Exercise 1:

Motivation: Brazil is the world's biggest sugar producer and hence generates considerable volumes of bagasse wastes. Previously these were disposed of by burning, but now are used as the principal raw materials in co-generation plants for production of electric power. This process generates around 2.7 million tons of ash every year, which are accumulated in landfills waiting for alternative ways for its reutilization. In general, the ashes of any industrial process are highly powdered of low density and high volume, which can cause the contamination of adjacent soils, underground water and problems of health, bearing serious social and environmental problems. However the sugar cane ashes have pozzolanic properties and can be used in concrete manufacture. Due to their positive influence on the microstructure and durability, pozzolan additions are routinely used for the manufacture of commercial high-performance concretes. The real importance of supplementary cementitious materials is their potential to improve the concrete durability, particularly the ability to limit the movement of fluid that can transport of aggressive ions into the concrete. However understanding water mobility in the pastes made using sugar cane ashes as supplementary cementitious is a technical challenge because of the complexity of the pore closure as the cement pastes hydrates.

Background. In concretes the role of water changes as the cement hydrates. Before cement hardens, most of the water is mobile, and after the initial set water becomes confined in the so-called capillary pores (pore diameters > 10 nm). As the cement sets gel pores form and the capillary pores decrease in volume. In good quality concrete the capillary pores become discontinuous after 7 days of hydration, and the water transmission though concrete is controlled by the smaller gel pores with pore diameters of less < 10 nm. At 28 days about 70% of the cement is hydrated while at 90 days about 90% of the cement is hydrated. However if the curing process is interrupted then the pores in the pastes are significantly larger allowing water to travel more freely in the pastes. Nowadays there is a considerable use of supplementary cementitious materials such as silica fume, pulverized fly ash (PFA) and granulated blast furnace slag (GGBFS) to replace cement and improve the concrete properties. These materials were all previously considered to be waste products and are now widely used to improve concrete durability and reduce the green house emissions. However the effectiveness of using sugar cane ashes as supplementary cementitious is not yet fully characterized.

Why neutrons? Water dynamics can be investigated by many experimental techniques, such as infrared and Raman spectroscopies, NMR and QENS, however QENS is a unique technique for the investigation of dynamic and geometric aspects of the movement of protons on very short time scales. Typical examples of successful results are the diffusion of water in zeolites, minerals, clays, but also concrete. In fact we have

shown that neutron scattering, and QENS in particular, is a powerful technique that can examine the interactions of the different pore waters found in cement paste. Here we allow for the complexity of the pore that evolves with time, by analyzing samples with different ages to separate and differentiate the water populations.

How will we proceed to achieve our objectives?

Now you should write your own approach to perform this experiment and why you want to use a particular instrument. To continue you should remember the following.

1) This research involves QENS
2) You want to compare the water mobility at different time scales, therefore consider the resolution Table
3) Maybe temperature is an important factor as it will modify (de-block) motions
4) You have the following instruments to choose from:

IRIS at ISIS, Workhorse high-resolution spectrometer at ISIS

High resolution quasi-elastic and inelastic neutron scattering spectrometer with long d-spacing diffraction capabilities.

See http://www.isis.stfc.ac.uk/instruments/iris/

TOSCA at ISIS is an indirect geometry spectrometer optimized for the study of molecular vibrations in the solid state.

See http://www.isis.stfc.ac.uk/instruments/tosca/tosca4715.html

IN6 at the ILL is a time focusing time-of-flight spectrometer designed for quasi-elastic and inelastic scattering covering motions on the ps time scale.

http://www.ill.eu/instruments-support/instruments-groups/instruments/in6/characteristics/

Exercise 2:

Background: The study of pain is, possibly, one of the larger and more important areas of Medicine. The conventional way to deal with pain is to induce anesthesia, being the pharmacological method the most used. ***Local anesthetics (hereafter LA and the objective of this work)*** are drugs that cause reversible local anesthesia and a loss of nociception1. When used on specific nerve pathways, effects such as analgesia (loss of pain sensation) and paralysis (loss of muscle power) can be achieved. Clinical LA belong either to the amino-amide (BVC2, RVC2...) or to the aminoester (benzocaine, procaine) class. Synthetic LA are structurally related to cocaine, but differ from it: they have no abuse potential and do not produce hypertension or local vasoconstriction. To improve the bioavailability of medicines liposomes have been successfully used as pharmaceutical drug carriers. LA encapsulated into liposomes show longer duration of action, reduction in circulating plasma levels, as well as reduced central nervous system and cardiovascular toxicity. Liposomes containing cyclodextrin (CD) are useful for encapsulation of biologically active substances, especially those are hydrophilic. The encapsulated CD aids a slow, controlled release of pharmacologic compounds from the liposomes. This novel method allows the treatment of a many physiological states.

CDs are rigid molecules with a hydrophobic cavity and hydrophilic exterior, which determine their ability to bind various low molecular weight compounds and parts of larger molecules, both in solution and in the solid state. Typical CDs contain a number of glucose monomers ranging from six to eight units in a ring, creating a cone shape: !CD, "CD and #CD. The pharmaceutical industry has taken great interest in using CDs as inclusion media, owing their ability to influence drug solubilization, stabilization, delivery, and toxicity. New CD-based technologies are constantly being developed and, thus, years after their discovery CDs are still regarded as novel excipients of unexplored potential [T. Loftsson, D. Duchêne, Int. J. of Pharm., **329**, (2007) 1-11]. Inclusion complexes of CDs can be studied by a variety of analytical methods that provide information on their kinetics and thermodynamics. Various studies indicate that the use of !-CD and some of its derivates increase the LA solubitily, as well as improve the therapeutic properties [See Daniele R. de Araujo,

Eur. J. of Pharm. Sc., 33, (2008), 60]. ***Encapsulated BVC and RVC can be used to eliminate the use of needle in local anesthesia dental treatment.***

What we propose and how we will proceed: Here we aim in getting information on the changes in the dynamics of the hydrogen bond (HB) reflected by changes of the measured density of states in the "CD and the LA-"CD systems, LA = BVC and RVC.

Now you should write your own approach to perform this experiment and why you want to use a particular instrument. To continue you should remember the following.

5) This research involves phonons, external vibrations
6) You want to compare the density of states (low frequency modes) for different samples
7) Maybe temperature is an important factor as it will modify (de-block) motions
8) You have the following instruments to choose from:

IRIS at ISIS, Workhorse high-resolution spectrometer at ISIS

High resolution quasi-elastic and inelastic neutron scattering spectrometer with long d-spacing diffraction capabilities.

See http://www.isis.stfc.ac.uk/instruments/iris/

TOSCA at ISIS or **LAGRANGE at the ILL** is an indirect geometry spectrometer optimized for the study of molecular vibrations in the solid state.

See http://www.isis.stfc.ac.uk/instruments/tosca/tosca4715.html

See http://www.ill.eu/instruments-support/instruments-groups/new-instrument-projects/in1-lagrange/

IN6 at the ILL is a time focusing time-of-flight spectrometer designed for quasi-elastic and inelastic scattering covering motions on the ps time scale.

http://www.ill.eu/instruments-support/instruments-groups/instruments/in6/characteristics/

9) Would diffraction help??? X-rays or neutrons???