KNOO

Keeping the Nuclear Option Open

Annual Report

Reporting period: 1st October 2005 - 31st September 2006

Principal Investigator: Professor Robin Grimes

Report compiled by: Dr. Mark Levy

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Introduction

The official start of "Keeping the Nuclear Option Open" (KNOO) was the 1st October 2005. At this point, equivalent financial contracts are in place with all collaborative institutions. Staff and students have been hired throughout the year. Almost all positions are now filled.

The first full meeting of KNOO members and stakeholders was held at Imperial College London, Department of Materials on the 21st and 22nd September 2005. This meeting allowed investigators and students to meet and appreciate the breadth of topics under study as part of the KNOO remit. This meeting also incorporated the first training session organised for students and PDRA's, held at the Imperial College Reactor Centre.

With most positions filled, we are on track for another good year of research. Several training events are being discussed with industrial contacts. Planning for the second annual meeting is underway. This will be hosted by HMS Sultan with arrangements being finalised in the new year.

This introduction is followed by an update of centrally focused events including a summary of our outreach activities. The main body of the report consists of technical updates on all projects which form KNOO. These are listed under their respective Work Package.

Mark Levy and *Robin Grimes*

KNOO Central Update

Financial Progress
Subcontracts were signed by all parties and spend is on track.

Outreach Publications
- Mark Levy "Maintaining nuclear skills" Public Service Review: Trade and Industry, number 10, p111 (2006)
- Robin Grimes, "This nuclear war is a waste of energy" Comment, The Guardian newspaper, Wednesday 21st June 2006.
- Lee W. E. & Grimes R. W. "Nuclear Waste: a UK Perspective" Energy Materials, volume 1, p22 (2006).

Meetings Attended
- Prof. Grimes was interviewed by the BBC World Service and discussed KNOO (10th November 2005 and 17th February 2006).
- Prof. Grimes represented KNOO at the EPSRC Energy Research, Public Dialogue workshop (12th December 2005).
- Prof. Grimes represented KNOO at a visit to South Africa organised through the British High Commission (20th February 2006 - 24th February 2006).
- Prof. Grimes represented KNOO at a visit to Canda organised through the British High Commission (5th March 2006 - 7th March 2006).
- Dr. Levy presented a poster detailing the activities of KNOO at the Topical Meeting on New Reactor Systems (TopNux) conference (Westminster 21st to 23rd March 2006).
- Dr. Levy represented KNOO at the UKERC Annual Assembly (Edinburgh 4th - 6th July 2006).
- Prof. Grimes represented KNOO at an EPSRC Energy day at at the call meeting for the Sustainable Nuclear Energy Programme (19th September 2006).

Industry/Governmental Interaction
- Prof. Grimes and Dr. Levy were invited to attend a seminar as part of the Foreign Policy Centre programme on Energy Security on the Future of British Nuclear Power, the House of Commons, Committee Room 16 on 15th November 2005.
- Prof. Grimes was a witness at the first evidence session of the Select Committee on Trade and Industry's investigation into the energy review and the issues relating to nuclear new build on 16th May 2006
- Dr. Levy was invited to attend the House of Commons evening reception on the subject of Energy entitled Powering the Future on 27th June 2006.

Public Engagement
- Prof. Grimes was a panel member in a debate at the University of Surrey on the topic of future energy sources entitled "Nuclear Power or Renewables: do we have a choice?", hosted by the Vice-Chancellor, Prof. Christopher Snowdon, and chaired by Prof. Al-Khalil on 3rd May 2006.
- Prof. Grimes gave a public lecture on Nuclear Power at the Chemistry department of University College London on 14th March 2006.

Annual Meeting
The first full meeting of KNOO was held at Imperial College London on 21st and 22nd September 2006. The meeting on the 21st was held at the Imperial College Reactor Centre at Silwood Park (see Training Activities).

The second part of the meeting involved research presentations, primarily from the Work Package Leaders and Senior Investigators, however several students and PDRA's also presented. The meeting was a great success and nine industrial stakeholders attended.

Training activities
PhD students and PDRA's were invited to the Imperial College Reactor Centre at Silwood Park on the 21st September for a training day. This involved a tour of the reactor facility, a half day of practical radiological experiments run in the reactor centre and two lectures by industrial experts. The first of these was Dr. Kurt Atkinson, a fuel performance engineer from British Energy, and the second Dr. Matrin Briggs from Rolls Royce Marine. Both aspects of the training were very well received by all attending.

Other details
A website for KNOO was setup and is now available at www.knoo.org. Publicity materials have been produced and are available upon request.

Work Package 1

Work Package Leader: Dr. Simon Walker

Project title: Fuel, thermal hydraulics and reactor systems

Researchers:
We have at present appointed six research students (Chatzikiriakou, Masson, Maudarboucas Sfikas, Belhouachi & Zeng). A further post is currently being interviewed for. We have appointed two PDRA's, one focussing on the experimental side (Dr. Hale) and one on analysis / CFD (Dr. Hu).

Supervisors:
Dr. S. P. Walker, Prof. G. F. Hewitt

Resarch progress:
The projects underway are:

- A CFD and experimental study of the cooling of hot surfaces by saturated droplet impingement. (Chatzikiriakou)
- The application of advanced (fast multipole) mathematical methods to model elastodynamic wave propagation for nuclear non-desctructive testing. This project has cross-cutting links with WP2 (Materials), which has a NDT component. (Maudarboucas)
- A computational study of the propensity of droplets to be diverted when the vapour flow in which they are entrained is itself diverted. (Masson)
- An experimental study of fluid/particle flows in simulated rod bundles (Zeng)
- The development of a coupled multi-pin TRACE – Mabel model of the behaviour of the core, and mechanical response of the pins, during reflood. (Belhouachi, Zeng)
- The study of the effects of crud deposition on fuel on reactor performance (Sfikas)
- (Names in brackets indicate the principal PhD students involved, although there is much interaction between projects. PDRAs, work more broadly across several projects.)

Collaborations/interactions with stakeholders:
In addition to the Britsh Energy plc. & Serco Assurance collaboration, we have developed especially good links with CD-Adapco over provision of CFD codes and technical support (Dr. Simon Lo).

Associated matters:
Serco Assurance have been awarded an Engineering Doctorate position, with us as the university partner, to work on the incorporation of advanced CFD methods into nuclear safety analysis. This is intended to link into / provide technology transfer with the KNOO projects noted above.

