SKC

Svenskt Kärntekniskt Centrum

Årsredogörelse

2003

Årsredogörelse 2003

SVENSKT KÄRNTEKNISKT CENTRUM

Allmänt

Statens Kärnkraftinspektion, Westinghouse Atom AB, Forsmark Kraft AB, Ringhals AB, OKG AB samt Barsebäck Kraft AB har beslutat samarbeta i syfte att stödja kärnteknisk verksamhet vid svenska högskolor. Dessa parter har slutit avtal om att fr o m 2002-01-01 bilda ett fristående samarbetsorgan, Svenskt Kärntekniskt Centrum (SKC). Stödet ges dels i form av basfinansiering till professorer och lektorer i grundläggande kärntekniska ämnen vid KTH, Chalmers och Uppsala Universitet och dels, liksom tidigare, i form av finansiering av doktorandprojekt med deltagande från svenska högskolor. Basfinansieringen regleras av särskilda avtal med respektive högskola.

Fr o m 2002 finns också nya kärntekniska kompetenscentra vid KTH (CEKERT) och Chalmers (CKTC). Dessa skall lokalt samordna högskolans grundutbildning och forskning i kärntekniska ämnen. SKC arbetar i nära kontakt med dessa centra, bl a genom att SKC föreståndare är medlem i styrelsen för respektive centrum.

SKC verksamhet har under året i huvudsak omfattat initiering, finansiering och uppföljning av forskningsprojekt samt åtgärder för rekrytering av teknologer och civilingenjörer. SKC har också givit ekonomiskt stöd till teknologers och doktoranders studieresor.

Tre nya forskningsprojekt (se nedan) initierades under året.

Fem styrelsesammanträden har hållits under året varav ett per capsulam. Styrelsens ledamöter, med mandat fram till 2004-12-31 framgår av *bilaga 1.* Ordförande har varit Bertil Dihné, VD Vattenfall Bränsle AB och föreståndare professor Tomas Lefvert, Elproduktion,Vattenfall Norden.

Forskningsprojekt

En förteckning över de forskningsprojekt som fick SKC stöd under 2003 återfinns i *bilaga 2*. Dessa projekt presenteras närmare i *bilaga 3*. Under året har stöd till tre nya forskningsprojekt beviljats av SKC styrelse enligt följande:

- "Positronteknik för analys av strålskador och mikroporositet i material", professor Imre Pázsit, Reaktorfysik, Chalmers
- ”Measurements and analysis of dry-out and film thickness in a tube with various power distributions”, adj.prof Wiktor Frid, Reaktorteknologi, KTH
- "Modelling of radiation damage in FeCr alloys." Doc. Jan Wallenius, Reaktorfysik, KTH

Två doktorsexamina avlades under året:

- Tim Lundström, Chemical Physics LiU, Radiation chemistry of aqeous solutions related to nuclear reactor systems and spent fuel management
- Martin Kroon, Hållfasthetslära KTH, Probabilistic and micromechanical modelling of cleavage fracture

Två studenter har avlagt teknologie licentiat examen:

- Rosa Pérez-Jerlerud, Materialvetenskap KTH, Thermodynamic database for zirconium alloys
- Per Seltborg, Reaktorfysik KTH, External source effects and neutronics in accelerator-driven systems

Forskar- och vidareutbildning

Fyra svenska studenter deltog i Eugene Wigner Course on Reactor Physics (5p). Deetta är en ny, europeisk kurs i regi av ENEN där studenterna bl a gör laborationer vid forskningsreaktorer i Wien, Budapest och Prag. I KSU-kursen i kärnkraftteknologi deltog under året sammanlagt 5 studenter.

Grundutbildning

Forskarskolans studierektor deltog i arbetet med den ansökan till EU som inlämnades och godkändes under 2003 beträffande European Master i Nuclear Engineering.
Bidrag har lämnats för kursutveckling vid Energiteknik, KTH i mätning av tvåfasflöde.

Information om Centrets verksamhet

SKC deltog som huvudsponsor i årets ARMADA vid KTH tillsammans med CEKERT. Hemsidan har vidareutvecklats. Ett pris för bästa examens- och doktorandarbete vid svensk högskola/universitet har instiftats och kommer att utdelas fr o m 2004.

Stöd till tjänster

Ersättning har utgått till KTH, Chalmers och Uppsala Universitet enligt avtal för stöd till professurer och lektorat. Medel har utbetalats även fast vissa tjänster ej var besatta. Dessa medel har använts dels till vikariatersättning , dels till satsningar inom grundutbildningen. En del av

dessa medel användes också för att finansiera en gästprofessur (deltid) vid Energiteknik, KTH.

Stöd har lämnats för anställning av en post-doc under två år på Reaktorfysik, KTH.

