R&D for a new concept EIC nucleon polarimetry and polarised target system based on chemically hyperpolarised droplets

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Talk outline

- Chemical hyperpolarisation – a brief primer
- Status of York ChHYP R&D programme
  - MRI system for polarisation measurement of ChHYP media
  - Key early results
  - Bubbling ChHYP cell – status and development plans
- The proposed polarised dripper prototype
- Potential use of ChHYP at the EIC
- Addressing reviewers questions

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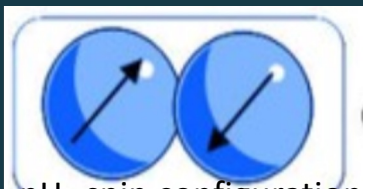
Chemical hyperpolarization (SABRE)

- Transfers nuclear spin order from pH_2 to target nuclei – protons (or nuclei) bound in e.g. pyridine (C_5H_5N)
- Polarisation of H (60%) [1], D, ^{13}C, ^{15}N (80%) [2] has been demonstrated
- Operates at RT
- ChHYP media aligns with weak applied field (earth's magnetic field if none applied)
- Ongoing York R&D to optimise substrates, catalysts, cell design
  > Volume of polarised fluid
  > Polarisation degree
  < Dilution
  > Relaxation time



pH_2 spin configuration

[1] P. J. Rayner *et al., Proc Natl Acad Sci U S A*, vol. 114, no. 16, pp. E3188–E3194, Apr. 2017, doi: 10.1073/PNAS.1620457114.

[2] M. Fekete, F. Ahwal, and S. B. Duckett, *J Phys Chem B*, vol. 124, no. 22, pp. 4573–4580, 2020, doi: 10.1021/acs.jpcb.0c02583.

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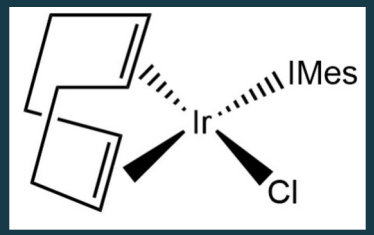
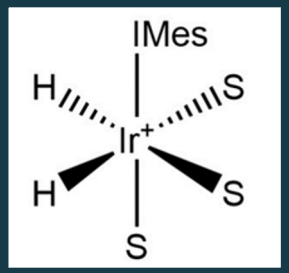
Signal Amplification By Reversible Exchange (SABRE) Spin Transfer



[Ir(IMes)(COD)Cl] precatalyst

Activation

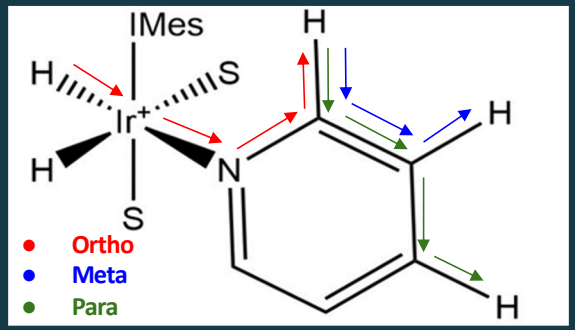
With H_2 addition

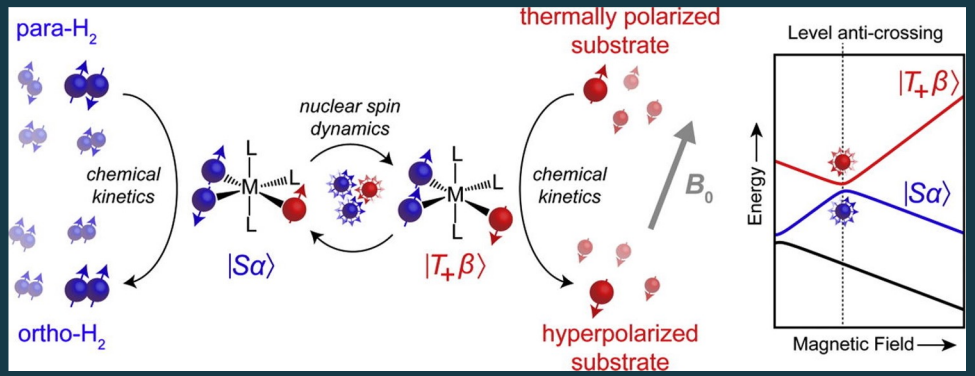


[Ir(IMes)(Substrate)$_3$(H)$_2$] active catalyst

^{1}H Pol. transfer

@ 6mT & 298K





Spin order transfer makes use of level anti-crossings

We have direct collaboration in the project from the director of a leading centre internationally for SABRE studies (ChYM)