Project title: Generic coupled methods for fault and severe accident studies in GenIV systems (see also WP4 for applications research)

Researcher:
Dr. Jeff Gomes

Supervisors:
Prof. Tony Goddard, Prof. Chris Pain (Leader of AMCG group) assisted by Dr. Matthew Eaton, Dr. Matthew Piggott

Research progress:
The strategic aim is to develop the FETCH 3D transient coupled FEM unstructured mesh nuclear/fluids/structural code (which had been demonstrated for VHTR in 2D axysymmetric transient fault modelling) into a 3D unstructured mesh fully coupled nuclear/CFD (single and multiphase))/structural interactions code for innovative reactor severe accident studies. In May 2006 (note that PhD students had been appointed in October 2005) Dr. Jefferson Gomes was appointed the the PDRA post. His past work had covered validation of the FLUIDITY CFD sub-code of FETCH and work on a number of projects coupling multiphase flow in FLUIDITY with radiation transport models (EVENT). His work since then has covered assisting the two KNOO research students appointed, code architecture of FETCH to meet the project needs and the incorporation of space-dependent burnup for PBMR type VHTRs.

Research aim:
During the year from October 06 Prof. Goddard has addressed on behalf of WP4 the consequences of the DTI's withdrawal of the UK from active membership of GIF and he has organized a visit to meet European Commission staff. Steps are being taken that this project continues to directly serve the needs of UK industry. The generic code research objectives are: to introduce the group's unstructured mesh adaptive-parallel LES technology into the coupled framework for modelling within-vessel flows and heat transfer; modelling individual channel flows for block type VHTR and GCFR systems; explicit modelling of control rods and their movement within the radiation transport framework; plan the integration of the RADIANT next generation radiation transport code in to FETCH and continuing consideration of the most suitable 1D whole circuit model with which to interface FETCH. Such interfacing should be straightforward in that all code modules of FETCH are written within the group.

Financial progress:
The use of the full budget allocated to Prof. Pain's group is covered under WP4.

Presentations given/conferences attended:
Two papers were presented at the 2006 American Nuclear Society's Topical Meeting on Reactor Physics (PHYSOR) conference.

Collaborations/interactions with stakeholders:
Collaboration has been maintained with AMEC NNC in GenIV reactor systems specification. Excellent interactions in closely related research matters have been maintained with Rolls Royce, British Energy, Serco Assurance, Nexia Solutions, AWE plc.

Project title: Fuel, thermal hydraulics and reactor systems / Application of advanced CFD

Researchers:
Dr. Yacine Addad, Stefano Rolfo, Amir Keshmiri (50% with WP4)

Supervisors:
Dr. Mark A. Cotton and Prof. D. R. Laurence

Research progress:
The PDRA, Dr. Yacine Addad was appointed in Feb 2006. He has 5 years' experience in LES and RANS with application to nuclear reactors through collaborations with British Energy, EDF and CD-Adpaco. The PhD student, Stefano Rolfo, just started this October and is being trained on running our software, in LES mode in particular.

An extensive literature review has been conducted. The Idaho National Labs and International VHTR committee reports were found particularly rich and useful, and their recommendations allowed the Investigators to identify key challenges for CFD applications to advanced reactors where we can contribute: fluid behaviour in the lower and upper plenum, fluid by-pass within the core, hot channel characteristics in normal operation, and in accident conditions, as well as natural circulation both inside the reactor pressure vessel and in relation to cooling of the containment building.

A parallel computer with 36 nodes (72 CPU) has been purchased and installed. Some housing and cooling problems are still currently being resolved using investment from the School. On the software side the RA has become very proficient in administering the machine and installing our software which runs efficiently in parallel. Several natural convection LES cases have been run (up to 2 million cells) on a geometry suggested by British Energy corresponding to cold gas inlet pens of an AGR. This is similar to the coaxial inlet-outlet of a VHTR gas reactor, yet at lower temperatures.

Research aim:
Refined LES of strongly heated tubes will provide a database for RANS models evaluation and improvement. Interactions with British Energy has highlighted additional challenges in AGRs that can be related to VHTR, namely: modelling carbon deposition on fuel pin ribs, effect of injection of sleeve gapping flow on cluster conditions, use of steady state heat transfer coefficients in transient conditions. Liquid metals remain a strong possibility in GenIV systems. Hence, a refined LES of thermal stripping will be conducted on a wall jet or stratified pipe-flow geometry, to be used in developing a synthetic reconstruction model for unsteady thermal loading as planned in the proposal.

Presentations given/conferences attended:
5th International Symposium on Turbulence, Heat and Mass Transfer Dubrovnik, CROATIA 25-29 September 2006

Publications emanating from project:
A joint presentation with British Energy Ltd was delivered, acknowledging the KNOO project.
Y. Addad, D. Laurence, and M. Rabbitt (British Energy Ltd)
Turbulent Natural Convection in Horizontal Coaxial Cylindrical Enclosures: LES and RANS Models, Turbulence Heat, 5th International Symposium on Turbulence, Heat and Mass Transfer Dubrovnik, CROATIA 25-29 September 2006, K. Hanjalić, Y. Nagano and S. Jakirlic (Editors).

Collaborations/interactions with stakeholders:
Discussions with British Energy are underway, these being aimed at further defining fuel element geometries, and, more broadly, examining the possibility of identifying test cases that might be relevant both to currently operating gas-cooled reactors and to Gen. IV designs.
Some collaboration with staff of CEA – Marcoule who are focusing on the same test cases (Shehata & McEligot) has been initiated.

Work Package 2

Work Package Leader: Prof. Andrew Sherry

Project title: Innovative Approaches to Nuclear Industry Inspection and Monitoring

Researcher:
Frederic Cegla – started Oct 2005 but took leave of absence for 6 months to do a project at University of Queensland. Restarts Nov. 2006.

Supervisor:
Prof. Peter Cawley

Research progress:
The first tool developed is an ultrasonic thickness gauge based on propagation down strip waveguides that isolate the active piezoelectric elements from the hot and/or radioactive measurement zone; the waveguides simply clamp onto the structure – they do not need to be welded in place. The method has been extremely successful with a great deal of interest from both the power and petrochemical industries:

- successful tests have been carried out on structures up to 600 ˚C;
- a patent application has been filed;
- prototypes have been installed on petrochemical plant – this will provide very valuable operating experience that will feed across to the much more heavily regulated nuclear sector.

