MBASE- The Molecular Basis of Advanced Nuclear Fuel Separations

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Lancaster University
National Nuclear Laboratory
Serco
University of Manchester
University of Reading

CEA
Idaho National Laboratory
Karlsruhe Institute of Technology
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Original Objectives

• To explore aspects of both established and innovative separation processes, linking them through the common theme of minor actinide separation

• To adopt an integrated approach, encompassing both physical and chemical phenomena

• To link both experimental and multiscale (molecular to process) modelling studies and

• To use molecular scale knowledge to improve separation performance in current or future processes

• Started 1 April 2010; End Date 30 Sept 2013

Structure of the Research Programme

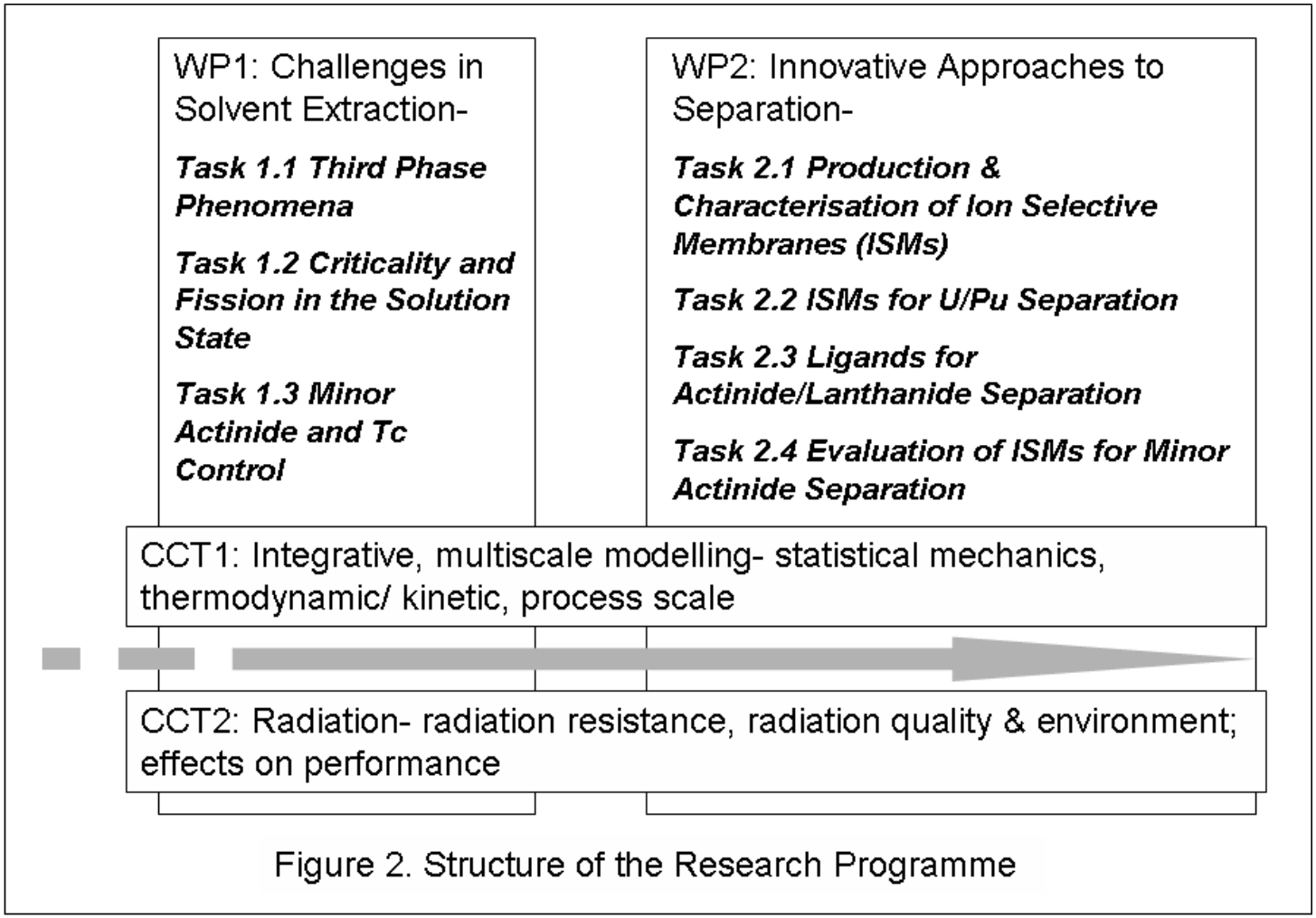


Figure 2. Structure of the Research Programme

The Core Team

Manchester Chemical Engineering- Clint Sharrad, Sven Schroeder, Andy Masters, Megan Jobson

