Neutron Scattering from Porous Materials and Confined Fluids: Applications to CO_2 Sequestration and Oil Recovery

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Introduction

- **Elastic neutron scattering techniques** such as **neutron diffraction**, **total neutron scattering**, **small-angle neutron scattering (SANS)** and **ultra-small-angle neutron scattering (USANS)** are powerful tools to probe and reveal the structure of porous materials at length scales from interatomic distances up to a few micrometers as well as the location, the structure and the phase behaviour of fluids confined within their pores.

- We highlight the benefits of utilising *in situ* CO_2 sorption and neutron scattering methods in porous systems to explore the pore morphology, the pore accessibility and the structural properties of confined CO_2.

- This information is very important in the case of sedimentary rocks for the design of optimal CO_2 sequestration as well as gas and oil recovery projects.

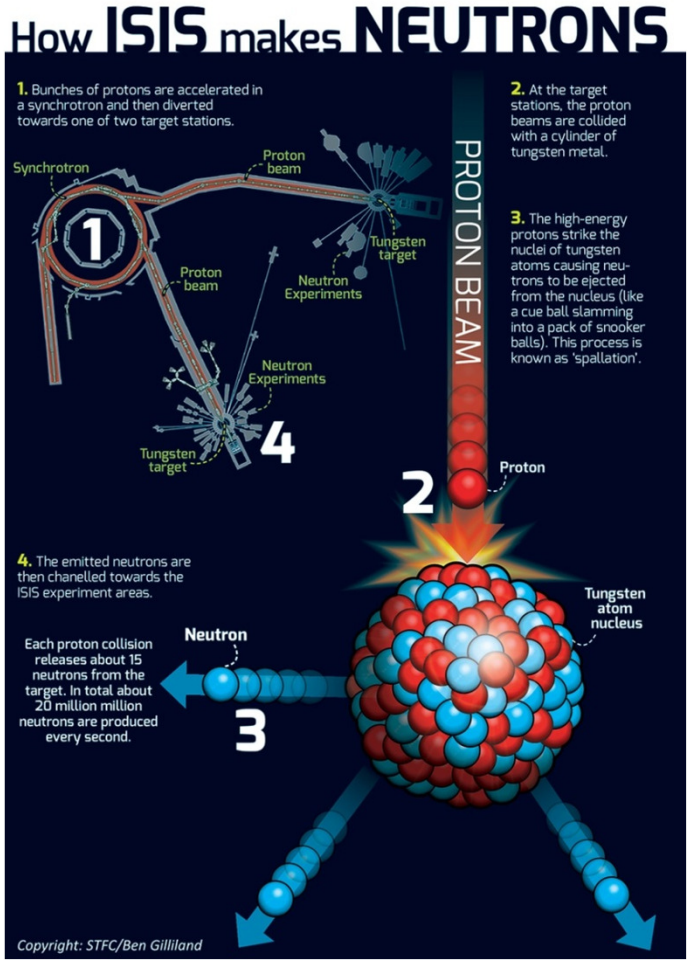
Methodology (I)

Getting access to neutron sources (reactors or accelerators)

- Applying for neutron beam time: calls for proposals are usually twice a year
- All proposals are peer-reviewed by a panel of experts
- Beam time allocation for the neutron scattering experiment in case of a successful proposal

Rutherford Appleton Laboratory, ISIS Neutron Source, Harwell Campus, Oxfordshire, UK

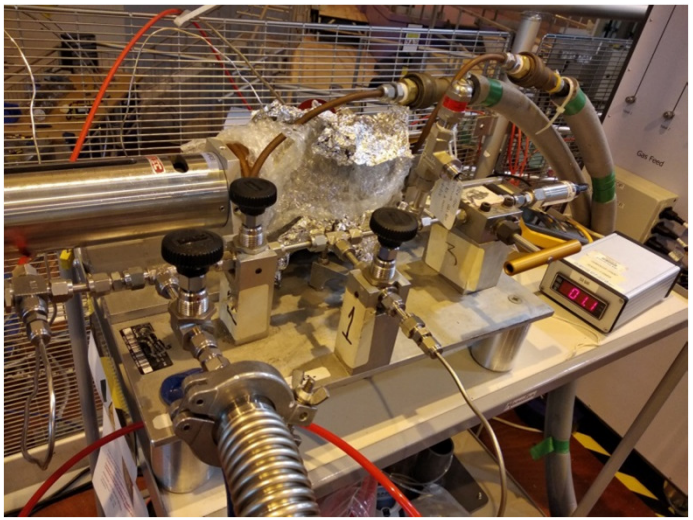
How neutrons are produced in an accelerator



