Keeping the Nuclear Option Open

2007 Annual Meeting

Abstracts

Session 1

Introduction

Robin Grimes

Imperial College London

Key events of the year will be reviewed and key events for the forthcoming year outlined. General comments will be made concerning the meeting structure and what we expect to achieve during the course of the two days.

EPSRC Keeping the Nuclear Option Open: Materials Research

Andrew H. Sherry

The University of Manchester

The materials work package within the EPSRC KNOO programme is undertaking research into new methods for the remote monitoring and the reliable prediction of materials condition in nuclear applications.

Due to the severity of the local environment in nuclear plant (e.g. high temperatures and neutron irradiation), research into new condition monitoring approaches are focusing on the need for a *remote* capability. Ultrasonic methods that utilise wave-guides to facilitate remote monitoring are being developed at Imperial College (London). One end of the wave-guide is attached to the component of interest, whilst the ultrasound generator and receiver are located at the other, i.e. outside the ‘hot’ area. A combination of experiment and finite element analysis is enabling the development of approaches to monitor wall thickness and defect development. Remote monitoring of in-service material property changes and residual stress levels are the focus of researchers at Bristol University who are developing a fully autonomous miniaturised ‘pod’, which would be located at/near the location of interest and activated remotely. The project is developing a prototype which draws on new research into energy storage/power management approaches, protective materials able to withstand the challenges of nuclear environments and miniaturisation of monitoring equipment – including hole drilling approaches for residual stress assessment, e.g. in nuclear graphite and glasses used for the immobilisation of HLW.

Research on materials performance in nuclear applications is based on developing an understanding of the mechanisms of mechanical, microstructural and electrochemical degradation in a range of materials, including nuclear graphite, austenitic stainless steels, zirconium alloys and rare earth halides and oxides for radiation sensor materials. Research into the *microstructural* degradation of nuclear graphite and the development of internal (Wigner) energy arising from neutron irradiation is being undertaken through collaboration between the Universities of Manchester and Cardiff. This work is highlighting the importance of radiation-induced microstructural changes (e.g. closure of Mrozowski cracks) on macroscopic behaviour. Research into the m*echanical* degradation processes that occur during service, including creep behaviour of structural materials as influenced by residual stress, are being undertaken by the Open University. This incorporates research into the calculation of residual stress levels due to welding and the deformation mechanisms of zirconium alloys. Research into the *electrochemical* degradation mechanisms includes atmospheric and irradiation effects on the stress corrosion cracking (SCC) behaviour of ILW container and fuel cladding materials, respectively. Novel test samples are being used at the University of Manchester to assess the critical combinations of stress, relative humidity, chloride concentration and temperature for SCC development in 304 and 316 stainless steels. Mesoscale modelling of initiating SCC cracks is shedding new light on the coalescence behaviour of multiple short cracks to form propagating long cracks. Additional research at Imperial College (London) is using atomic-scale modelling approaches to understand and develop new radiation sensor materials.

Work Package 4

Tony Goddard

Imperial College London

Focussing on safety and performance of Innovative reactors, this work package is heavily cross cutting with other Packages. Although paying special attention to VHTR and GFR systems other systems are being addressed such as compact plate LWR systems eg the Imperial CONSORT system, while the emphasis on graphite systems should help to maintain expertise in gas-cooled technology. The Investigators are Profs Pain and Goddard (Imperial, coupled transient safety modelling), Dominique Laurence and Mark Cotton (Manchester, nuclear fluids modelling), Barry Marsden (Manchester, nuclear graphite), Mike Fitzpatrick, (Open University , metallic materials for GenIV) and Ray Allen (Sheffield, design implications of hydrogen production).

Session 2

The Nuclear Decommissioning Authority

Neil Smart

The NDA remit as set out within the Energy Act includes – "*promote, and where necessary fund, research relevant to nuclear clean up"*. The NDA need to underpin delivery and / or accelerate programmes to fulfil the overall mission and technical underpinning of these activities is critical. Firstly, NDA set the requirement for nuclear sites to write down within the Life Time Plans (LTP) at a high level, the proposed technical baseline underpinning the LTP activities; furthermore we required technology gaps / opportunities in the technical baselines to be outlined in a R&D requirements section to the LTP. Criteria were established to categorise the R&D in three areas:

- "needs" - those development activities needed to underpin the proposed technical solutions
- "risks" – those activities required to reduce / eliminate key risks to the proposed technical solutions
- "opportunities" – innovations / changes to the technical baselines

The purpose of production of the technical baselines and underpinning R&D requirements is to establish an auditable trail through the LCBL from programme components into how the programme will be delivered. The LTP 05 was the first programme to attempt this process. NDA believe the production of the technical baselines and R&D requirements will be of benefit to the SLC's in terms of ensuring a focus on overall programme delivery and not just short term activities. Furthermore, we can ensure that investment in technology is targeted at priority areas, with common issues and requirements identified and solutions on a broader scale will be achievable.

Structure And Defect Stability Of Calcium Phosphate Minerals

Emily Michie, Robin W. Grimes

Department of Materials, Imperial College London

The choice of material for radioactive waste immobilization depends both upon the chemistry of the waste type and the physical environment in which the waste form is to be stored. Consequently, natural mineral phases are attractive due to their proven long time scale stability.

Apatite is of interest because (i) it is the most abundant phosphatic mineral, found in almost all igneous, some sedimentary and metamorphic rocks and (ii) it exhibits a large chemical variability. Indeed, due to the difficulty of incorporating halides in conventional materials, chloroapatites and fluorapatites are being considered as potential hosts for radioactive waste streams containing both actinides and halides. These subgroups of apatite demonstrate considerable non-stoichiometry, providing significant compositional flexibility, ideal for incorporating a range of waste species. β-tricalcium phosphate (whitlockite) is used as a precursor for preparing apatites. It is therefore useful to better understand the stability of these structure types and the relative solubility of different ions.

Atomistic scale computer simulation is used to examine both the apatite and the whitlockite structures and the defect mechanisms associated with incorporating both alkali halide and various cation species. Initially, the structures for various fluorapatites were established by comparing quantum based calculations (CASTEP) and experimental values. Subsequently, for apatite and whitlockite, a modified interatomic potential parameter set was derived that is able to reproduce structures and quantum derived defect behaviour.