In-kind access to facilities

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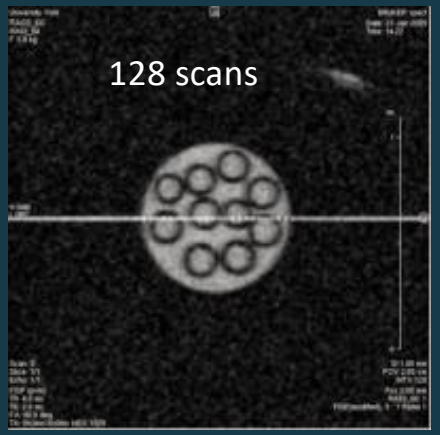
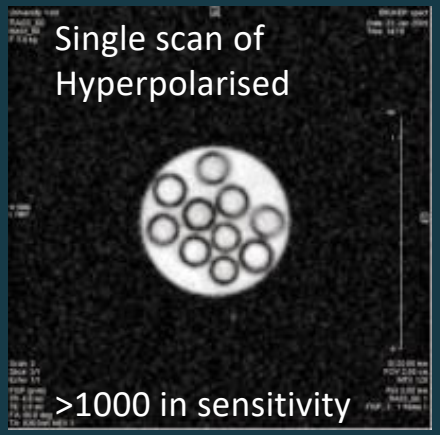
CHyM@York – Centre for hyperpolarisation in magnetic resonance

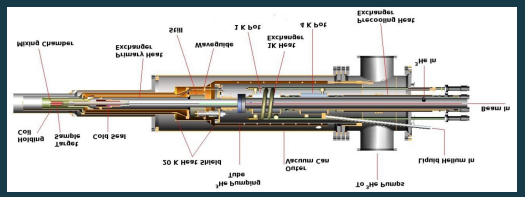


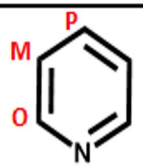
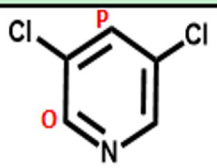
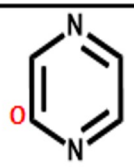
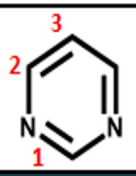


ChHYP substrate comparisons

For comparison, butanol used in DNP
has 10/42 protons polarisable (24%)

DNP - cannot currently
operate at intensity frontier (e.g. CLAS12)



Pyridine	3,5-Dichloropyridine	Pyrazine	Pyrimidine
C_5H_5N	$C_5H_3Cl_2N$	$C_4H_4N_2$	$C_4H_4N_2$
Polarisable proportion of protons (%)			
11.9	4.1	9.5	9.5
T1 relaxation rate (s)			
O/M/P = 41.2/39.5/37.0	O/P = 69.4 / 112.6	O = 42.0	1/2/3 = 69.5/49.8/37.8
			

Some results from the initial R&D

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Measuring the polarisation of ChHYP media

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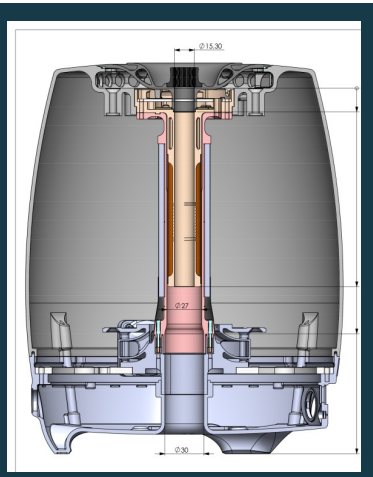
York MRI system