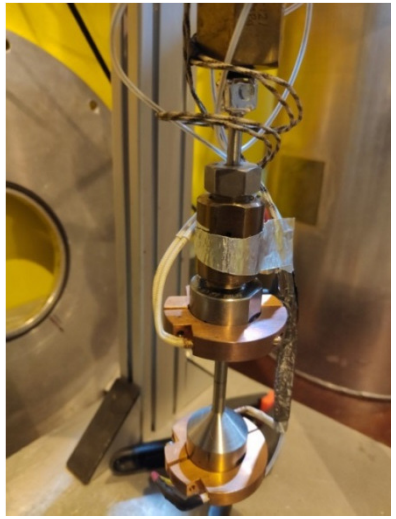
https://stfc.ukri.org/research/our-science-facilities/isis-neutron-and-muon-source/

Methodology (II)

Experimental set-up for performing *in situ* gas sorption and neutron scattering measurements in a porous material



Gas handling panel



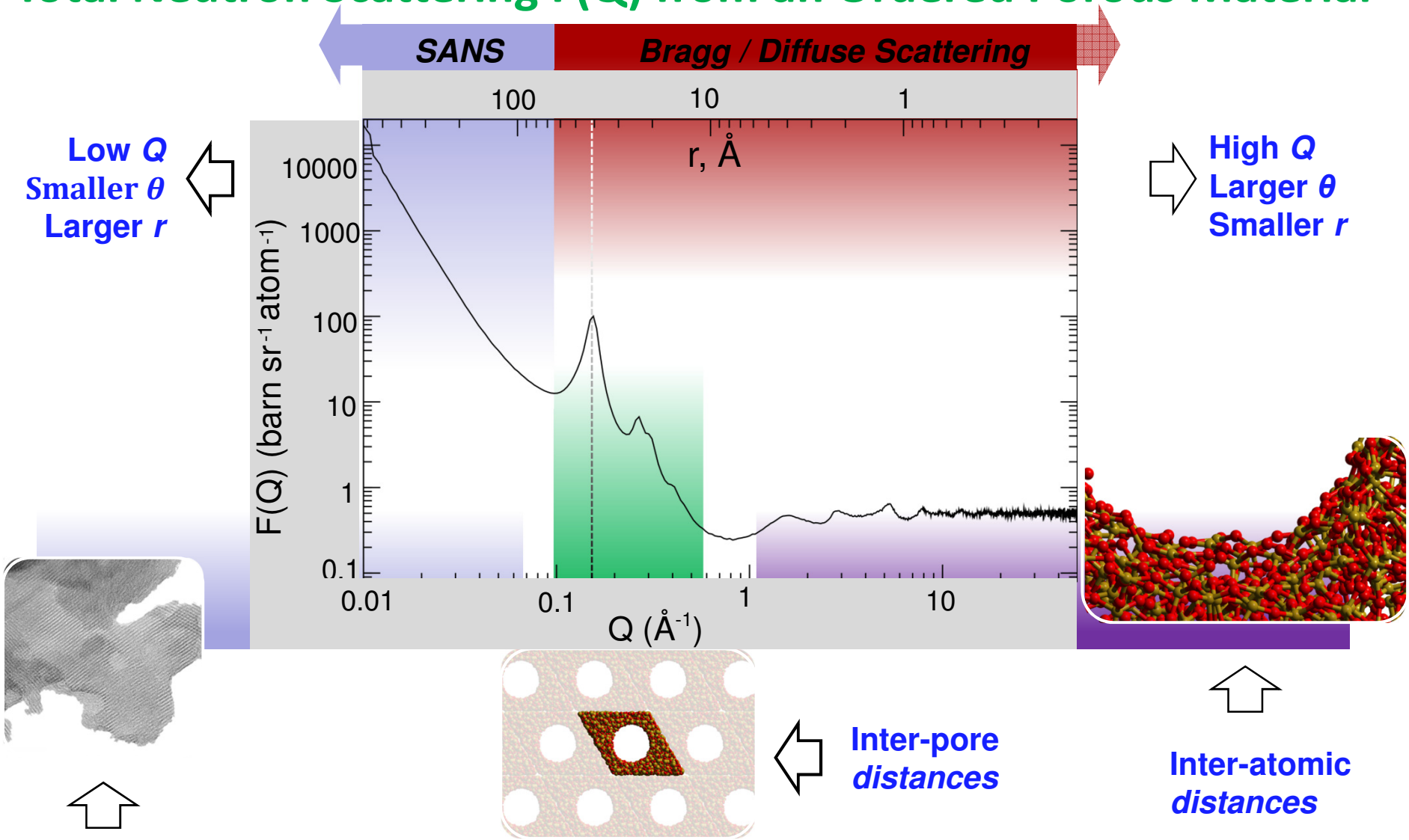
High-pressure sample cell

A stick connected to the gas handling panel and to the sample cell is inserted in the neutron beam under vacuum