Of particular interest was the substitution of Sr^{2+} onto the two non-equivalent Ca^{2+} cation sites in fluoroapatite. Previous experimental studies are unclear as to which site Sr^{2+} substitutions are most likely to occur. Here it was found that there was no energetic difference between substituting Sr^{2+} onto either site. Mg^{2+}, Ba^{2+} and Zn^{2+} substitutions were also investigated, however these showed a significant difference between the cation sites. Al^{3+} and Ga^{3+} substitution was also considered.

Microstructural Characterisation of Nuclear Grade Graphite using High Resolution Techniques

Abbie Jones, Barry Marsden and James Marrow.

Nuclear Graphite Research Group, Materials Performance Centre, The University of Manchester

Graphite has been used as a moderator and reflector in more than 100 nuclear power plants worldwide and in many research and plutonium-production reactors. It is used primarily as a moderator and reflector, although graphite is also used for other features of reactor cores, such as fuel sleeves, spacer rings, shield-wall graphite or other carbon-bearing material in certain cases. Fast neutron irradiation induced changes to the graphite crystal structure within nuclear graphite have been shown to lead to disruption of the bonding across the basal planes and closure of micro-cracks (Mrozowski cracks) resulting in similar graphitic structures to that seen during manufacture before the graphitisation process.

The objective is to obtain microstructural Transmission Electron Microscopy (TEM) thermal strain measurements by image correlation, with which to validate irradiation models for structure and property relationships. Sample preparation methods have been compared using both traditional mechanical polishing and state of the art Focused Ion Beam FEG-SEM. Image correlation analysis of data and relationship to thermal expansion coefficient has been used to calculate the crystal strain of the graphite. It is envisaged that this may lead to the development of improved graphite products for the nuclear industry.

Characterisation and sorption properties of $Mg(OH)_2$ colloids; ^{152}Eu(III)-Humic Acid-Hematite ternary system

A. Pitois[1], P. Ivanov[1], L. Abrahamsen[1], D. Farrelly[1], N. Bryan[1], R. Taylor[2] and H. Sims[3]

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The removal and processing of the highly contaminated Magnox sludges accumulated at UK facilities require that the chemistry of fission products and transuranic elements is fully understood. The speciation and associated solubilities of these elements and hence their distribution between solution, colloidal and solid phases under alkaline storage pond conditions are obviously key factors controlling their behaviour. This work investigates the effectiveness of $Mg(OH)_2$ bulk in trapping radionuclides and of $Mg(OH)_2$ colloids for radionuclide transport in the pond environment. A thorough characterisation of colloids (size, size distribution and morphology) as well as a study of the sorption properties of both bulk and colloids have been performed in this study.

Humic acids (HA) bind virtually all metal ions, and interact particularly strongly with the transition metals, the lanthanides and actinides, affecting their migration behaviour in natural systems. The main object of the present work is to examine the behaviour of nanogram amounts of ^{152}Eu(III) and its distribution between the solid phase and the solution in the Eu(III)–HA– hematite ternary system. The stability constant of the Eu(III)–HA complex has been determined in the binary system in accordance with the Charge Neutralization Model. The influence of pH, hematite and HA concentrations on the distribution of Eu between surface and solution has been studied for the ternary system. A mathematical model has been developed that can predict the binding on organic colloids and metals in ternary system experiments.

Simulation Approaches for Sludge Rheology

Martin Whittle, Karl P. Travis
Immobilisation Science Laboratory, University of Sheffield
Mark Bankhead, Scott L. Owens
Nexia Solutions Ltd.

In the UK, the corrosion of Magnox fuel cans stored in underwater silos over decades has created significant quantities of radioactive sludge that must be retrieved and immobilised for long-term storage. Other types of legacy sludge and slurry materials pose similar disposal problems in nuclear sites globally. The design of systems capable of retrieving these materials with minimal incidence of pipe blockage requires an understanding of their rheology. Mesoscale simulations offer one route for achieving this, and recent advances in the parameterisation of Dissipative Particle Dynamics (DPD) simulation suggest a promising approach. We examine some preliminary results from two possible realisations using Dissipative Particle Dynamics. The stress response in Couette flow establishes the viscoelastic nature of both model fluids while the development of plug characteristics in Poiseuille flow demonstrates the potential usefulness of the model in geometries of engineering interest. Possible extensions of the current models are briefly discussed.

Potential cements for high water content sludges

NB Milestone

Immobilisation Science laboratory, University of Sheffield

The current cements used for encapsulation of intermediate level nuclear waste (ILW) are based on Portland cement (OPC) with high replacement levels of supplementary cementing materials (SCMs), chosen to reduce the temperature rise encountered when large volumes of cementitious material are used. Typically around 90% blast furnace slag or 75% pulverised fuel ash are used, well above the levels used in construction. Much of the SCM remains unreacted due to the low level of activating OPC so that the porosity of the hardened matrix is high and filled with alkaline pore solution which causes corrosion of metals and dissolution of compounds such as zeolites and desiccants.

Encapsulation of slurries and sludges with their high water content necessary to transport them will result in a highly porous, weak wasteform which is not likely to exhibit the long term durability needed.

Development of activated slags provides a potential alternative. Using sulfates, the binder is ettringite which binds up to 5 molecules of water compared to the C-S-H of OPC systems where only 1 is bound. These systems which include calcium sulphoaluminate and supersulphated cements are slow to develop initial strength but continue to hydrate, eventually forming a dense impermeable matrix. Preliminary leaching studies show they are comparable to dense OPC based systems and may provide the answer to handling the high water content sludges.

Session 3

Overview of Nexia Solutions

Graham Fairhall

Nexia Solutions provides nuclear R&D and technical services to a wide range of UK customers across the fuel cycle. It has a technical capability which includes fuel manufacture, reactors, fuel recycle, waste management and disposal. Nexia has a long history having been formed from R&D departments within BNFL and has experience of developing fuel cycle supporting Magnox, AGR and LWR reactors as well as advanced systems such as Generation IV.

In October 2006 the UK Government announced their intention to establish a UK National Nuclear Laboratory founded out of Nexia Solutions and utilising the British Technology Centre. Work is still ongoing to finalise the scope and detail of the NNL although an announcement on the way forward is imminent.