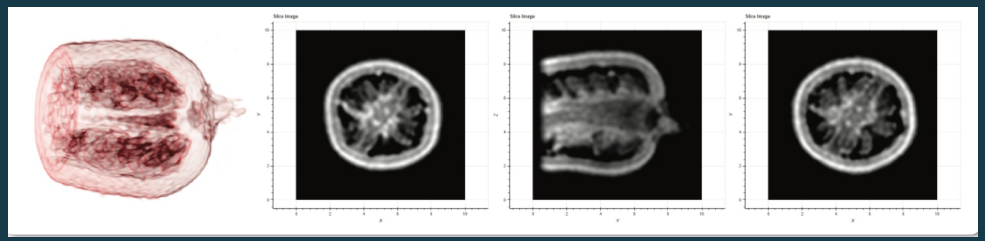
Benchtop Ilumr system

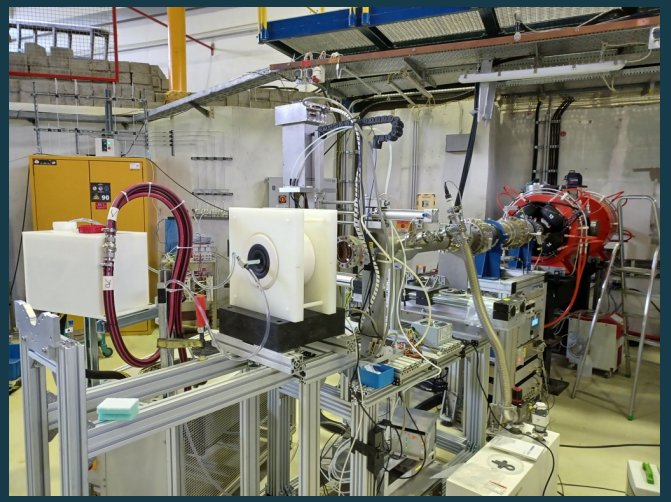
0.3T Field from Halbach array of permanent magnets; 14 MHz
0.25mm spatial resolution

15 mm diameter Bore. Dedicated design - open at both ends

Bespoke scan protocols developed to measure polarisation in 20 time intervals with only few % polarisation loss