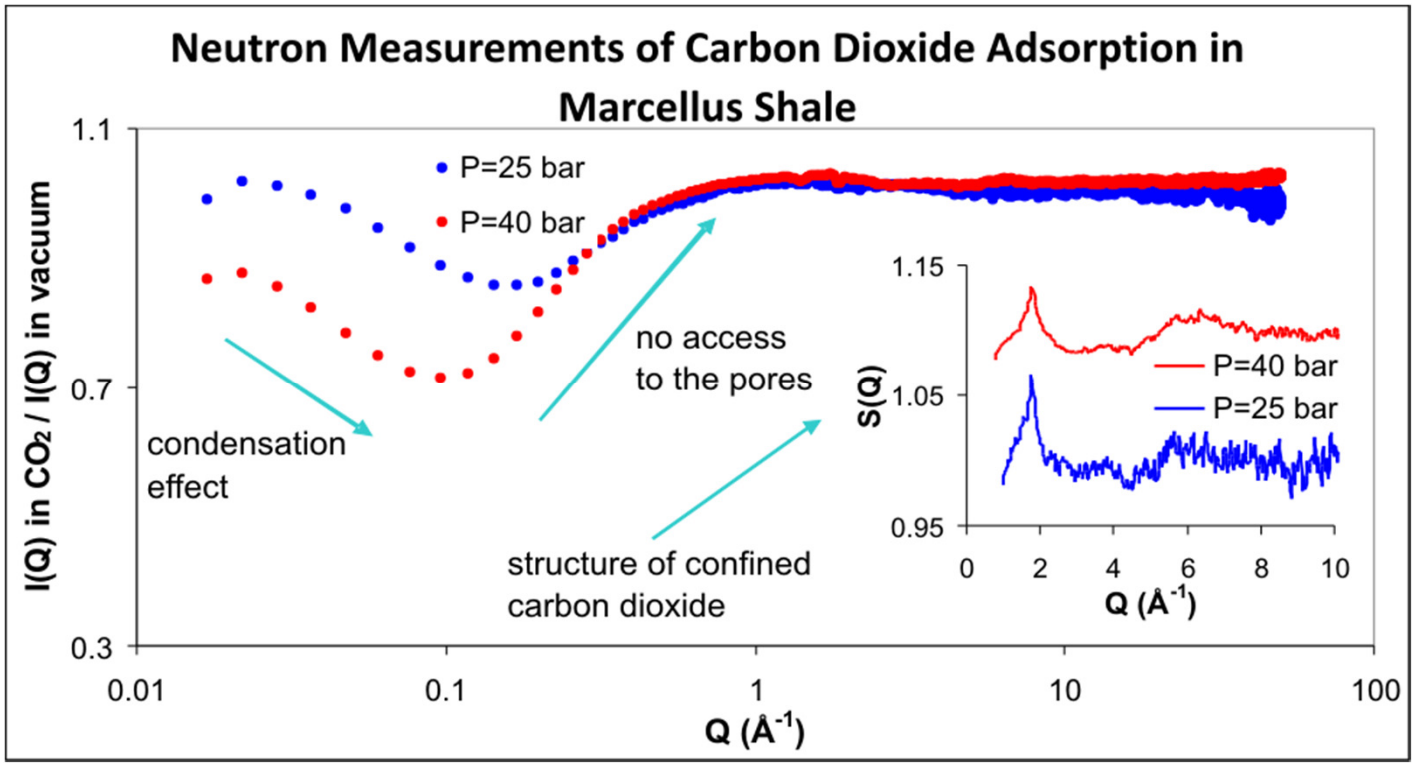
Science & Technology Facilities Council
ISIS

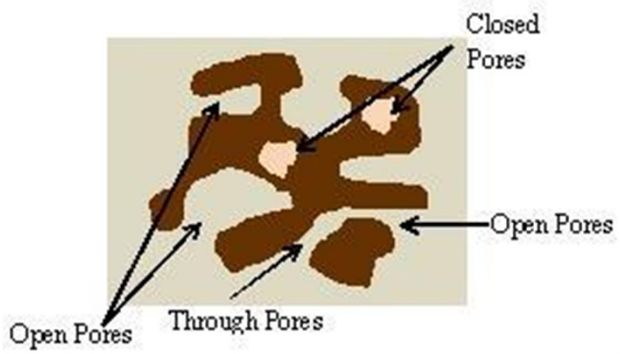
Theory

Total Neutron Scattering F(Q) from an Ordered Porous Material



Results





- Liquid-like properties of confined CO_2
- Shale micropores (<2 nm) are inaccessible or closed to CO_2 – unlikely sites for geologic CO_2 sequestration
- CO_2 Enhanced Oil Recovery (CO_2-EOR) is also unlikely to displace petroleum from shale micropores

K.L. Stefanopoulos et al., Environmental Science & Technology, 51 (2017) 6515–6521

Conclusions

- Elastic neutron scattering techniques are powerful tools for probing structural details of porous materials and pore-confined fluids.
- In particular, revealing the complex pore architecture of sedimentary rocks, the pore accessibility to CO_2 and the structure of confined CO_2 are of great importance because the microstructure and evolution of porosity plays a critical role in many geological processes including CO_2 sequestration and oil recovery.
- It would be challenging to further utilise the potentiality of neutrons to monitor *in situ* structural changes, phase transitions and molecular interactions in the nanopores during various processes such as sorption, flow, catalytic reactions and by *in operando* charging-discharging batteries.

Acknowledgements

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