Ekonomi

Kostnaderna under 2003 blev ca 16.8 MSEK.

Övrigt

Styrelsen har under året diskuterat ny strategi med mer fokusering regionalt och vad beträffar ämnesområden för den forskning som SKC stödjer. Mer preciserad strategi formuleras fr o m 2004.

Svenskt Kärntekniskt Centrum i april 2004

Bertil Dihné
Ordförande

Bilagor

1. SKC styrelse under 2003
2. Förteckning över forskningsprojekt som stöds av SKC
3. Presentation av pågående projekt

Svenskt Kärntekniskt Centrum

Styrelseledamöter 2003-01-01--2003-12-31

Ordinarie:

Ordförande	**Bertil Dihné**	Vattenfall Bränsle AB
	Gustaf Löwenhielm	SKI
	Per-Göran Nilsson	Forsmarks Kraftgrupp AB
	Björn Gustafsson / Anders Helmersson	OKG AB
	Leif Johansson	Ringhals AB
	Agneta Wellmar	Barsebäck Kraft AB
	Nils-Olov Jonsson	Westinghouse Electric Sweden

Suppleanter:

	Oddbjörn Sandervåg	SKI
	Thord Rooth	Forsmarks Kraftgrupp AB
	Peter Jonsson	OKG AB
	Eva Telg	Barsebäck Kraft AB
	Stig Andersson	Westinghouse Electric Sweden

Adjungerade:

Professor	**Bo Höistad**	Inst. för Strålningsvetenskap Uppsala Universitet
Professor	**Waclaw Gudowski**	Reaktorfysik KTH / AlbaNova
Professor	**Imre Pázsit**	Reaktorfysik Chalmers Tekniska Högskola

Forskningsprojekt Svenskt Kärntekniskt Centrum 2003

Kat.	Projekt	Institution / avdeln. Projektledare	Lic/doktorand	Examina
	KTH - Kungliga Tekniska Högskolan i Stockholm			
RF	Investigation of Neutron Source Effects in Sub-Critical Media	Reaktorfysik Prof. Wacek Gudowski	Per Seltborg	Tekn.lic. sep-03
MV	Termodynamisk databas för zirkoniumlegeringar	Termodyn. modellering Prof. Bo Sundman	Rosa Pérez-Jerlerud	Tekn.lic. mar-03
HL	Mikromekanisk modellering av klyvbrott	Hållfasthetslära Univ.lekt Jonas Faleskog	Martin Kroon	Tekn.dr. sep-03
RT	Mechanistic Modelling of Dry-Out in Fuel Assemblies	Reaktorteknologi Adj.prof. Wiktor Frid	Mattias Hemlin, Vattenfall Bränsle	
RS	Distribution av vätgas och ånga under reaktorhaverier,med fokus på stratifi-ering och kondensationseffekter	Reaktorteknologi Adj.prof. Wiktor Frid	Kristofer Karkoszka	
HL	Detection of Stress-Corrosion Cracks by means of Non-Linear Scattering of Ultrasonic Waves	Wallenberglab. PhD Claudio Pecorari	Milan Poznic´	
RT-7	Measurements and Analysis of Dryout and Film Thickness in a Tube with Various Axial Power Distributions	Reaktorteknologi Adj.prof. Wiktor Frid	Carl Adamsson Westinghouse	
	CTH - Chalmers Tekniska Högskola			
RF	Avancerade analysmetoder för icke-stationära härdprocesser	Reaktorfysik Prof. Imre Pàzsit	Carl Sunde	
RF	Utveckling av Cf-252 metoden för reaktivitetsmätning under härdladdning	Reaktorfysik Prof. Imre Pàzsit	JohannnaWright	
RT	Use of intelligent computing methods fo flow measurements and 2-phase flow diagnostics	Reaktorfysik Prof. Imre Pàzsit	Håkan Mattsson	

MV	Positronteknik för analys av strålskador och mikroporositet i material	Reaktorfysik Doc Anders Nordlund	Elisabeth Tengborn	
	GU - Göteborgs Universitet			
KE	In-Situ bestämning av oxidationskinetiken för Zircaloy mha impedansspektroskopi	Oorganisk kemi Prof. Elisabet Ahlberg	Ulf Andersson	
	LiU - Linköpings Universitet			
KE	Utbildning av doktorand i strålningskemi, radiolys av vatten vid hög temperatur m.m.	Fysik och mätteknik Prof. Anders Lund	Tim Lundström	Fil.dr. sep-03
	Malmö Högskola			
HL	Modelling of intergranular stress corrosion cracking	Hållfasthetslära Prof. Per Ståhle	Andrey Jivkov post-doc	Fil.dr. dec-02
	Mälardalens Högskola			
MTO	Projekt ORCCA	Adj.prof Carl Rollenhagen	Irene Eriksson	

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Kategoribeteckningarna har följande innebörd:

RF	Reaktorfysik
RT	Reaktorteknologi
RS	Reaktorsäkerhet
MV	Materialvetenskap
HL	Hållfasthetslära
CS	Reglerteknik
MTO	Människa-Teknik-Organisation
KE	Kemi

Presentation av SKC projekt under 2003

Electrochemical Impedance Spectroscopy as a tool for *In-situ* determination of the oxidation kinetics for Zircaloy.