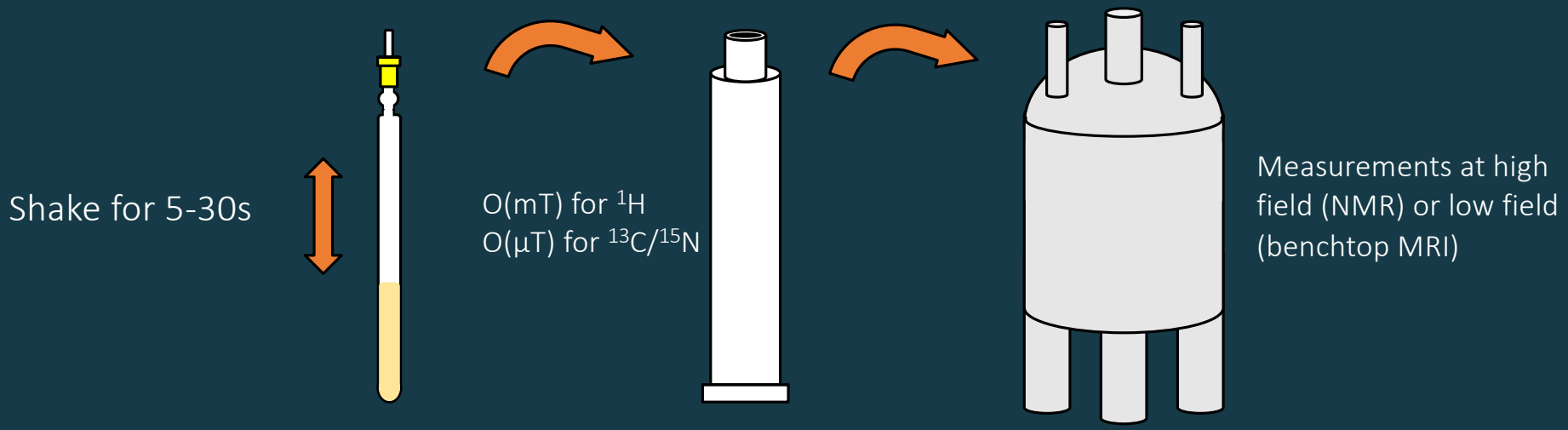






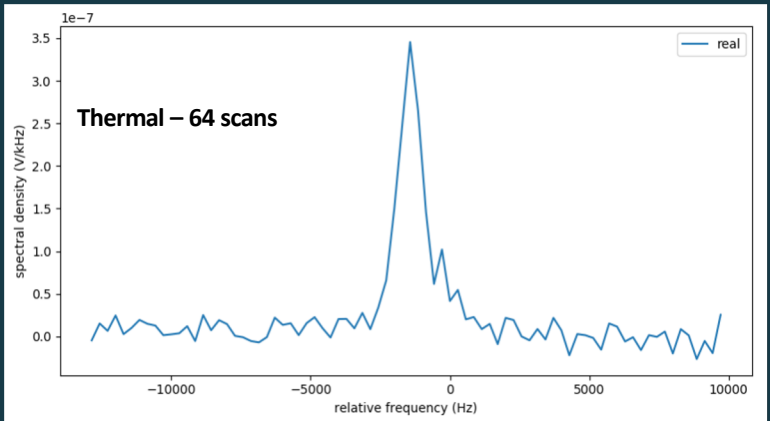
SABRE ‘Shake and drop’ method

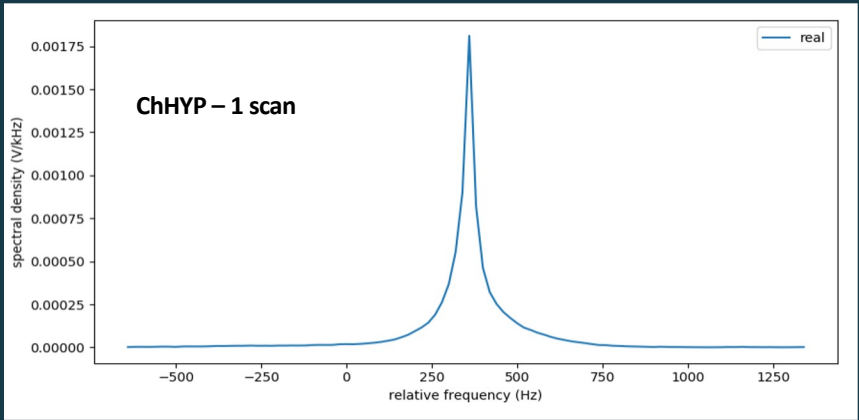
- Prepare sample with substrate, catalyst and solvent.
- FIll sample with pH_2 (4 bar)
- Shake sample in polarisation transfer field using a handheld helmholtz array (6 mT for ^{1}H polarisation).
- Rapidly transfer sample to NMR/MRI for measurement.



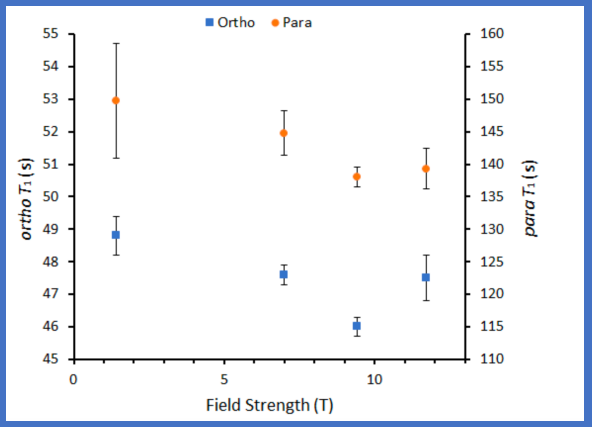
Determination of degree of polarisation

- Area of MR signal from from thermal and hyperpolarised -> Calibrate polarisation
- These results from simple shake of ingredients > 11% ^{1}H polarisation (pure pyridine substrate)
- Shake cells to be used for first in beam tests (photon beam A2@MAMI – Dec ‘23)