The next step will be to develop the technique for crack sizing using time of flight diffraction, so addressing the nozzle weld example. The current devices use strip waveguides which have flexibility in one plane; application of thin rod/wire waveguides will also be investigated, together with different attachment methods.

Research aim:
To provide proof of concept for remote acoustic inspection technology, including consideration of optimal waveguide geometry and material, signal quality, and waveguide end coupling. To develop a prototype inspection tool trialed using two instrumented test cases: signal propagation in highly irradiated graphite and crack growth measurement in nozzle welds.

Financial progress:
Spend is largely on staff and consumables and tracks PDRA months.

Publications emanating from project:
Patent application PCT/GB2006/003415; other publications held awaiting patent clearance.

Collaborations/Interactions with stakeholders:
Discussions with Dr. S. Worthington (Nexia Solutions), Dr. N. Habgood (Rolls-Royce Naval Marine).

Project title: Intelligent Automated In-Situ Monitoring Capabilities

Researcher:
Mr. Soheil Nakhodchi

Supervisor:
Prof. David Smith

Research progress:
Exploration of methods of measuring interior residual stresses in graphite and glasses. Design of test samples and rigs to undertake trials. Trials being conducted using applied stresses to a variety of graphite samples, including porous graphite representative of graphite part through life.

Design of systems for mounting the equipment and sample extraction are underway also.

Research aim:
To develop intelligent, automated, in-situ monitoring capabilities. This is a viewed as highly ambitious and yet essential if the requirement is to minimise human operational exposure, minimise human risk and hence improve overall safety. A step change through innovative monitoring will facilitate reduction of risk and costs in the maintenance and operation of nuclear fission systems, and safe and effective management of nuclear waste. Task 1 will establish a "proof of concept" for installing diagnostic equipment in an independent "hardened" shell to protect sensitive equipment from nuclear environments and radiation. Task 2 will focus also on developing monitoring tools for in-situ measurement, and for extraction of small samples and in-situ analysis.

Collaborations/Interactions with stakeholders:
British Energy is providing additional support for exploratory studies on capability of residual stress measurement in graphite.

Project title: Mechanical Performance of Nuclear Cladding and Structural Materials

Researchers:
PDRA Supriyo Ganguly started on 1st Sept 2006.
PGRS Jamalulail Ismail, PhD Title "High Temp Mechanical Properties of Nuclear Structural Materials" started on 1st October 2006.
PGRS Amil Jain, PhD Title "Weld Stress modelling in Nuclear Structural Materials" will start on 1st January 2007.

Supervisors:
Prof. Lyndon Edwards and Dr. Mike Fitzpatrick

Research aim:

1. **Zirconium Alloys**
   Develop understanding of microstructure/property relationships in current and likely future Zr alloys. Then acquire critical mechanical properties and develop models to predict effects of microstructure on mechanical performance.
2. **Future nuclear structural materials (including cladding)**
   Study, measure and model mechanical behaviour of candidate materials include F/M and ODS stainless steels, high temperature nickel alloys, monolithic ceramics and ceramic matrix composites
3. **Weld residual stresses in nuclear components**
   Design and perform critical experiments to develop validated models of weld structural integrity – initially for zirconium alloys and SS structural materials but eventually including future nuclear structural materials
4. **Effect of H and He on mechanical behaviour of nuclear structural materials**
   Initial paper study leading to possible future funding bid.

Presentations given/conferences attended:

1. Lyndon Edwards presented one of only eight Keynote Lectures at the next ICNS: - International Conference on Neutron Scattering to be held at Sydney on 27 November to 2nd December 2005.
2. Lyndon Edwards gave Plenary lecture at 2006 UK Neutron and Muon users conference Warwick, March 2006

Current collaborations/interactions with stakeholders:
Current KNOO relevant collaborations with:
British Energy, Barnwood, UK
Rolls Royce: Marine , Derby, UK
JRC, Petten, Netherlands
ANSTO, Sydney, Australia
Nuclear Materials Group, Kingston University, Canada
CNEA, Bariloche, Argentina

Project title: Mechanistic Understanding of Chloride-Induced Atmospheric Stress Corrosion Cracking (AISCC) in Austenitic Stainless Steels

Researcher:
Dr. Anthony B. Cook

Supervisors:
Prof. Andrew H. Sherry and Dr. Stuart B. Lyon

Research progress: As indicated above our approach will address the key factors controlling AISCC. Progress to date includes:

i) Design of wedge shaped samples, humidity enclosure and suitable tension rig to determine the stress range, critical chloride and relative humidity levels at which AISCC occurs.
ii) The identification and design of suitable (novel) electrochemical systems to study crack tip chemistry/electrochemistry in order to determine the importance of the local environment to the initiation and propagation of AISCC.

Research aim:
Extend the current understanding of AISCC and related phenomena in austenitic materials by carefully quantifying the key factors (chloride concentration, relative humidity, stress and temperature effects) controlling its initiation and propagation. Ultimately the intention is to apply such knowledge to produce realistic long-term predictive models pertaining to AISCC susceptibility in these materials.

Collaborations/Interactions with stakeholders:
Regular contact/discussion with peers/researchers involved in AISCC projects ongoing at Serco Assurance (Dr. D. R. Tice, Risley).

Project title: Mechanistic Understanding of Irradiation Effects on Stress Corrosion Cracking of Austenitic Stainless Steels

Researcher:
Abdulla Faisal Isa Al Shater

Supervisor:
Prof. Andrew H. Sherry

Research progress:
Experimenting with different heat treatments to simulate neutron irradiation effects and assessing the degree of irradiation damage (mainly sensitization) through double loop potentiodynamic polarization tests. Generating IGSCC through slow strain rate tests.

Research aim:
To study the effects of neutron irradiation on stress corrosion cracking of 20/25 Nb stabilized stainless steels (Advanced Gas Cooled Reactor Spent Fuel Cladding Material) which has been taken to high levels of burn up, and examining ways of simulating those effects (e.g. heat treatment, cold work and proton irradiation), and verifying the effectiveness of corrosion inhibitors.

