3) Remote NMR: Calculation details for carbon footprint of NMR instruments, https://csdm.dk/rnmr/details.html

# Helium monitoring

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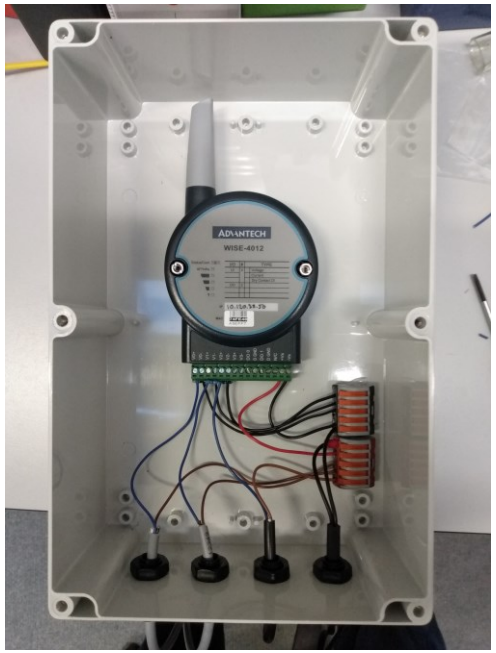
DIY monitoring system

- Pressure
- Temperature
- Liquid volume
- Magnet levels




# Acknowledgements

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