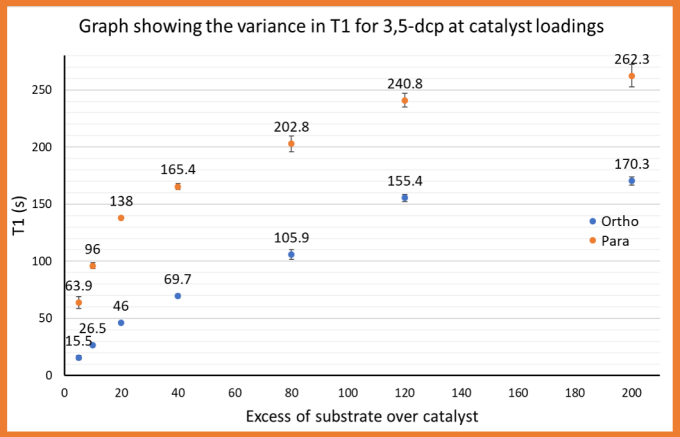


Polarisation degree - little dependence on holding B field



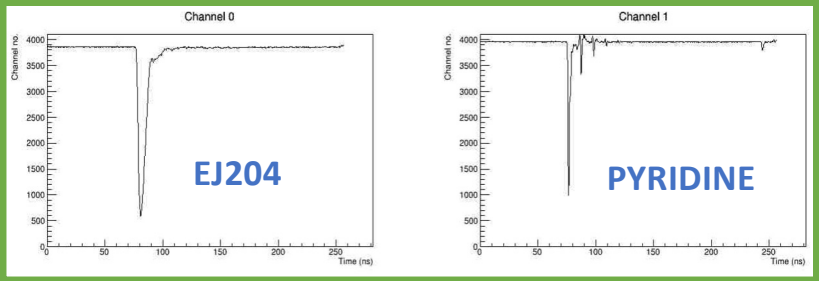
Submitted Nature Comms

Relaxation time increases with lower solvent conc



Submitted Nature Comms

Active polarized targets (Cerenkov or scint) feasible



Also:

Studies on the effect of temperature and sample concentration on the relaxation time

Studies on optimisation of polarisation yield

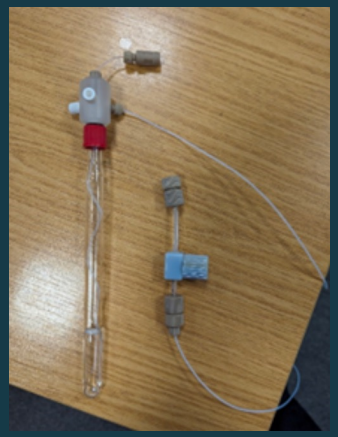
Bubbling cells prototyped -> next slide

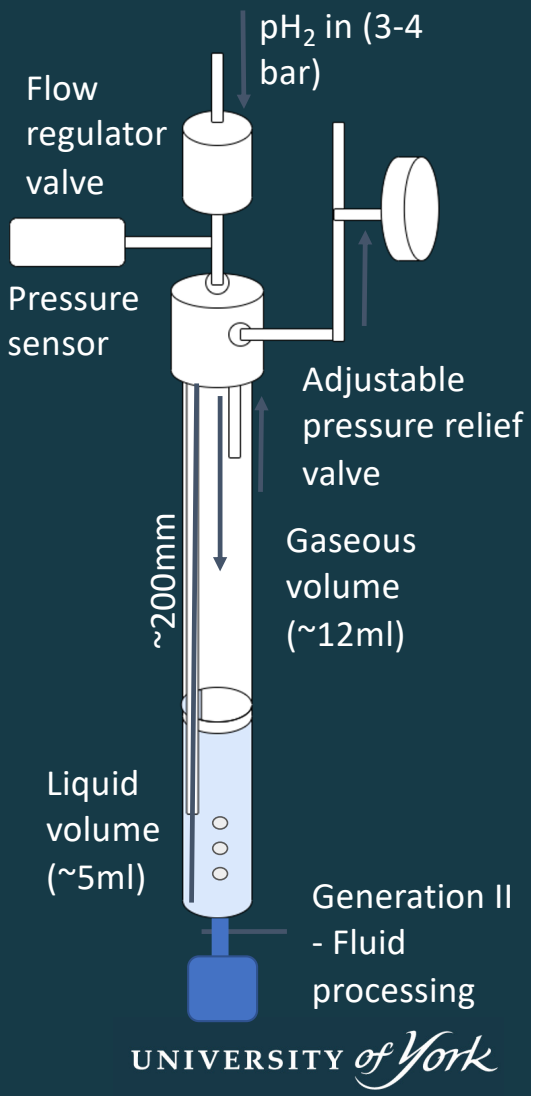
Bubbling cell prototype – Gen I

- Continuous source of polarised media via bubbling cell
  Cumulative polarisation (enhanced by longer relaxation times)
- Tests underway to establish location/stability of equilibrium
  (expect >60% polarisation achieved in unreplenished pH2 systems)
- Next stage (Gen II) designs

  Higher pH2 pressure (12 bar) -> Increase the polarisation
  Solvent evaporation following SABRE process
  Catalyst held in cell by polymeric resin