Presentations given:
- Regular SCC meeting presentations (Effects of Corrosion Inhibitors on IGSCC of 20/25 Stainless Steels in Storage Ponds) (April 2006)
- Postgraduate Progress Presentation (at University of Manchester) (May 2006)
- Project Progress Presentation (at Nexia Solutions, Sellafield) (August 2006)

Courses attended:
- Introduction to Research in the University of Manchester, Faculty of Engineering and Physical Science (16/2/2006)
- Academic Writing at the University of Manchester, Faculty of Engineering and Physical Science (14/2/2006)
- Carbon and Alloy Steel Metallurgy and Processing, at Corus and National Metals Technology Centre (NAMTEC), Sheffield (11^{th} and 12^{th} of April 2006).
- Introduction to Nuclear Technology course and seminar at the University of Manchester (April 2006)
- SEM, FIB, TEM, EPRT and SSRT training at the University of Manchester.

Industrial meetings and conferences attended:
- Several visits and meetings in Nuclear site such as (Springfields and Sellafield –plant and Nexia Solution-).
- Member of Corrosion and Science Division (CSD) at the Young ICORR Committee.

Collaborations/Interactions with stakeholders:
- 23-24 Aug. 2006 (Sellafield): Meeting and discussions with Nexia Solutions and British Nuclear Group
- 1 Sept. 2006 (Springfields): Visit to Oxide Fuels Complex plant.
- 26-27 October 2006(Sellafield): Meeting and discussions with Nexia Solutions and Prof. Gary Was (University of Michigan) and Dr. D. R. Tice (Serco Assurance)

Project title: Effects of Helium on Materials Performance in Nuclear Environments: Modelling of Helium Diffusion in Stainless Steel

Researcher:
Mark Simon, Robert Clegg

Supervisor:
Prof. Andrew H. Sherry

Research progress:
Researching information on, and using said information to produce a report that discusses in detail why the process of helium embrittlement occurs, the mechanism of exactly how this process works, and to provide a discussion and examples of the various methods used to model this and other processes.

Research aim:
To study, via modelling with particular computer software, the diffusion of helium through the material stainless steel in certain nuclear environments, and to investigate the effect that the various micro-structure defects that occur, such as dislocations, and certain processes that the material can succumb to, as an example, embrittlement caused by the Helium, have on this diffusion.

Project title: Nuclear Graphite

Researcher:
Dr. K. Wen

Supervisors:
Prof. B. J. Marsden and Dr. T. J. Marrow

Research progress:
Microstructure and mechanical properties of baked carbon and its graphitized counterpart were characterized by transmission electron microscopy (TEM), high resolution transmission electron microscopy (HRTEM), Raman spectroscopy and nanoindentation. It has been proposed that similarities in the propertiues of irradiated graphite and baked carbon may be understood in terms of microstructure. The elastic modulus measured by nano-indentation in the baked carbon is 18.83±6.85 GPa, which is higher than that measured in its graphitized counterpart (12.55±4.09 GPa). Also a much higher hardness was measured in the baked carbon (1.52±1.01 GPa) than in its graphitized counterpart (0.34±0.16 GPa). This significant difference in mechanical properties is a result of from their different microstructures. Baked carbon consists mainly of structures with discontinuous aromatic layer and occasional lamellae, in which continuous aromatic layers are stack with order. Few microcracks were observed in the baked carbon. On the other hand, numerous microcracks were observed in the graphitized structure.

Research aim:
Microstructure characterization of ion and/or neutron irradiated nuclear graphite and highly oriented pyrolytic graphite (HOPG). Observations of the deformation mechanism of graphite: using focus ion beam (FIB) to prepare TEM samples to study the microstructure of deformed graphite with deformation introduced by indentation.

Publications emanating from project:
"Microcracks in nuclear graphite and highly oriented pyrolytic graphite (HOPG)", K. Wen, T.J. Marrow and B.J. Marsden, presented by B. Marsden at INGSM-7 (7th International Nuclear Graphite Specialists Meeting in Oak Ridge, Tennessee, USA), and submitted to Journal of Nuclear Materials (2006).
Conferences attended: "Carbon 2006", July 16th-21st, Aberdeen, UK.

Presentations given:
"Microcracks in nuclear graphite and highly oriented pyrolytic graphite (HOPG)", K. Wen, T.J. Marrow and B.J. Marsden, presented by B. Marsden at INGSM-7 (7th International Nuclear Graphite Specialists Meeting in Oak Ridge, Tennessee, USA).

Project title: Nuclear Graphite

Researcher:
Dr. A. N. Jones

Supervisor:
Prof. B. J. Marsden and Dr. T. J. Marrow

Research progress:
The crystalline structures of unirradiated nuclear graphites and their thermal strain behaviour have been evaluated using HRTEM with in situ TEM thermal experiments. The objective is to obtain thermal strain measurements by image correlation, with which to validate models for structure/property relationships. Sample preparation methods have been compared using both traditional mechanical polishing and state of the art Focused Ion Beam FEG-SEM. The mechanical properties of the virgin graphites are being correlated with the microstructure through a series of compressive loading experiments using both in situ X-ray diffraction and Raman spectroscopy. In addition to analysis of the thermal strain experiments, the examination of neutron irradiated graphites by HRTEM will be undertaken following visits to Petten (Netherlands) and Nexia Solutions. Ion beam irradiated graphites from Cardiff, will be compared with neutron irradiated samples.. Three-dimensional studies of the structure/property relationships will be initiated at the University of Manchester (2007), using TEM tomography.

Research aim:
Microstructure characterization of ion and/or neutron irradiated nuclear graphite and highly oriented pyrolytic graphite (HOPG). Observations of the deformation mechanism of graphite: using focus ion beam (FIB) to prepare TEM samples to study the microstructure of deformed graphite with deformation introduced by indentation. To undertake an in-depth study of the relationship between the microstructure, dimensional change and materials properties of both unirradiated and irradiated nuclear graphites

Presentations given:
Two day training and conference at MicroScience (ExCel, London) 28th - 29th June 2006. Paper presented and submitted to the NGRSM-7 (Oak Ridge, Tennessee),
11th – 14th September 2006, for publication in the Journal of Nuclear Materials.

Work Package 3

Work Package Leader: Prof. Simon Biggs

Project title: Structure and defect stability of calcium apatites

Researcher:
Emily Michie

Supervisor:
Robin W. Grimes

Research progress:
Atomistic scale computer simulation is being used to examine the apatite structure and the defect mechanisms associated with incorporating both halides and actinides. Initially, the apatite structures for fluorapatite, chloroapatite and hydroxyapatite were established by comparing the calculated with experimental values. A variety of interatomic potential parameters are available in the literature and these were examined in order to assess their reliability.