PhD research into integrated uncertainty modelling (also poster)

Andrew Hagues

AMCG group, Imperial College

In recent years there has been a growing interest within the engineering community in modelling uncertainties associated with a wide range of problems. Traditionally the only way to analyse uncertainties is to run a simulation many times with varying the uncertain parameter e.g. boundary and initial conditions. This is very computationally expansive and the focus is now on being able to model uncertainties explicitly. Working with AMCG group staff Dr Eaton and Prof Pain, the aim of this project is to produce a fully 3D adaptive-stochastic finite element model that is capable of capturing multiple uncertainties in fluid properties and boundary conditions of the flows inside a nuclear reactor. Here we present some of the theory behind modelling uncertainties and the methods that will be used during the course of this project. Additionally examples will be shown of some classical problems where the models currently being developed could be applied such a Rayleigh-Bernard convection problem and flow past a bluff body.

Interactions of droplets with hot surfaces Modelling and Experiments

D. Chatzikiriakou

In some postulated PWR accidents, water droplets entrained in steam will flow through the core and will be the main means available for core cooling. As a droplet approaches a hot surface (the overheated fuel rod in this case), under certain conditions, a vapour layer can be formed by evaporation from the droplet. This layer acts like a cushion and can prevent direct contact between the droplet and the hot surface (Leidefrost phenomenon). Rather than hitting and wetting the surface, the droplet rebounds from the surface after a short 'near-contact' time, driven by its

elasticity due to surface tension. As a result, the hot surface cannot be wetted and the heat transfer from the hot surface to the impinging drop is rather poor. This project is addressing these topics, by a combination of modelling and experiment. The interaction of water droplets with a hot fuel rod is being studied computationally. The hydrodynamic behaviour of the droplet during the impact with the hot wall (the deformation process) and the heat transfer mechanism during the impingement are the main focus of a series of numerical calculations. Simulations of a single evaporating droplet approaching a hot wall, in the presence of superheated steam, are being performed with a finite volume solution of the Navier-Stokes equations for incompressible viscous fluid flow. The one-fluid formulation is employed, with the 'level set' method used for the tracking of the interface between the two phases. A series of forthcoming experiments is aiming to measure the amount of heat removed by the water droplet during its impact with the hot solid surface. These will employ infra-red thermography to measure wall temperature variation over the O (100 μm) region throughout the O (1ms) duration of the interaction. The dependence of that heat transfer on parameters such as the droplet velocity size will be investigated.

Corroded Magnox sludge and plutonium waste cementation

S.A. Parry and F.R. Livens

Corroded Magnox sludge waste

Corrosion of spent Magnox fuel rods in water filled storage ponds has produced magnesium-rich sludges contaminated with fuel and fission products. We have experimentally investigated the composition and evolution of an inactive corroded Magnox sludge (CMS) simulant.

Our characterisation of the sludge using infrared spectroscopy, X-ray diffraction, and environmental scanning electron microscopy (ESEM) has determined that CMS is mainly composed of brucite, $Mg(OH)_2$, and additionally artinite, $Mg_2CO_3(OH)_2.3H_2O$.

Plutonium association with CMS

Pu adsorption onto CMS colloids may provide a mechanism to enhance Pu mobility. Therefore, we have determined the associative behaviour of plutonium in solution with CMS in a model storage pond/ effluent treatment system.

The addition of carbonate to the system had the largest influence over Pu solubility, allowing >90% of the Pu to pass through a filter membrane. The presence of CMS, and polyelectrolyte increased Pu filter hold-up. Silica at 1 ppm produced no observable effect. Solution pH was also found to influence Pu filterability. Over the pH 7 to 11.5 range examined, more Pu was held up on the filter at higher pH.

Cementation of Pu contaminated CMS

For long-term storage it is intended that the CMS waste be immobilised in a cementitious wasteform. Therefore, our research has continued to examine CMS evolution, and we have begun to examine the microstructure of ordinary Portland cement (OPC) based samples. Our samples doped with CMS, Zr, U (and later Pu) have been analysed using SEM and EMPA to establish the phases present and with which phases the Zr and actinide elements associate.

Refined Large Eddy Simulation for reactor thermal-hydraulics studies

Yacine Addad, Stephano Rolfo (presented by D. Laurence)

Large Eddy Simulation (LES), whereby the larger turbulent structures are resolved and only smaller ones modelled, provides a much richer collection of results (e.g. time series, spectra), than the Reynolds Averaged Navier Stokes (RANS) approach, and this level of detail is now required in many industrial problems, e.g. thermal fatigue, aero-acoustics, and turbulence induced fluid-structure coupling. In wall resolved LES (WR-LES) the mesh is such that all boundary layer structures are computed as in Direct Numerical Simulation, and WR-LES are now used in addition to, or even in place of experiments. WR-LES previously confined to small Reynolds numbers when using structured grids (since spacing in the near-wall layer must capture Kolmogorov scales), can now be applied to higher Reynolds numbers thanks to extensive use of local refinement with unstructured grids. As highlighted by previous applications of LES to more complex configurations, present WR-LES also shows that adequate design of the mesh is a most important condition for a trustworthy simulation. Some guidelines for optimal usage of unstructured mesh features for WR-LES will be highlighted, as well as an application to mixed convection in piping systems.

Supporting research – towards a KNOO CFD benchmarking activity – contribution from FLUIDITY (also poster)

Matthew D. Piggott

AMCG Group Imperial College

I am a Research Council funded Fellow whose work helps underpin KNOO. FLUIDITY is a state-of-the-art CFD model which has been developed by the AMCG group at Imperial College London for the past 15 years. It is based upon flexible finite element discretisation methods on unstructured meshes which are able to accurately conform to complex geometries. Some of FLUIDITY's most important capabilities stem from its use of in-house adaptive mesh techniques, including topological mesh operations and mesh movement, which seek to optimise the accuracy and efficiency of an entire simulation. To enable efficient calculations on large parallel computational platforms load-balanced domain decomposition algorithms are used in tandem with mesh adaptivity. A suite of advanced discretisation options are available, as are a range of newly developed LES turbulence models which act as natural partners to the highly variable and anisotropic numerical resolutions possible with unstructured adaptive meshes. In this presentation the adaptive mesh technology and error measures will be reviewed, as will discretisation and LES options. With any new modelling technology validation, verification and benchmarking are of paramount importance and these will form the focus of this presentation.