Research leader: Professor Elisabet Ahlberg, Scientist: Ulf Andersson
Department of Chemistry, Electrochemistry, Göteborg university

Introduction

Development of new or modified fuel cladding materials is a continuous task for the nuclear industry and the performance of these materials needs to be characterised. Also, utilization of nuclear fuel to a higher degree of burn-up entails new problems regarding the performance of the existing cladding materials. Consequently, methods for quantification of oxide growth under reactor conditions are desired. One such method is Electrochemical Impedance Spectroscopy (EIS).

The general aim of this project is to determine the most important parameters responsible for the oxidation and hydration of zirconium alloys under nuclear reactor conditions. In order to do this EIS is used to follow the oxidation process in real time and to determine electric and ionic properties of the growing oxide. The physical interpretation of experimental data is complicated by the complex nature of the process and different models are utilised for analysis, taking into account also electron and mass transfer in porous media.-

This project is running in collaboration with Stefan Forsberg at Studsvik Nuclear AB.

Reference group for this project

Karen Gott, SKI, Magnus Limbäck, Westinghouse Atom, Pål Efsing, Barsebäck Kraft AB, Lars Björnkvist, Vattenfall bränsle, Lotta Nystrand, Studsvik, Gunnar Lysell, Studsvik

Methodology

Three different Zircaloy materials are investigated at 160, 225 and 280ºC in an autoclave system, simulated PWR environment, see Figure 1.

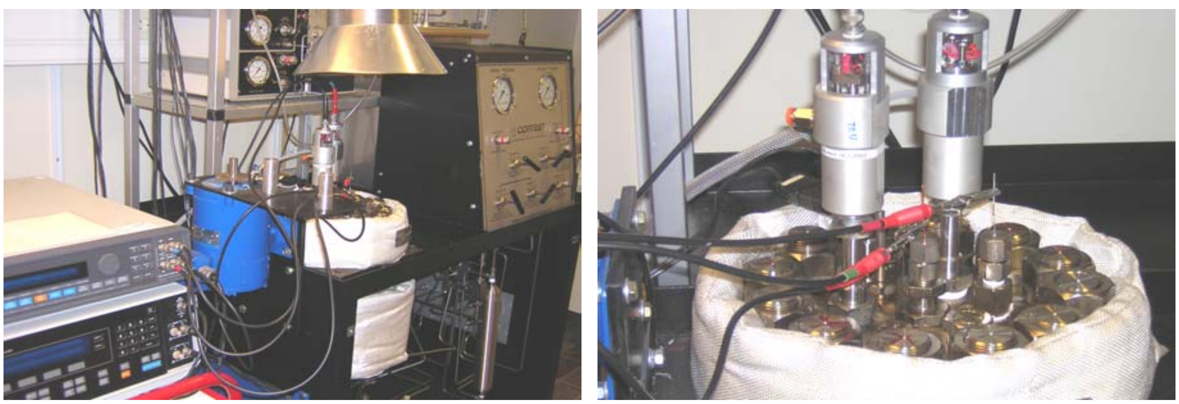


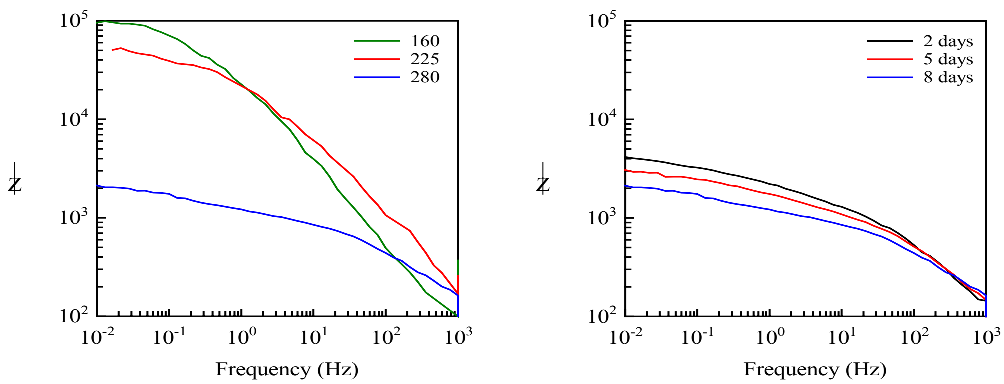
Figure 1. The autoclave system with the potentiostat and frequency response analyser in the left figure. The right figure shows the cell lid with the mounted electrodes.