Quantum mechanical simulations are also being carried out using the plane wave code CASTEP. Internal solution energies were calculated, investigating the substitution of strontium onto the two non-equivalent cation sites. Energetically there was no difference found between substituting Sr on to either site.

After examining the apatite structure and the solid state transport mechanisms associated with both halide and actinide loss, modelling will be extended to consider the effect of radiation damage and the influence of an aqueous environment.

Presentations given/conferences attended:
- RCS Christmas Meeting, University of Surrey, December 2005
- Eighth European Society of Glass Science and Technology conference, Sunderland UK, 10-14 September 2006
- AWE Materials Science Research Day – Poster Session, 25th October 2006, Thames Room, Aldermaston.
- International Symposium on Structure-Property relationships in Solid State Materials, Bordeaux, France June 2006.

Courses Attended:
The CCP5/Marie Curie Actions Molecular Simulation Summer School, Cardiff University 17-25 July 2006 (took the Advanced Course Option in First Principles Simulations).

Project title: Colloidal Ternary Systems in Nuclear Waste Processes

Researcher:
Dr. Peter Ivanov

Supervisor:
Dr. Nick Bryan

Research progress:
Work started on this part of the KNOO project in April 2006. This aim of this project is to study the thermodynamics and kinetics in colloidal ternary systems that are relevant to nuclear industry legacy waste systems. In addition to a generalised simple ternary system with quartz sand, organic colloids and Eu^{3+} which has been used for initial model development, two ternary systems of specific relevance are also being studied: magnesium hydroxy/carbonate, which is relevant to Sellafield Magnox fuel sludge ponds; and iron oxide phases (hematite, goethite and magnetite), which are important in many nuclear waste systems, for example EARP sludges, corrosion products in plants and in waste repositories.

The behaviours of the ^{152}Eu/organic colloid/quartz sand and ^{152}Eu/organic colloid/iron oxide (hematite, goethite and magnetite) ternary systems have also been studied. $^{152}Eu^{3+}$ is being used as an analogue of Am(III). Ion exchange, UV spectrophotometry, γ-spectrometry and ultrafiltration have been applied to these systems, and the kinetics of the interactions in the systems have been determined over a wide range of pH (2 - 11) and colloid concentrations (10 ppm - 100 ppm).

Much less is known about the behaviour of the magnesium hydroxy/carbonate system. Therefore, our initial studies have examined the evolution of the populations of inorganic colloids in solutions that are in contact with the bulk magnesium phases as a function of pH and ionic strength.

A computer based kinetic mathematical model has been developed that can predict the uptake of colloids onto bulk surfaces and the interactions of metal ion with colloids and bulk phases. Therefore, it can be used to predict the change in the solution/solid phase partition of radionuclides in colloidal ternary systems with time.

Research aim:
The main efforts in the next period (until 01/10/2007) are going to be applied to the use of the Field Flow Fractionation (FFF) method for a better understanding of the behaviour of these ternary systems. Also, we will be extending the magnesium system work to include metal ions.

Publications emanating from project:
A number of papers are in preparation

Presentations given/conferences attended:
N.D. Bryan et al "A simple ternary system model" Second International Conference on Natural Aquatic Colloids and Nanoparticles: Structure and Interactions with Pollutants and Pathogens, University of Plymouth, September 2006.

Collaborations/interactions with stakeholders:
Nexia Solutions are involved with the planning and progress of the project: in particular the study of the magnesium hydroxide (Magnox) systems.

Project title: Behaviour of plutonium-contaminated fine particle wastes

Researcher:
Dr. Stephen Parry

Supervisor:
Prof. Francis Livens

Research progress:
This element of the project has focused so far on corroded Magnox sludge (CMS) and particularly on the behaviour of plutonium in CMS systems. Three different aspects are being studied:

Factors controlling plutonium solubility. In the ponds, chemical conditions vary as a result of treatment processes (*e.g.* pH is adjusted, a flocculant is added, trace silica can enter the system) and plutonium solubility varies substantially as a result of these changes. Experiments, with a full factorial design, have been carried out to define key controls on plutonium behaviour and the results are presently being analysed using analysis of variance.

Carbonation of CMS. The first corrosion product of Magnox alloy is brucite but some of the storage ponds are maintained at high pH (*ca* 11) and, in these circumstances, atmospheric CO_2 is absorbed by the pond water. This produces artinite, a mixed Mg hydroxide/carbonate. In addition, pond effluents are treated with CO_2 to reduce the pH before passing through the SIXEP ion exchange plant at Sellafield and it is unclear how particulate CMS responds to this treatment. Energy dispersive (time resolved) X-ray diffraction (EDXRD) at the Daresbury synchrotron has been used to explore the carbonation reactions of brucite and has shown that the brucite-nesquehonite-hydromagnesite transformations occur readily.

Evolution of cemented CMS waste (collaborative with Neil Milestone, Sheffield). CMS is a reactive solid and one candidate immobilization process is cementation. Preliminary EDXRD experiments under hydrothermal conditions have shown that CMS stimulant reacts readily with Ordinary Portland Cement/Blast Furnace Slag to form a complex mixture of phases.

Research aims:
- Complete analysis of variance; spectroscopically define Pu redox and complexation behaviour as a function of key variables.
- Define carbonation reactions of CMS, understand the role of artinite, obtain rate and activation parameters, resolve inconsistencies in the Mg-CO_2-OH^- phase diagram.
- Analyse phase assemblage in cemented CMS stimulant, assess the relevance of cementation reactions in hydrothermal conditions to transformations at lower Temperature and Pressure.

Financial progress:
The major capital item (FFF) has now been ordered.

Publications emanating from project:
One paper is currently in preparation.

Presentations given/conferences attended:
S Parry *et al.* "Plutonium Behaviour in Corroded Magnox Sludge" Plutonium Futures 2006, Asilomar, USA, July 2006.

Collaborations/interactions with stakeholders:
Nexia Solutions (Luke O'Brien, Robin Taylor, Mark Sarsfield) are involved with the work, in particular defining plutonium behaviour.

Project title: Large Eddy Simulation of Liquid-Particle Flows

Researcher:
Dr. Jun Yao

Supervisor:
Prof. Michael Fairweather

Research progress:
The researcher joined the KNOO project on 1st September. From September 06 to October 06, the researcher had outlined research objectives and contents; set-up computer and program systems; trained on safety courses and KNOO programme and built up literature review.