Session 4

The Current Generation of Nuclear Power Stations

Bob Ainsworth

British Energy

British Energy is the largest UK electricity generator and generates around one fifth of the UK electricity supply. It operates 8 nuclear power stations with a capacity of 8,800MW and one coal-fired station with a capacity of 1,940MW. Total annual output of electricity has been about 59-74TWh over the past five years with a typical nuclear contribution of about 60,000 million kWh/year.

British Energy is a major UK company employing approximately 6000 staff with a turnover of £3billion in 2006/07. Nuclear generation plays a key role in reducing CO_2 emissions: the complete life-cycle CO_2 emissions for Torness nuclear power station have been estimated as 5.05g/kWh, compared with operational emissions of 900g/kWh for a typical coal-fired plant and 400g/kWh for a typical gas-fired plant.

Increased wholesale prices in the UK electricity market in recent years have made investment in new plant of all types more attractive, and this includes new nuclear build. The increases also make life extension of existing plant more attractive enabling investment in existing plant and in research.

Computer Simulation Of Helium Gas Bubbles In Uranium Dioxide

David Parfitt, Robin Grimes

Imperial College London

Helium is formed in nuclear fuel as a product of the alpha-decay of actinides during long-term storage and normal operation. The high heat of solution of this helium drives the precipitation of the atoms into gas bubbles; these act as reservoirs, absorbing helium from the lattice, and through thermal and radiation-enhanced resolution, returning it back to the lattice. Understanding the effect of these bubbles upon the thermal and mechanical properties of uranium dioxide is important for safe and economical storage and operation.

Here we present molecular dynamics simulations of helium gas bubbles and their interaction with displacement cascades within the uranium dioxide lattice. A simple two-body effective potential has been used to successfully model the dynamics of several different bubbles sizes and morphologies with a range of internal gas pressures. The interaction of these bubbles with recoil cascades, representative of radiation damage due to alpha-decay and nuclear fission, has been examined with initial recoil energies of up to 30 keV.

We propose several new mechanisms here that will significantly impact upon models of the gas resolution rate and the mobility of bubbles in uranium dioxide. In particular, the combination of re-absorption of helium into the disordered regions of the lattice and the transfer of uranium and oxygen atoms across the bubble will lead to the net migration of these bubbles along any anisotropy in the radiation field.

Ultrasonic crack monitoring using SH waves in extreme and inaccessible environments

Frederic Cegla

The development of SH waveguide probes that can work under extreme conditions (Temperature>500°C, radiation) has opened up the possibility to carry out ultrasonic monitoring using SH waves on plant components that cannot be expected otherwise. The deployment of such monitoring devices can results in substantial economic benefit by continuously supplying information about the state of a critical plant component rather than only at periods of shut down, which can be years apart.

This paper presents two different crack size monitoring techniques using SH waves and highlights their advantages and disadvantages. The method of time of flight diffraction (TOFD) that uses the diffracted signal from the crack tip is analysed for cracks on the near and far side of the specimen relative to the probes. In the other method used to estimate crack size the amplitude drop of the received wave between two receiving probes due to shielding of the incoming wave by the crack is used. Theoretical and experimental results are presented.

Towards multiscale fully coupled modelling of innovative reactors

Christopher C. Pain and Jefferson L.M.A. Gomes

AMCG Group, Imperial College London

As part of the WP4 of the KNOO programme, the AMCG at Imperial College London is investigating possible accidents scenarios in innovative reactors in order to ensure passive safety. GIF has selected GFR and VHTR as one of the possible designs for the forth generation of nuclear reactors which may be commissioned by 2040. There is a general UK interest in the 'virtual' or 'numerical' nuclear reactor. In the design of such reactors, the main focus are: passive safety, reliability and economic sustainibility. As part of the WP4, we have developed a coupled neutron-radiation and multiphase flow model to ensure that these objetives may be achieved. The integrated neutrons/fluids method embodied in the Finite Element Transient Criticality (FETCH) model has been successfully validated in a number of applications including transient criticality experiments. The neutronics model in FETCH solves the neutron Boltzmann transport equation in full phase-space (space, time, angle and speed travel) using a variational finite element approach based on the second order even parity equations. The computational multifluid dynamics model is a high-resolution multi-phase compressible flow model which solves the conservation equations for both fluids and solid phases. Fully integrated turbulence models (based on 4th order Smagorinsky LES), mesh adaptivity, shock-capturing schemes, material interface tracking and domain decomposition parallel computing technologies have been incorporated into FETCH in order to investigate detailed dynamics in complex geometries. The approach is being extended to coupled structural effects. This numerically robust technology has incorporated several submodels that may allow us to successfully model multiscale physics from detailed turbulent heat transfer and flow dynamics in individual channels to whole core reactor. In addition, we are collaborating with stakeholders to integrate FETCH with a 1-D whole circuit model, which may help the full understanding faulty accident scenarios.

Supporting research - integration of innovative reactor physics/radiation transport methods into transient modelling

Matthew Eaton

AMCG group Imperial College London

I work on advanced deterministic radiation transport methods and coupled nuclear/thermo-fluid methods for nuclear criticality, reactor physics, shielding and dosimetry and my work helps underpin the KNOO research and training in the AMCG group. I have recently been awarded a Royal Academy of Engineering Fellowship to lead the UK in developing coupled methods for uncertainty propagation within complex engineering, multi-scale, multi-physics simulations. This research will cover applications to CFD, to radiation transport and to coupled transient modelling. The novel numerical methods that characterise the new radiation transport methodology embodied in the numerical framework RADIANT will be described. This new numerical radiation framework which is optimally robust across all radiation regimes, uniquely able to deal with arbitrary angular discretisation methods and utilises the latest hierarchical solution methods is currently being integrated into the "virtual" numerical reactor framework FETCH. This will lead to greater levels of realism in reactor physics modelling yielding new insights into the behaviour of generation four nuclear reactors such as the VHTR and GFR concepts.