Reading- Mike Hudson, Laurence Harwood

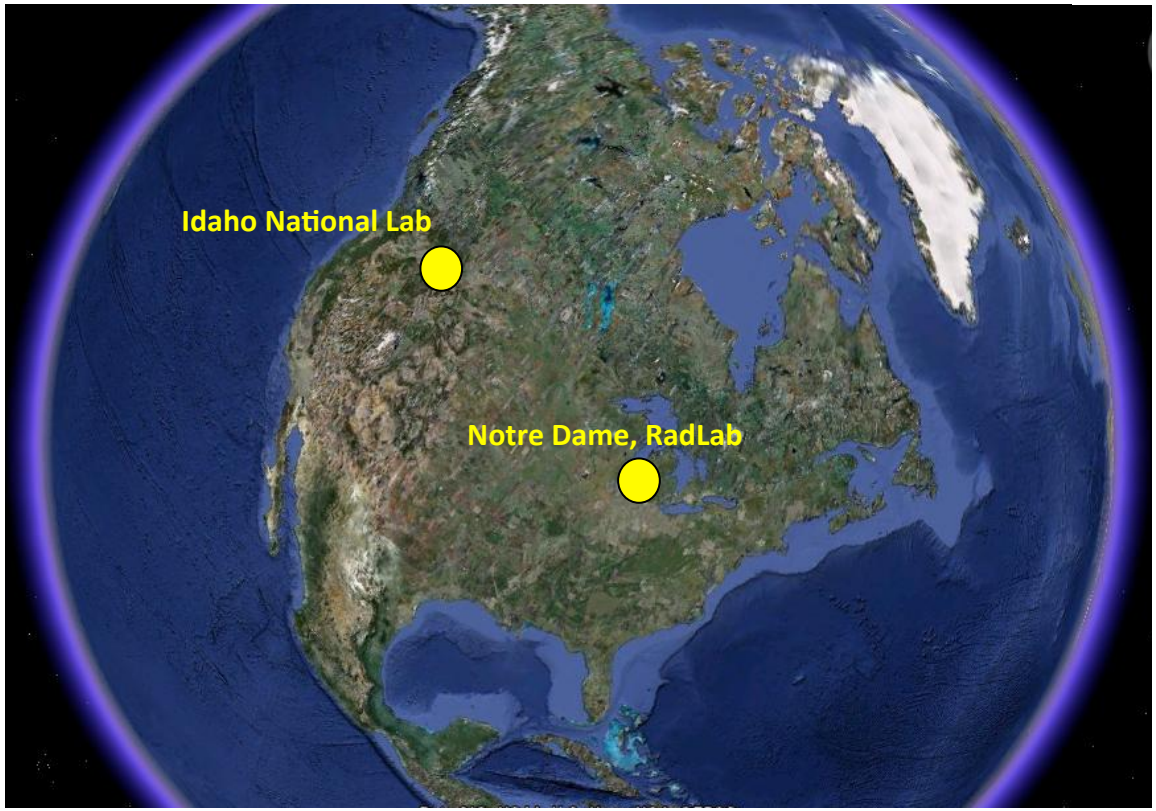
Lancaster- Colin Boxall

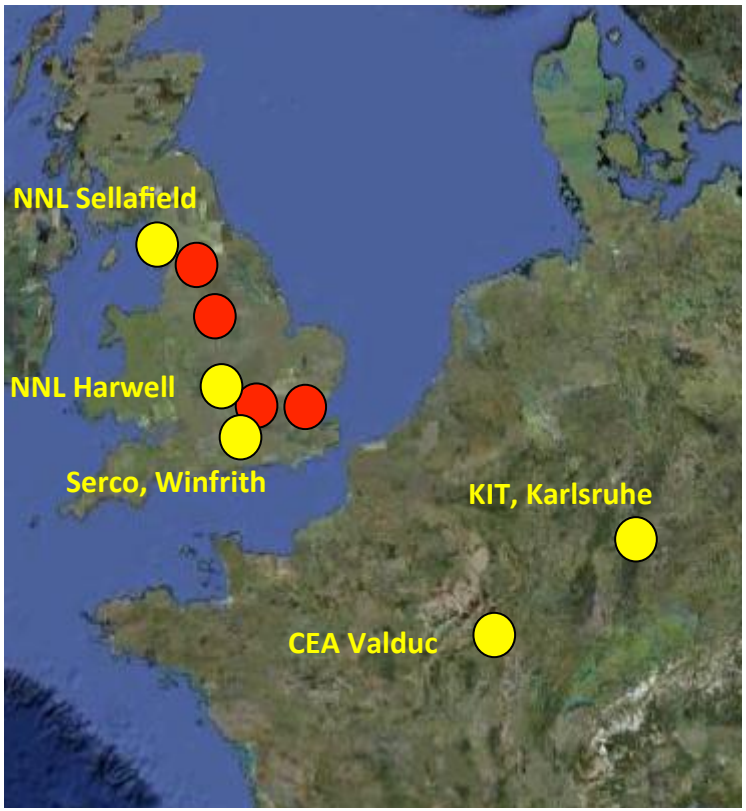
Imperial College- Chris Pain, Tony Goddard, Matt Eaton

NNL- Robin Taylor, Mark Sarsfield, Howard Sims

Manchester Chemistry- Simon Pimblott, Francis Livens

Collaborations





NNL Sellafield- flowsheet development; active separation facilities; *NNL Harwell*- radiation effects; *Serco, Winfrith*- criticality modelling; *CEA Valduc*- criticality data; *KIT, Karlsruhe*- transuranic synchrotron facility; *Notre Dame RadLab*- experimental radiation science facilities; *Idaho National Lab*- active laboratory facilities, minor actinide chemistry and spectroscopy, radiation effects

Links To The EPSRC Nuclear Fission Doctoral Training Centre (DTC)

What is the DTC?

- 50 PhD students over 5 years
- 4 year programme- 1 year taught then 3 years full time PhD
- Students 'own' their PhD- develop their own proposal which is reviewed
- All projects must be cross-disciplinary

DTC PhDs linked to MBASE

- Extension of the NDDO (Neglect of Diatomic Differential Overlap) semi-empirical Molecular Orbital (MO) theory formalism to f-orbitals.
- Model-directed ligand design for nuclear element coordination chemistry.
- Relating electronic and structural properties of complexants to actinide binding efficiency
- Investigation into the Radiolysis of PUREX Solvent Systems

MANCHESTER 1824

The University Of Sheffield.

The University of Manchester
Dalton Nuclear Institute

MANCHESTER 1824

Dalton Cumbrian Facility

Joint £20m investment with the Nuclear Decommissioning Authority to establish a unique experimental research capability near Sellafield:

- Radiation Science
- Nuclear Engineering Decommissioning
- Academic access to 10% of the NNL Central Laboratory