From November 06 to January 07, it is planed to work on three-dimensional liquid flow (single phase); to review experimental/simulation work in single phase flow; to write/adjust LES simulation code for a liquid flow; to compare LES results with experimental measurement and improve the simulation accuracy; to use different LES models and choose the best one for the next study and to help related postgraduates to study and research.

Research aim:
To investigate the mechanism of particle transport in large eddy simulations (LES) of three-dimensional turbulent liquid flows:

- To investigate the mechanism of particle dispersion, sedimentation and re-suspension in liquid flows, using LES for simulating the flow and Lagrangian particle tracking under the condition of one-way coupling;
- To study the physics of three-dimensional particles dispersion patterns, particle-turbulence interactions in developed turbulent flows under the condition of two-way coupling. Particularly, to understand the near-wall particle interactions with turbulence effect on particle deposition, re-suspension and preferential concentration.

Ultimately, to acquire a comprehensive understanding of the working mechanism of dilute liquid-particle flows and to use this as the basis for the following study on dense liquid-particle flows under the condition of four-way coupling (i.e. including particle-particle interactions).

Publications emanating from project:
1 conference paper to be submitted to ICEM'07
1 paper to be submitted to *Chemical Engineering Science*.
1 paper to be submitted to *Physics of Fluids*.

Project title: The influence of mixed salts on the zeta potential and rheology of titanium dioxide (TiO_2)

Researcher:
Miss Qanitalillahi Omokanye

Supervisor:
Prof. Simon Biggs

Research progress:
In this work, so far aims and objectives have been outlined. All necessary safety and equipment (Colloidal Dynamics ZetaProbe, Malvern Rheometer, Lumi Fuge and Turbi scanner) training that would aid the research have been completed. Literature review is building up and experiments from previous papers have been repeated to test apparatus, in addition aid interpretation of data.

By studying the stability control of particulate dispersions in mixed electrolytes, for example NaCl and Na_2SO_4, we are able to design and control waste processing efficiently. The electroacoustic and shear yield stress response of concentrated titanium dioxide suspensions have been measured across a range of pH (10^{-3} - 10^{-12}) conditions and electrolyte concentrations (0.001 M - 1.0 M). The yield stress as a function of pH for titanium dioxide in single system electrolytes showed a correlation in the shift in the position of the isoelectric point for the ζ potential results.

Research aim:
Future work to be done includes mixed electrolyte shear yield stress measurements including divalent salts. In addition first year interim report due at end of January is in the process of being completed.

Publications emanating from project:
1 paper to be submitted to ICEM DECOM 07 conference to be held in September 2007
1 paper to be submitted to 6th European Chemical Engineering Conference to be held in September 07

Presentations given/conferences attended:
- Visit to Sellafield Cumbria (Nexia Solutions), December 2005
- Presentation for IPSE postgraduate seminar, March 2006.
- Malvern Instruments Seminar, Tadcaster, March 2006
- Sheffield Nuclear Forum Conference, April 2006

Collaborations/interactions with stakeholders:
Discussions held with Nexia Solutions staff (Dominic Rhodes and Graham Fairhall)

Work Package 4

Work Package Leader: Prof. Tony Goddard

Project title: Safety Performance for VHTR and GCFR (see also WP1 for code development research)

Researchers:
Mr. Jason Dunstall (KNOO PhD from 1st Oct 2005)
Mr. Brendan Tollit (PhD BNFL Energy Group funded for KNOO – from 1st Oct 2005)
Mr. Andrew Hagues (KNOO PhD appointed – starts work 1st Jan 2007)

Supervisors:
Prof. Tony Goddard (Leader of WP4), Prof. Chris Pain (Leader of AMCG group) assisted by Dr. Matthew Eaton, Dr. Matthew Piggott, Dr. Jeff Gomes and Dr. Andrew Buchan

Research progress:
Prof. Goddard has organised a meeting of Work Package 4 participants which was held in Manchester on 19th June 2006.

Mr. Dunstall has focused initially on analyzing the historical DRAGON reactor transient data with a view to it acting as a transient benchmark for FETCH. When this training exercise has been prepared for publication he will switch to applying FETCH to transient modelling of a generic GCFR design agreed with stakeholders. For pastoral reasons Mr. Dunstall has changed to half time work for the next two years and his PhD project will therefore end in September 2009.

Mr. Tollit has, as a training exercise and aided by the whole team, successfully created a 3D transient natural circulation model of the Imperial College reactor CONSORT where all fuel elements and control rods are represented together with 3D water flows in the surrounding tank. This work is now being prepared for publication. Mr. Tollit's main brief is transient modelling of block-type VHTR systems in consultation with stakeholders.

Research aim:
Steps are being taken that, despite the DTI's withdrawal from active participation in GIF, this project continues to directly serve the needs of UK industry and has industry/international inputs. The related development of FETCH and its major constituent codes has been outlined under WP1. Mr Dunstall will work to assess the multiscale reactor physics issues needing to be addressed for GCFR and the generation of the necessary models. He will take part in agreeing with stakeholders a generic code design that he should model. He will broaden his experience from reactor physics to include CFD (FLUIDITY).

Mr. Tollit will continue with a science emphasis on FLUIDITY but will broaden his experience to include more reactor physics. He will take part in agreeing the generic core design to be studied for a block type VHTR and (with the involvement of the whole team) carry out 3D within-vessel, whole core transient modelling

Mr. Hagues – who has an industry computational fluid dynamics background – will focus on reactor CFD and will begin research (as part of the group's effort) to understand the formal basis of modelling/data-driven uncertainties for innovative reactors. This research will employ stochastic FEM.

Financial progress: (excluding the BNFL Energy Group studentship)
From a EPSRC KNOO budget of £371,286 the expenditure to 1 October 2006 was £61,512

Presentations given/conferences attended: (including the name of the conference)
Both Mr. Dunstall and Mr. Tollit attended the 2006 Frederic Joliot' Otto Hahn Summer School at Caderache France. They also presented PhD papers on DRAGON and CONSORT reactor modellilng at the 2006 UNTF meeting

Collaborations/interactions with stakeholders:
Collaboration has been maintained with AMEC NNC in GenIV reactor systems specification. Excellent interactions in closely related research matters have been maintained with Rolls Royce, British Energy, Serco Assurance, Nexia Solutions, AWE plc.