Buoyancy effects on turbulence in VHTR channels

Stefano Rolfo, Amir Keshmiri, M. Cotton

Ascending and descending vertical turbulent flows occur in the cores of currently operating gas-cooled reactors of the Magnox and Advanced Gas-Cooled Reactor (AGR) types. Under post-trip conditions, the heat loading may be relatively high in relation to the flow rate, and the thermal hydraulic regime is one of combined forced-and-free, or ‘mixed’ convection. Significant impairment or enhancement of heat transfer can occur, depending upon the flow orientation (upward or downward) and the degree of buoyancy influence. In the present work, which uses an in-house code, ‘CONVERT’, different low-Reynolds number turbulence models are employed. These include the Launder-Sharma k model, the Non-Linear Eddy-Viscosity Model of Suga, and the Strain Parameter model (k S) of Cotton and Ismael. The flow geometry consists of a long vertical pipe that is heated uniformly, and a wide range of buoyancy influence is examined. The model results have been compared with ‘Direct Numerical Simulation’ data and significant variations in model performance have been found. Moreover, in order to check the accuracy of the numerical implementation of the models, the same cases have been tested using industrial and commercial CFD packages, ‘Code_Saturne’ and ‘Star-CD’, respectively. While the Cotton-Ismael model is not available in these codes, other turbulence models including the k omega and v2f formulations have also been examined and compared to the Direct Numerical Simulation data of You et al. I. J. of Heat and Mass Transfer, 46 (2003). In numerical terms, CONVERT is a parabolic ‘marching’ code, while both Saturne and Star-CD employ cyclic boundary conditions.

Session 5

Mark Cheeseman

Rolls-Royce Marine

Rolls-Royce, a world-leading provider of power systems and services for use on land, at sea and in the air, operates in four global markets - civil aerospace, defence aerospace, marine and energy. In the Marine sector, the Company has a primary focus on power, propulsion and motion control solutions, serving over 2,000 customers and has equipment installed on 20,000 commercial and naval vessels operating around the world.

The Rolls-Royce Submarines business is the pioneer of one of the most important technological advances in naval propulsion - the use of nuclear propulsion for the Royal Navy's submarine flotilla. As the UK Technical Authority for the Nuclear Steam Raising Plant, Rolls-Royce manages a team of over 1,000 engineers delivering all aspects of the plant design, safety, manufacture, performance and through life support. This role is undertaken in close co-operation with the Ministry of Defence to achieve maximum benefits to the submarine programme - improving affordability, reliability, availability and sustainability.

Multi-pin Coupled Reflood Model

B. Belhouachi, D. Morico

Realistic analysis of a large break loss of coolant accident (LOCA) requires modelling complex phenomena such as a coupled study of the 3-D transient two phase reflood flow, and the mechanical response of the fuel. These last two processes are coupled. The deformations of the pins change the coolant flow passages, and this changing of the cooling conditions modifies the subsequent mechanical response of the pins. This feedback needs to be incorporated into both the thermofluids and the structural/thermal mechanics models.

In this framework, a literature review of the main experimental programs related to Fuel Behaviour under LOCA conditions (conducted from the seventies until now) is being performed. The first part covers aspects of clad ballooning and burst and resulting flow blockage, including burst-induced fuel relocation. The second part is devoted to the question of the coolability of blocked regions in a rod bundle after ballooning in a LOCA. Clad oxidation, resistance to quench and post quench loads and safety criteria are discussed in a third part.

In this paper, main results from the first and second part are presented here; we will discuss the thermal hydraulic calculations performed with the USNRC TRACE code for the analysis of the ACHILLES experiment. ACHILLES is a single-rod LOCA test which has been carried out at AEA Technology Winfrith.

The comparison and combination of conclusions drawn from the ACHILLES experiment results and system simulation studies were used to improve our understanding of the physical phenomena governing the behaviour of a partially blocked rod array.

Towards a Mechanistic Understanding of Atmospheric Stress Corrosion Cracking (AISCC) in Austenitic Stainless Steels

A. B. Cook, S Lyon and A H Sherry

Materials Performance Centre, Materials Performance Centre, University of Manchester

Intermediate level waste (ILW) containers consist of components fabricated from both AISI 316L and AISI 304L austenitic stainless steel (ASS). Such materials are employed because they display suitable structural characteristics, and generally excellent resistance towards both atmospheric corrosion and the highly alkaline conditions found in cement-based encapsulants. This said however, all grades of ASS are susceptible, to a greater or lesser degree, to localized corrosion; i.e. pitting/crevice corrosion and associated phenomena such as stress corrosion cracking (SCC). The choice of ASS is based largely upon the assumption that the threat posed to the integrity of the ILW container by such processes during service lifetime (>200 years) is minimal. However, ASS have recently been shown to be susceptible to atmospheric-induced stress corrosion cracking (AISCC), a sparsely studied phenomenon that occurs under certain combinations of sea-salt deposition, temperature and relative humidity (RH). In this project we seek to address the impact, if any, of AISCC on ILW materials by quantifying the key issues that lead to its initiation and propagation. The ultimate goal is to construct a model to predict AISCC susceptibility over long timescales. In this presentation, and associated poster, we discuss the progress to date, particularly research associated with the development of novel experimental techniques for studying localized corrosion.

Internal strain measurement in graphite

David Smith,

Solid Mechanics Research Group,

University of Bristol

This talk provides details of a new development in the measurement of internal strain in graphite. Internal strain is measured using the deep hole drilling (DHD) where a reference hole is drilled into the material. In-situ measurement of internal strain is extremely difficult particularly down AGR graphite bricks. The purpose of our research is to undertake laboratory trials on graphite subjected to known applied strains. Rectangular graphite beams with high and low levels of porosity where subjected to four point bending. Strain gauges adhered to the beams, were used to measure the strain distribution through the beam. The distortion of the through thickness reference hole was measured and compared with surface strains. The measured distortions were very similar to the surface strains for the graphite beams with low porosity. For high porosity graphite larger errors were found although the overall trends were similar.