The creation of almost pure (polarised) pyridine from a Gen-II cell is a technical rather than scientific challenge





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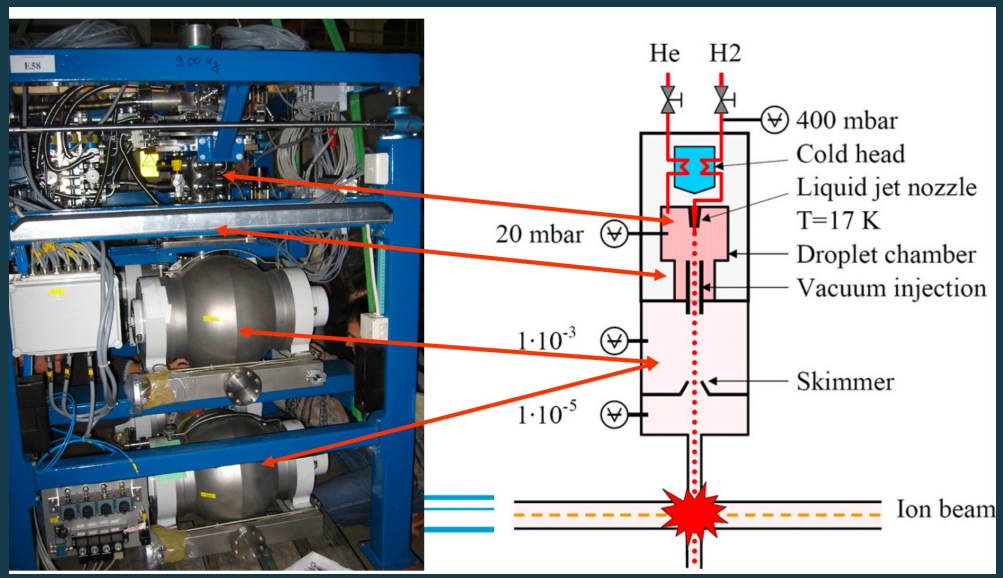
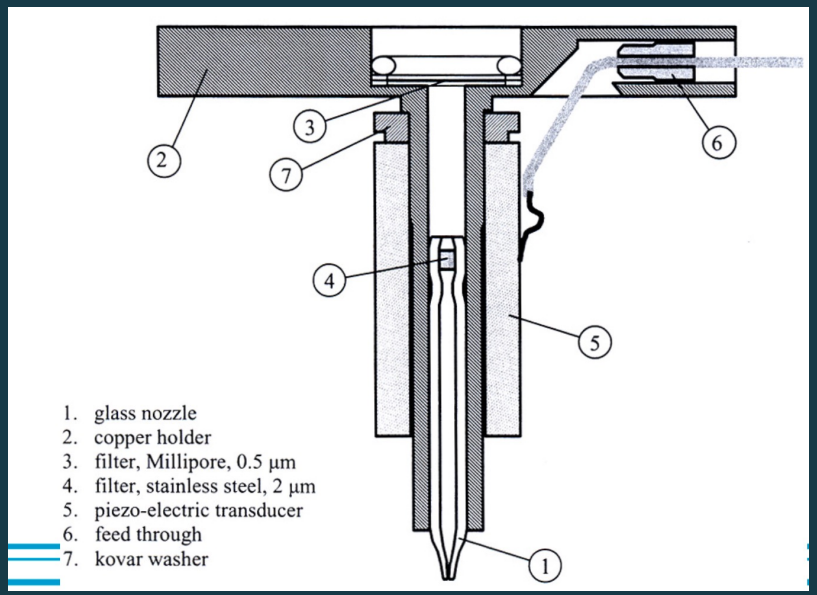
The key R&D – towards the world's first polarized dripper system

- **Unpolarised** Dripper systems which create hydrogen droplets to intercept ion beams have shown utility and success at many facilities (e.g. WASA@COSY). Also planned for PANDA@GSI





- Member of team (Bashkanov) has extensive experience/ontacts through decade spent at COSY

