Green Chemistry Centre of Excellence

Alternative Solvents
Recent estimates by the pharmaceutical and fine chemical industry have suggested solvents account for the majority of the waste produced in a typical batch process. Solvents are also subject to a number of regulatory controls. For these reasons there has been a large amount of interest in ways to reduce hazardous solvent use and find benign substitutes.

The “Alternative Solvents” technology platform in the Green Chemistry Centre of Excellence (GCCE) promotes the use of more sustainable solvents as replacements for conventional organic solvents. Here lies an opportunity to reduce the environmental impact of industrial processes as well as making them safer.

Our goal is to develop, apply and promote the implementation of safer, greener and more sustainable solvents (supercritical/liquid CO₂, bio-based solvents and solvents made from waste) into industry. The platform focuses on the use of alternative solvents in a wide range of applications.

Some of the applications already developed using supercritical or bio-based solvents include:

- Extraction of waxes and botanicals (for food and beverage, cosmetic and personal care products)
- Recovery of liquid crystals from end-of-life electronics
- Synthesis of aroma molecules using biocatalysts in alternative solvents
- Use of modelling tools to predict the properties and behaviour of a solvent
- Use of bio-based solvents for conducting industrially relevant organic reactions
- Chromatography in supercritical fluids

### Reactions in Alternative Solvents

Traditional catalytic and biocatalytic processes can be performed in supercritical CO₂ and bio-based solvents, providing a number of advantages over conventional solvents including:

- Reduced hazards
- Lower rates of catalyst poisoning
- Enhanced catalyst stability
- High enantioselectivity
- Simple product and catalyst recovery

### Carbonates as Alternative Solvents

The use of wastes to make low cost solvents is a highly appealing concept. The utilisation of CO₂ to make carbonate functionalised solvents is well established. In recent years, organic carbonates (both cyclic and acyclic) have been highlighted as highly promising alternatives to typical VOCs. Solvent selection guides concur that carbonates pose few environmental, health and safety hazards. Current projects within the GCCE are investigating the use of carbonates as alternative solvents in various synthetic transformations, including solid phase peptide synthesis.
SUPERCritical FLUID CHROMATOGRAPHY AND EXTRACTION

The “Alternative Solvents” technology platform also operates a state of the art semi-preparative supercritical chromatography system. This system runs extractions, reactions and analysis all in the supercritical phase.

Carbon dioxide is a non-polar solvent once pressurised into a liquid or supercritical state. The density and polarity of CO₂ is completely tuneable to selectivity separate mixtures.

Supercritical CO₂ has several distinct advantages over traditional organic solvents in extractions, including:

- Tuneable for fractional separations
- High permeability for extraction of raw biomass
- Low surface tension
- Low viscosity
- High mass transfer rates
- Simple product recovery with no solvent residue

Supercritical CO₂ extractions have been successfully developed for:

- Herbs and spices for food and beverage use
- Waxes for cosmetics and personal care products
- Oils (nutraceuticals)
- Purification of active pharmaceutical ingredients
- Recovery of liquid crystals from end-of-life electronics

Bio-Based Solvents and Modelling

Solvents from biomass and food waste are viewed as one of the most promising types of alternative solvents. A key feature of this work is the use of modelling software to predict the properties and behaviour of a solvent. The use of these tools allows for the prediction of solvents offering the most favourable performance for a target application. They also guide the synthesis of novel solvents designed for specific processes.

We prepare new bio-based solvents at lab-scale within the GCCE and at demonstrator scale using the BDC facilities. Our discoveries include Cyrene™, a replacement for toxic polar aprotic solvents in materials science and synthesis, and tetramethyloxolane, a broad substitute for toluene.
S4 - SUSTAINABLE SOLVENT SELECTION SERVICE

The GCCE has developed the S4 (Sustainable Solvent Selection Service) programme to replace hazardous solvents and to promote benign alternatives. This service is provided to businesses that are looking to develop applications for waste streams or new bio-based products, and those who find access to their favoured solvents has become restricted due to regulations. We have worked on projects with SMEs and international corporations, ranging from 2 week exploratory studies to 3 year funded PhD studentships.

We have expertise in the design and synthesis of new solvents, and a catalogue of applications with which to test them. Laboratory and pilot plant facilities are available to carry out extractions and fractionation in liquid or supercritical CO₂. Supercritical chromatography and reactions systems are also available in addition to routine analytical equipment.

www.york.ac.uk/res/s4/