Deformation characteristics of Zircaloy-4

O. Zanellato, M.E. Fitzpatrick, L. Edwards

Zircaloy-4 is commonly used for nuclear applications such as fuel cladding tubes or reactor vessels. Like most Zirconium alloys, it combines a small neutron cross section with good mechanical properties and corrosion resistance. However its crystal structure is hexagonal close packed below 800°C and thus shows a strong thermal and mechanical anisotropy [1]. This can give rise to misfits between grains in the material which can lead to failure after thermal and/or mechanical cycling.

This work is mainly the result of neutron diffraction experiments carried out on a hot rolled Zircaloy-4 plate. It was aimed at measuring and understanding the orientation dependent behaviour of the crystal and of the bulk material. Several compression tests were performed in-situ in the neutron beam using the ENGIN-X diffractometer at the UK's ISIS pulsed neutron source. For each load increment the interatomic distances for families of grains with a given orientation (reflections) were measured using the neutron diffraction technique [2][3]. The strain evolution for various crystal reflections was monitored.

As expected it was found that some grains were bearing much more load than others. The resulting intergranular elastic strains could reach up to 5000 microstrain at the end of the tests and were responsible for high type II (intergranular) residual stresses after unloading. Considering the macroscopic behaviour, the direction normal to the plate had better mechanical properties than the other two processing directions.

The strong crystallographic texture (measured separately by electron backscatter diffraction (EBSD)) suggests that the crystal anisotropy has been transferred to a macroscopic level.

[1] K. Linga Murty and Indrajit Charit, *Texture development and anisotropic deformation of zircaloys*, Progress in Nuclear Energy, Volume 48, Issue 4, May 2006, p. 325-359

[2] M.E. Fitzpatrick, A. Lodini, *Analysis of Residual Stress by Diffraction Using Neutron and Synchrotron Radiation*, Taylor and Francis, 2003

[3] E.C. Oliver, M.R. Daymond, P.J. Withers, *Effects of Texture and Anisotropy on Intergranular Stress Development in Zirconium*, Materials Science Forum 495-497, p.1553-1558

Session 6

Overview of AWE

Gary Burnell

The presentation offers a brief general overview of AWE based upon its mission to deliver the UK's requirements for nuclear warheads and support for national security, and its vision to be internationally recognized for scientific, technical and business excellence.

Heat Transfer and Fluid Dynamic Processes in PWR Reflood

Caroline M. D. Masson, Yiyun Jessy Zeng,

In the case of a Loss-of-Coolant Accident inside a pressurised water nuclear reactor, four main phases take place, namely blowdown, refill, reflood and long term cooling. We are here mainly interested in the reflood phase, where water droplets are entrained in the vapour flow and contribute greatly to fuel cooling before it is quenched. Due to a rapid change in pressure, the fuel rod claddings are likely to balloon and it is important to know how this ballooning would divert the two-phase flow. The vapour flow will necessarily be diverted by the balloons, but it is yet unknown if the droplets would follow, or if their greater density would cause them to carry on and wet the balloons. These projects comprise experiments and computational modelling addressing these questions. An experiment will be carried out to visualise the macroscopic flow and droplets diversions using essentially a Particle Image Velocimetry system. The results collected will be coupled with Computational Fluid Dynamics calculations in order to validate the data obtained. The transient two-phase flow CFD studies are computed with the CFD code STAR-CD. The studies of the cooling of the fuel rods by means of droplets-wall heat transfer will be following these investigations.

Modelling and Simulation of Single-Phase and Particle-Laden Impinging Flows and Flows in Straight Ducts

Mike Fairweather and Jun Yao

Institute of Particle Science and Engineering, School of Process, Environmental and Materials Engineering, University of Leeds

Work underway on the Reynolds-averaged Navier-Stokes (RANS) modelling and large eddy simulation (LES) of single-phase and particle-laden two-phase flows will be described. Two flow geometries are considered. The first is the impingement of a jet on a flat plate, of relevance to applications of impinging flows in the nuclear industry where they are used to prevent the settling of solid particles in waste storage tanks, and to re-suspend particles that form a bed, prior to waste processing and long term storage. The second is flows within ducts, of direct relevance to waste transport and processing, which will be extended to circular pipe flows at a later date. For the impinging flow case, reasonable agreement between the RANS and LES approaches, and available data, will be demonstrated, although the requirement for further reliable data sets is identified. Preliminary results for the LES of duct flows, with and without particles, will also be described, and the potential of LES demonstrated in terms of its ability to yield high quality turbulent flow field predictions, and to predict the deposition and re-suspension of particles within the flow. Comparison with data will also be provided. Finally, future developments and links to ongoing experimental programmes will be discussed.

PhD research into coupled fault modelling for GFR

Jason Dunstall

AMCG Group Imperial College London

The Gas-cooled Fast Reactor (GFR) is one of the six innovative reactor systems selected by the Generation IV International Forum (GIF) for R&D work as part of the Generation IV programme. Under the selection criteria, the GFR is ranked top for sustainability, and rated good for safety, economics, non-proliferation and physical resistance. In order to analyse proposed GFR designs and model transient safety performance under accident conditions, the coupled radiation-fluids finite element code FETCH will be used. Developed by the AMCG group at Imperial College, FETCH allows asymmetrical, three dimensional transient modelling of scenarios such as control rod movement, depressurisation and structural faults, as applied to GFR. A overview of the reference GFR designs and the modelling of GFR using FETCH will be given, along with examples of the use of FETCH in analysing the Dragon Reactor Experiment for method validation.

PhD research on coupled fault modelling for HTR/ VHTR

Brendan Tollit

AMCG Group Imperial College London

The VHTR is designed to push the boundaries and capabilities of existing HTGR technology to higher levels, challenging the desired inherent and passive safety mechanisms. The VHTR design will represent an evolutionary step from existing HTGR designs, such as the PBMR and GT-MHR. To ascertain the viability of the VHTR design requires a detailed understanding of the complex multi-physics dynamics within the core.The Finite Element and Transient Criticality (FETCH) code developed by C. Pain et. al. is a coupled multi-physics (Neutronic, CFD /Multiphase) code based on FEM. It has a variety of applications including 3D within vessel reactor transient studies – and is being extended to include structural impacts. As part of KNOO WP4 a range of models within FETCH are being developed to simulate various svariey evere accidents and faults for generic VHTR/GCFR designs (to ascertain temperature and flux profiles). These include cylindrical RZ, 1/6th 3D and full 3D models to capture asymmetric effects. Accidents that will be modelled include fast reactivity initiated accidents (such as control rod ejection), passive decay heat removal capabilities and water/steam ingress.