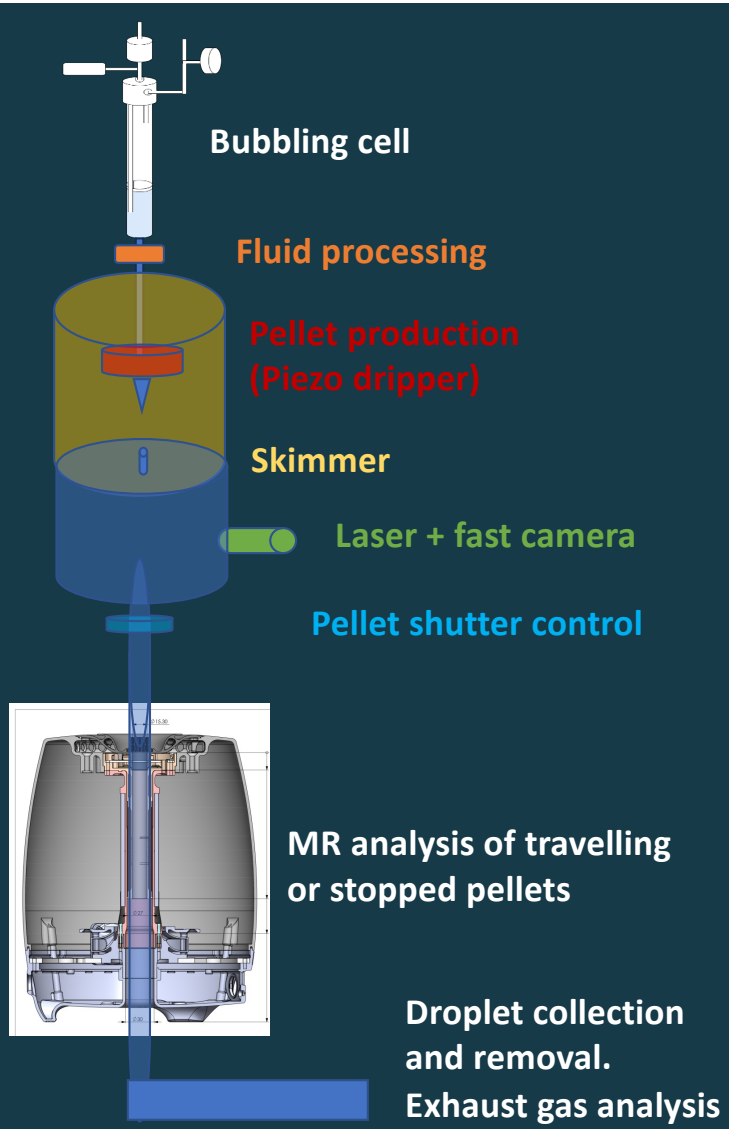
The ChHYP Dripper protoype

Accurate characterisation of relaxation time from frozen ChHYP media -> expected increase

What droplet sizes are optimal? Minimise and quantify drop-to-drop variation in polarisation. (nozzle prototyping, cell design,..)

Test droplet tracking system and optimise

Data to benchmark (predicted low) contribution from flash evaporation to the exhaust gases



~20 mbar

10^{-3}

10^{-5}

Potential for ChHYP at EIC

Rapid proton polarimetry

- Measurements with C foils have technical challenges
- With ChHYP droplets -> single shot pellets (ingredients are cheap!). Use standard LS methodologies from C, N nuclei in the pellets?

Absolute proton polarimetry

- Higher densities of polarised protons than gas jet systems (order of ~1000)
- Complimentary technology to jet system with faster measurements (x50 FoM)?
- Polarisation oriented arbitrarily drop-by-drop (or unpolarised). Benefits to systematics?
- How does dilution affect the characterisation of CNI elastic (p,p'), detector requirements, rates, .. ?
- Droplet size – potential down to ~20 microns -> beam profiles? Measure in the beam halo?
- Spin-spin asymmetries for higher-t scattering may be large – can they be exploited in parallel?

Simulations to address these (and other) questions are part of proposed R&D programme

Polarised fixed target possibilities ?

- Droplets with polarised heavier nuclei (e.g. ^{15}N, ^{117,119}Sn..) are realisable
- Research at York in parallel with this programme -> potential for ChHYP fixed target facility to fill the "gap" in polarised electron-ion scattering above A=3 ?

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Questions from reviewers

Assuming a 1% statistical measurement of the beam polarization in 1 hour, would the machine luminosity be significantly reduced by the target droplets? (If it is not possible to answer that question by the time of the presentation, perhaps one can start with an easier calculation: what would be the amount of material in g/cm2 seen by the proton beam during that hour from droplets versus residual gas?)