Project title: Atomistic modelling of fission gas release in uranium oxide

Researcher:
David Parfitt

Supervisor:
Robin Grimes

Research progress:
This project commenced in July 2006. To date work has been carried out in two key areas: Firstly, identifying a set of inter-atomic potentials which can be used to accurately reproduce the bulk and microscopic behaviour of uranium dioxide (UO_2). This includes modelling the energies of fission gas atoms, produced as part of the natural decay processes, within the host UO_2 lattice.

Secondly, developing simulation techniques to use these potentials in making accurate predictions about the dynamics of fission gas release from within UO_2. A key element of this has been the use of the molecular dynamics simulation code DL_POLY which is being used to examine fission gases within voids in the crystal lattice.

Research aim:
Work in the future will extend the characterisation of the fission gases contained within the crystal voids and also look at the processes which can lead to the release of the gas into the surrounding environment. In particular the interaction between these voids and the displacement cascades formed from recoil fragments of fission events will be simulated.

Collaborations/interactions with stakeholders:
An on-going collaboration with British Energy. The release of fission gas is important in the operation of current and future nuclear reactions and we are working with them to better model this release and to understand the associated microscopic structures found in high-burnup fuels.

Project title: Massive Scale Hydrogen Manufacture using Nuclear Power

Researchers:
PDRA1 & 2 are identified and will start Jan 2007 and August 2007.
Two DTA funded PhD students have started.

Supervisors:
Prof. Ray Allen, Dr. Bruce Ewan and Dr. Geof Priestman

Research progress:
Sheffield has worked in a number of international consortia examining the thermodynamics of the two main cycles. For the SI Process, the partners include: CEA (France), DLR (Germany), Emprasarios Agrupadas (Spain), University of Virginia (USA) and INEL. For the Westinghouse /HyS process, partners include: Westinghouse (USA), SRNL (USA), Shaw, Stone & Webster (USA), PBMR (RSA), M-Tech (RSA) and the University of the North West (RSA). In addition, Sheffield has had a major methodological input into European Study of routes to hydrogen (via INNOHYP). A PhD student has started (DTA funded) looking at membrane separations/reactors. Process flow sheet calculations have been performed and established that an overall efficiency increase of up to 4% in the process is possible by feed dewatering. This has been part funded by HYTHEC. A joint benchmarking project has been initiated with University of Virginia (US). SRNL and CEA have agreed to act as technical sponsors. A Funding application has been drafted and will be submitted to EPSRC for UK activities and DoE for US activities. A PhD student (DTA funded) has started and is focussed on alternative separation approaches in the HIx section. Initial results are encouraging. Significant work has been done in collaboration with the Westinghouse Corporation. A wide range of alternative process configurations were considered and only HyS showed promise. This phase of the work is finished and was published in the Ewan and Allen paper at Cincinnati. Resources are now re-focussed on the oxygen separation stage using a DTA funded PHD Student.

Research aim:
As part of developing the forward strategy for the UK in this field, 3 new research proposals have been prepared submitted to DTI Programme of Research into Advanced Nuclear Reactor System, Supergen Plus and EPSRC.

Financial progress:
Extremely light spend pending appointment of PDRA's

Presentations given/conferences attended:
Allen RWK and Zimmerman, WBJ. "Challenges in the Use of Process Heat from High Temperature Nuclear Reactors" Invited Keynote Lecture, Turbulence, Heat and Mass Transfer Conference, Dubrovnik, September, 2006,
Ewan, B.C., and Allen, R.W.K., "A representation of Limiting Efficiencies of Thermochemical Cycles" Presented to the A I Chem E Annual Meeting, Cincinnati, November 2005
Allen, R.W.K., Le Duigou, A., Roeb, M et al, "A Search for a long Term, Massive Scale Hydrogen Production Route" Presented to the A I Chem E Annual Meeting, Cincinnati, November, 2005
Elder, R.H., Borgard, J.M., Ewan, B.C. and Allen, R.W.K. "Use of Membranes and Reactive Distillation for the Separation of HIx in the Sulphur Iodine Cycle" Presented to the A I Chem E Annual Meeting, Cincinnatti, November, 2005.

Collaborations/interactions with stakeholders:
Mainly with international stakeholders.

Project Title: Safety Performance for VHTR and GCFR

Researcher:
A PhD Studentship: "Mechanistic Modelling of Irradiated Graphite Behaviour" is being advertised at present. It is hoped to recruit a student as soon as possible, early 2007.

Supervisor:
Prof. B. J. Marsden and Dr. T. J. Marrow

Research progress:
Nuclear graphite is manufactured from "coke" a bi-product of the oil or coal industry. The coke is mixed with a pitch and then extruded, or moulded, into large blocks which are baked at about 800°C, re-impregnated, at least once, and then graphitised at about 1800°C. The final product is very pure polycrystalline "artificial graphite" with about 20% porosity. The properties, both unirradiated and irradiated, of the final product are mainly defined by the original "coke". As coke supplies vary with time, the properties and irradiation behaviour of the final product changes. At present irradiated graphite properties are based on empirical data obtained on samples irradiated in a material test reactor (MTR). The cost of such a programme may take about 6 years and amount to £8m. It is therefore desirable that the relationship between irradiation induced changes to graphite structure and change in property are fully understood, thus reducing the scope and size required of MTR programmes. In addition, such an understanding may lead to the development of "new types of graphite" that will have longer lifetimes. This would reduce the amount of irradiated graphite waste in future VHTR designs.

Research aim:
This project involves investigation of graphite irradiation data from international and UK MTR programmes. Semi-empirical mechanistic models will be developed to determine the important parameters that govern the graphite behaviour. This project interacts directly with a postdoctoral project in KNOO, which is a study of the microstructure of unirradiated graphite and the microstructural changes in irradiated graphite. This PhD project aims to develop mechanistic models for the prediction of irradiated behaviour in nuclear graphite.

It is intended to recruit a student as soon as possible.