Posters

Development of the RADIANT radiation transport/reactor physics code.

Andrew Buchan and colleagues

AMCG group, Imperial College London

The RADIANT code has been developed at Imperial College in order to address accuracy and robustness limitations of current codes. Simulating the transport of neutral particles can often lead to a vast array of problems when numerical techniques are used to discretise the 7-dimensional phase space of the Boltzmann transport equation. Typical problems encountered can range from unphysical oscillations forming within the solution, caused by both Gibbs oscillations and ray-effects, to the computational resource limits due to the huge matrices generated by the discretisation process. The code already has adjoint and forward options. Three other aspects are presented. The first is the finite element (FE) Streamline Upwind Petrov Galerkin method (SUPG) which is designed to provide stable solutions across all material regimes (from transparent to opaque material cross-sections). In addition to this a Riemann method for satisfying bare surface boundary conditions is given. This is particularly important as the method allows any arbitrary angular approximation scheme to be used. Finally a new spherical wavelet method that enables adaptive anisotropic resolution to be applied to the angular phase-space is presented. A numerical example of a shielding problem using these numerical methods is given. We show that a stable solution that is fully converged in the angular domain can be obtained efficiently using the adaptive wavelet approximations. This results in matrices that are significantly reduced in size, therefore placing minimal strain on computational resources.

Modelling SCC in Corrosion-Resistant Materials

Yi Zhang, A. Jivkov, A. Sherry and J. Marrow

Intergranular stress corrosion cracking (IGSCC) of irradiated austenitic steels is accompanied by compositional changes due to radiation-induced segregation at grain boundaries, and this may be responsible for decreased resistance to cracking. The degree of resistance depends on the structure of the grain boundary. This project is using experimental analysis and finite element modelling to address: (i) irradiation-assisted SCC (IA-SCC) of core internal materials in high temperature water and (ii) atmospheric-induced stress corrosion cracking (AI-SCC) of ILW container material under intermittent chloride supply. This poster presents the implementation of a three-dimensional model for intergranular crack propagation to the nucleation, growth and coalescence of cracks.

Interactions of droplets with hot solid surfaces

D. Chatzikiriakou, S P Walker, G F Hewitt

The initial stages of the modelling and experimentation on droplet interactions with hot surfaces are presented. The series of experiments scheduled to begin soon are aiming to reveal the spatial and temporal variation of the temperature of a hot solid due to its interaction with a tiny (order of microns), near-saturation water droplet, by employing an infrared spectroscopic method. The time of the interaction is expected to be of the order of msecs and the variation in temperature of the order of a few degrees. This will enable us to determine the local heat transfer coefficient that

characterises the phenomenon and associate it with the droplet size, the droplet impingement velocity, the temperature of the hot surface as well as the degree of subcooling of the droplet. Preliminary experiments using the infrared spectroscopic method for the observation of the interaction of cold water droplets with a beyond Leidenfrost temperature solid surface show encouraging results as the vapour layer preventing direct contact of the droplet with the solid is observable and the temperature drop throughout the solid is measurable. Numerical experiments with FE commercial software are also being conducted in order to provide information regarding the optimisation of the experimental setup. In the numerical modelling field, under-millimetric droplets sustained by a vapour cushion are simulated. Those droplets, called sessile, unlike larger droplets, can be considered to be evaporating uniformly from their whole surface, as already shown by previous experimental work. The computed vapour layer thicknesses show considerable agreement with experimental data. These initial-stage simulations are employing a finite volume code solving the Navier-Stokes equations for incompressible viscous fluid flow. The onefluid formulation is used and the Level Set method is employed for the tracking of the

interface between the two phases.

Alexander Theodosiou

Cardiff University

AGR reactor grade graphite is bombarded with inert gas ions, under UHV, in an attempt to disrupt the molecular lattice and generate stored, Wigner-like energy. The prescence of stored energy is detected through differential scanning calorimetry (DSC).

Bristol University Wireless Sensor Node

Neville McNeill

Department of Electrical Engineering, University of Bristol

The design and development of a remote sensing node for monitoring quantities such as temperature, corrosion and strain is presented. Principal features are that system is to be low-cost, autonomous, have high life expectancy and be able to withstand harsh environments, particularly high temperatures. The IEEE 802.15.4 wireless communications standard is used and the power management scheme used to energise the transmitter at the sensing node is described. Particular challenges in this application include the efficient management of energy at very low power levels and voltages, and also circuit design for high temperatures. Energy may be supplied from storage elements (batteries, capacitors or by mechanical means) or derived from the ambient environment (solar cells, thermoelectric elements). A configurable hardware arrangement for evaluating these alternative schemes is presented with preliminary results.

Internal strain measurement in graphite and glass

Soheil Nakhodchi

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Graphite and glass has been used widely in the nuclear industry. Graphite is used as a moderator, reflector and structural component in power plants, whilst, glass mostly is used in immobilization of high level radioactive wastes (HLW). The level of the internal stresses/strains in these structures has a critical role in their structural integrity. In this study, the feasibility of using the deep hole drilling (DHD) technique to measure internal stresses/strains in graphite is investigated and applicability of the technique on glass is under exploration.

Finite element (FE) analysis was carried out in order to evaluate the capability of the deep hole drilling method to measure thermal stress/strain distributions in AGR graphite bricks. The simulation was applied to a hollow cylinder subjected to a thermal gradient thus introducing thermal (or secondary) stresses. Effects of the changing the material properties (E) in the cylinder and influence of the variation of Young’s modulus through the wall thickness was investigated. The results show that the DHD method can be used to determine internal stresses.

Laboratory experiments were carried out on PGA graphite, parallel and perpendicular to brick axis, and PG25 porous graphite. Graphite beams were subjected to the known loads and the DHD method applied to measure applied stresses through the depth of the beams. The measured linear stress distribution agrees well with the applied stresses.