The effective (average) media from the pellets offered to the beam can be controlled by the frequency to keep luminosity effect within desired limits

The pellets can exploit the beam halo

We aim to minimise the pellet size during the R&D. We note that sizes down to nm have been achieved for water [Hakimian et al, Nature Comms 12 6973 (2021)

The atoms per cm^2 compared to the Carbon foil at RHIC are presented in the proposal for a large diameter pellet (60 microns). For 20 microns each pellet (while in the beam) has atoms/cm^2 factor 30 larger than the C foil for a diameter of 20 microns. This is the upper limit (when the beam is interacting with the pellet diameter and a continuous stream is used).

Questions from reviewers

Is the flash evaporation during droplet freezing expected to increase the residual gas in the beamline

This is expected to be negligible

We have calculated the sublimation rate from 1kHz 20μm diameter pyridine pellets– it is 10^{12} atoms/sec compared to 10^{15} atoms in cold arc of beam (higher for warm arc)

The flash evaporation would happen in a vacuum chamber 1-2 m above the beam line which is connected to a beampipe with a thin (10mm bore) pipe and 0.7mm collimator at the entrance. The flash evaporation occurs in a well pumped location distant from the beampipe, so negligible residual gas is expected to leak into the beamline from flash evaporation. This is already established at Wasa@Cosy where a range of pellet media were investigated.

We will obtain data to accurately quantify the residual gas during the R&D programme

Questions from reviewers

Details of the proposed simulation remain fairly vague. The spin-dependence is not of major concern for the event generator or detector response; this can usually be achieved through reweighting. More importantly, background from other processes or unpolarized contributions need to be understood for such high density targets. How pure are the hydrogen pellets? Are there any remnants from the catalyst, i.e. other nuclei?

Minimal solvent and catalyst is expected in the Gen-II bubbling cell. The backgrounds are therefore dominated by C, N nuclei in the pyridine in ratio 5:1.

The simulations will characterise contributions from unpolarised backgrounds (and their utility in parallel polarimetry) in a variety of analysing reactions and establish baseline detector requirements. It is crucial to model the polarisation dependence on the polarised proton reactions processes but also scattering on the unpolarised nuclei – all for a range of chosen polarisation orientations in the pellet. We do not see a simple way to reweight - and do not think it would save much work.

The simulation programme would include:

1) Standard CNI methods
2) Other methods made possible due to the flexible spin orientation with ChHYP e.g. higher-t elastic p,p scattering at 90^{o} CM shows very strong longitudinal-longitudinal asymmetries. Hyperon production also offers new opportunities (pp->Λ +X)
3) Explore possibilities for utilising the scattering from C, N for simultaneous measurement using standard LS methods
4) Carry out first simulation exploring possibilities for polarised heavy nuclei fixed target programmes

Questions from reviewers

While the size of the pellets is smaller than the beam size, how narrow can the pellet stream be focused in the beam-pipe? It is not necessary to synchronize pellets with individual beam bunches. What is the speed of pellets through the beam-pipe?

We expect to achieve similar pellet size, frequency as the WASA target (pellet system there was successful with water, nitrogen, deuterium and hydrogen with similar pellet properties)

The narrowness of the pellet stream would be determined by the collimator size. At WASA this was 0.7mm diameter to make pellets compatible with the WASA beam dimensions. Part of the R&D is to optimise the Pyridine pellet stream diameter – but we see 0.7mm as the starting baseline.

The speed of pellets is adjustable with the pressure gradients on the pellet path (20-100m/s) achieved at WASA). We see no reason why similar (or larger) pellet speeds could not be achieved with pyridine

Summary

- We have a strong interdisciplinary team leading efforts to establish ChHYP in nuclear and particle physics – collaborating with one of the leading international ChHYP centres
- The dripper system prototyping requested here - is the key gateway R&D to establish the capabilities for future use at the EIC
- The system could underpin novel new complementary polarimetry methods to help reach the sub % accuracy in ion polarisation identified in the yellow report
- It has the potential to underpin a next generation EIC polarised electron-ion capability beyond A=3
- Proving this novel polarised dripper system has exciting potential more widely in the field - e.g. with intense e^- beams at JLAB, MESA (where DNP fails), polarised annihilation at PANDA, muon beams,…

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