Publications emanating from project:
Although no student has not yet been recruited, the following publication related to the RAPHAEL project have been issued:

- Hall G., Marsden B J, Marrow T.J., MummeryP, Vreeling J.A. and van der Laan J. Possibilities for the Microstructural Modelling of the Irradiation Properties Of Graphites For Future High Temperature Reactor Proceedings. HTR2006: 3rd International Topical Meeting on High Temperature Reactor Technology October 1-4, 2006, Johannesburg, South Africa. A joint paper with NGR Petten Netherlands.
- Hall G. Status of Development of modeling method for graphite. RAPHAEL-0604-D-ML3.5-1

Presentations given/conferences attended:
Reference 1 was presented at HTR-2006 in South Africa.

Collaborations/interactions with stakeholders:
This projected is related to the European Union FP6 RAPHAEL initiative. This EU FP6 project

funds a post Doctoral Research Associate working at the University of Manchester (Dr. Graham Hall). Graphite irradiated in the FP5 and FP6 programme is being examined under WP2 and the irradiation damage observed will be modelled under this work package. There is particularly close collaboration with NRG Petten as part of the RAPHAEL project and British Energy Plc who are irradiating and investigating property changes in AGR graphite. There is also close collaboration with HSE (NSD) who are funding work on microstructural studies in graphite and modelling of stresses in nuclear graphite components. It is also hoped that irradiated UK graphite will be examined using TEM at the Sellafield Technical Centre in conjunction with Nexia Solutions.

Project title: Safety Performance for VHTR and GFR Nuclear Structural Materials

The Open University is not specifically funded for GenIV work but several areas in the Open University WP2 structural Nuclear Materials remit are relevant to GenIV materials issues and this work is described here.

Researchers:
PDRA Supriyo Ganguly started on 1 Sept 2006
PGRS Jamalulail Ismail, PhD Title "High Temp Mechanical Properties of Nuclear Structural Materials" started on 1 October 2006

Supervisors:
Prof. Lyndon Edwards and Dr. Mike Fitzpatrick

Research progress:
Review of US GenIV Structural Materials work started but GenIV as PhD student only just appointed
Research aim (next year from 1st October 06)
Gen IV related work is concentrating on the development of state of the art creep facilities to

Collaborations/interactions with stakeholders:
Current WP4 relevant collaborations with:
JRC, Petten, Netherlands
ANSTO, Sydney, Australia
Nuclear Materials Group, Kingston University, Canada

Project title: Safety Performance for VHTR and GFR – Application of RANS methods

Researcher:
Mr. Amir Keshmiri (50% with WP1)

Supervisors:
Dr. Mark A. Cotton and Prof. D. R. Laurence

Research progress:
Amir Keshmiri was appointed only recently (October 2006); however, the taught elements of his MSc in Thermal Power and Fluids Engineering (2005/06), and also his MSc project on conjugate heat transfer, should accelerate progress in the training period. In the meantime, a series of publications by McEligot and co-workers at Idaho National Labs, as well as those by colleagues at Manchester (often cited by Idaho National Labs and the International VHTR Committee), have enabled us to identify a series of test cases (experimental, DNS, and LES data) on strongly heated gas channels to begin the validation process for advanced RANS models (relaminarization due to the increase of gas viscosity with temperature, as well as the effects of favourable/adverse buoyancy forces on turbulence are particularly challenging).

Some collaboration with staff of CEA who are focusing on the same test cases has been initiated, as well as collaboration with the Russian Nuclear Labs in Sarov. Discussions with British Energy are ongoing to refine the definition of WP4 with particular reference to the issues of riblets on fuel elements (see 'Collaborations/interactions with stakeholders', below).

Research aim:
Amir Keshmiri is currently running 'Star-CD' and the open-access EdF code 'Saturne', applying both codes to some of the 'building block' test cases referred to above. (Both Amir and Stefano Rolfo [PhD student commenced Oct. 2006; 100% WP1] are currently using RANS and LES methods to provide them with appropriate background experience.)

Over the coming year Amir's work will be extended to encompass RANS studies of heat transfer for innovative fuel element surfaces. Initial designs will be based upon AGR-type 'multi-start' fuel pins and will also draw upon experimental and computational work conducted at Manchester that was concerned with internal flow in spirally-fluted tubes.

Financial progress:
The bulk of the Manchester 'Fluids' expenditure comes under WP1 (1 full-time PDRA; 1.5 PhD students as detailed above). Spend is currently on track with predictions.

Collaborations/interactions with stakeholders:
As noted above, preliminary discussions with British Energy are underway, these being aimed at further defining fuel element geometries, and, more broadly, examining the possibility of identifying test cases that might be relevant both to currently operating gas-cooled reactors and to Gen. IV designs. It is intended that WP4 leadership (and other interested parties) will be fully involved in these discussions.

Abbreviations

AGR – Advanced Gas cooled Reactor
AISCC – Atmospheric Induced Stress Corrosion Cracking
CEA – Commissariat à l'Énergie Atomique
CFD – Computational Fluid Dynamics
CMS – Corroded Magnox Sludge
DTA – Doctoral Training Account
DTI – The Department of Trade and Industy
EARP – Enhanced Actinide Removal Plant
EPRT – Electrochemical Potentiodynamic Reactivation Polarization Test
EPSRC – Engineering and Physical Sciences Research Council
F/M stainless steel – Ferritic/Martensitic stainless steel
FEM – Finite Element Modelling
FFF – Field Flow Fractionation
FIB – Focus Ion Beam
FIM – Field Ion Microscope
GCFR – Gas Cooled Fast Reactor
GenIV – Generation IV
HOPG – Highly Oriented Pyrolytic Graphite
HRTEM – High Resolution Transmission Electron Microscope
HSE (NSD) – Health and Safety Executive, Nuclear Safety Directorate
IGSCC – Irradiation Generated Stress Corrosion Cracking
INEL – Idaho National Laboratory
KNOO – Keeping the Nuclear Option Open
LES – Large Eddy Simulation
MTR – Material Test Reactor
NDT – Non Destructive Testing
ODS stainless steel – Oxide Dispersion Strengthened stainless steel
PBMR – Pebble Bed Modulated Reactor
PDRA – Postdoctoral Research Assistant/Associate
PGRS – Postgraduate Research Students
RANS – Reynolds-averaged Navier-Stokes
SCC – Stress Corrosion Cracking
SEM – Scanning Electron Microscope
SRNL – Savannah River National Laboratory
SS – Stainless Steel
SSRT – Slow Strain Rate Test
TEM – Transmission Electron Microscope
VHTR – Very High Temperature Reactor
WP1 – Work Package 1
WP2 – Work Package 2
WP3 – Work Package 3
WP4 – Work Package 4