Factors in the Disposal of Spent Gen IV VHTR Fuel Containing Zirconium Carbide

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Imperial College London, Department of Materials

Zirconium carbide (ZrC) has been proposed as a component in advanced nuclear fuels for the Generation IV Very High Temperature Reactor (VHTR). Specifically, ZrC is an important fission product retention layer in tri-structural isotropic (TRISO) coated fuel particles and would replace the less refractory silicon carbide layer currently used in TRISO. However, plans for final disposition of spent TRISO fuel are undecided, with direct disposal or vitrification under consideration. Retention of fission products by the ceramic layers and minimising the volume of waste are important considerations. Also, the effects of a ZrC component in TRISO on the properties of the spent fuel must be studied to enable sound decisions on safe disposal of a fuel with novel composition and properties. This work will discuss computational and experimental methods of investigating thermal, mechanical, and thermodynamic properties affecting ZrC behaviour in VHTR fuel.

Study of Residual Stress Field in a Stainless Steel Bead-on-Plate (BOP) Simulation Benchmark Sample

S. Ganguly, M. E. Fitzpatrick, L. Edwards

Dept. of Materials Engineering, The Open University

Welds in reactor pressure vessels and the surrounding heat exchangers are one of the primary sources of structural integrity problems in nuclear power plant. Improved understanding is needed of the residual stresses around welds, and how they can be modelled accurately. Welded joints are often the regions most likely to contain fabrication defects or cracks that initiate and grow during service. Welding also introduces complex residual stress field, which has profound influence on the in-service life of critical engineering components. Simplified fracture assessment procedures usually assume a representative stress profile along a line through the wall thickness, however, these lead to very conservative results. Recently finite element (FE) based approach of weld residual stress simulation was allowed for more realistic profiles, however, the simulation results are to be supported by detailed residual stress measurement.

The experiment presented here was aimed to characterise the 3-dimensional residual stress field generated due to deposition of a single weld bead on a rectangular stainless steel plate. The work carried out forms a part of an international round robin exercise of parallel measurement and simulation in order to develop a residual stress validation benchmark. A single weld bead deposited on a plate will create a strongly varying three-dimensional residual stress field and have many characteristics of a repaired weld. The experimental work reported was carried out at SALSA, the strain scanner at the ILL neutron source, France. A monochromatic wavelength of ~1.5 Å was used to measure the lattice spacing of the {311} family of crystallographic planes. A stress-free reference was measured by measuring 3 cubes each of dimension 3×3×3 mm^3 in all the principal directions. The calculated principal strains were then compared with the measurements carried out at a spallation neutron source, to provide validation of the data obtained.

Turbulent natural convection between horizontal coaxial cylinders

Y. Addad, D. Laurence, M. Rabbitt

In several Advanced Gas-Cooled Reactors (AGRs), boiler penetrations run horizontally through the thickness of the reactor pressure vessel. At the bottom and top of the boilers, the penetrations contain tubes that carry water and steam respectively into and out of the boilers. In both cases the tubes are colder than the ambient pressurised carbon dioxide gas. The number of tubes within the penetrations ranges from three to 44, and tube size varies significantly. The gas flows within the penetrations are generally long range thermosyphons, driven by temperature differences. The rate of heat transfer of the thermosyphons crucially governs how far into the penetrations a thermosyphons might reach. The turbulence model used to calculate the gas flows is a vital component of the predictions, however, the accuracy of current predictions is not well quantified. Thus, the work described in this study has been undertaken to help define a suitable RANS turbulence model for use in calculations of such flows which are driven by temperature differences in horizontal penetrations. For the purpose of validation studies natural convection in “infinite” annular cavities is considered. This permits the use of periodic conditions in the pipe-axis direction for LES computations and also 2D simulations with Reynolds Averaged Navier Stokes (RANS) models.

The negatively buoyant wall-jet: LES results

Y. Addad, S. Benhamadouche, D. Laurence

The results of a Large-Eddy Simulation (LES) of a downward hot wall-jet injected against a cold upward channel flow are presented. Based on an experiment of He et al. [Int. J. Heat Fluid Flow 23 (2002) 487], this flow was suggested as an ‘‘application challenge’’ to the Qnet-CFD EU network by the industrial power generation sector. Indeed, numerical predictions vary significantly with the type of RANS model used, with only the most advanced models yielding reasonable agreement with the experiment: see the paper by Craft et al. [Int. J. Heat Fluid Flow 25 (2004) 809]. The present LES was undertaken to confirm and complete the experimental data, which in some areas can be sparse. Computational resources limited the LES simulation to 1/2 million nodes, and an optimal LES mesh was defined from RANS-derived scales. Then, to reduce uncertainties, two independent codes were used to perform the simulations: the commercial code *Star-CD* and the industrial program, *Code_Saturne*. Statistical quantities are compared with experimental data and show that both codes are able to return fairly satisfactory results for isothermal and moderately buoyant cases.

Application of the $\overline{v^2}-f$ turbulence model to forced, mixed and natural convection

J.C. Uribe, F. Billard and S. Rolfo

Previous applications of the $\overline{v^2}-f$ model to both academic and industrial test cases revealed that this model is quite superior to corresponding Reynolds Averaged Navier Stokes (RANS) 2-equation based models, this being the case in particular for heat transfer calculations. The model stems from a standard 2-equation k-espilon model, but instead of using damping functions as in many other low-Reynolds-number RANS models, an extra transport equation is solved for the wall-normal fluctuations, $\overline{v^2}$. An elliptic equation for the f variable enables one to take into account non-local effects due to the pressure/strain-rate correlation. The main drawback of this model is its numerical instability, especially in segregated solvers. Here, a new formulation of the $\overline{v^2}-f$ model is implemented in an industrial unstructured finite volume code with the aim of resolving this stability problem. Initial comparisons with the standard and highly popular k-espilon model and the k-omega SST model were made for three different test cases and revealed promising results. In fact, the predictions of the $\overline{v^2}-f$ model are in better agreement with DNS and experimental data for the cases carried out, namely: channel flow at Re*=395, the Betts Cavity at Ra = 0.86 10**6, and vertical pipe flow at Re = 2650 and Gr/Re**2 = 0, 0.063, 0.087, 0.241, 0.400 (Re and Gr being based on pipe radius and bulk velocity).