Impedance spectra are sampled over a wide range of frequencies and the oxide growth is measured as a function of time. For the oxidised samples the electric properties are investigated by measuring the impedance as a function of potential, giving information on the concentration of charge carriers and the flat band potential of the zirconium oxide formed.

The influence of alloy composition and water chemistry is investigated and also irradiated samples will be investigated primarily with emphasis on the electric properties of the oxide

Results

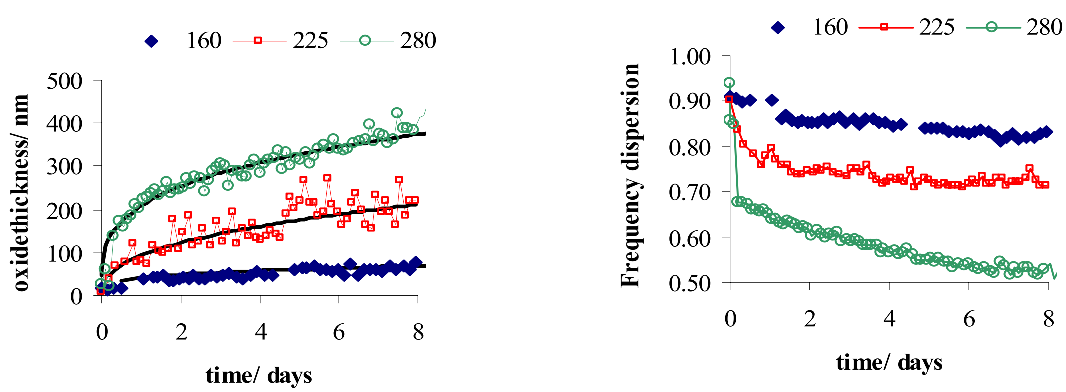
Analysis of the impedance spectroscopy data show that the oxide growth rate can be followed, *in-situ,* in a simulated PWR environment. The oxide resistance decreases when the temperature increases as seen in the Bode plot in Figure 2a. The oxide resistance decreases also as a function of exposure time in the autoclave, Figure 2b.



a) **b)**

Figure 2. Bode plots from one of the investigated materials. Increasing the temperature decreases the oxide resistance as seen in figure a (solution resistance subtracted). Figure 2b shows decreasing oxide resistance with time at 280°C (solution resistance subtracted).

The oxide growth follows a cubic growth law [1] independent of material composition. At increasing temperature the frequency dispersion increases in all investigated materials.



a) **b)**

Figure 3. a) Oxide growth curves follow cubic growth law. b)The frequency dispersion increases with increased temperature.

At room temperature, after the autoclave testing, the oxide thickness is determined by FIB/SEM, showing good agreement with the oxide thickness obtained from the impedance measurements. The information on charge carrier concentration in the oxide is still under discussion and also the electric properties of irradiated samples.

References

1. Göhr, H., et al. Long-term in situ corrosion investigation of Zr alloys in simulated PWR environment by electrochemical measurements. Zirconium in the Nuclear Industry: Eleventh International Symposium. 1996, p. 181-201.

Detection of Stress-Corrosion Cracks by Means of Nonlinear Scattering of Ultrasonic Waves

Research leader: Doc. Claudio Pecorari, Scientist: Milan Poznic´, Marcus Wallenberg Laboratory, KTH

Background

Conventional ultrasonic methods currently used to inspect components of nuclear power plants have shown serious difficulties in detecting stress-corrosion cracks, especially in the early stages of their development, and when such defects are imbedded in a medium with coarse microstructure. There are two main reasons behind this fact. The first one is the partial crack's closure caused by the removal of the tensile stresses that are responsible for the crack's growth, during inspection. The second reason is the inappropriate use of the probing waves which do not exploit the mode conversion of an incident SV wave into an evanescent longitudinal wave at the surface containing the crack. Indeed, in isotropic materials, it is customary using SV wave at 45 degree incidence or higher, instead of angles of incidence closer to the critical angle for longitudinal waves.

Objectives

This project has been set up to investigate the potential of nonlinear scattering phenomena as a new tool to detect and localize stress-corrosion cracks in components of nuclear power plants. In particular, the development of a realistic theoretical framework to investigate the magnitude of the second harmonic's generation upon scattering of both surface and shear waves, as well as to optimize the experimental configuration used during inspection has been given high priority. The validation of the theoretical predictions on both interfaces between rough surfaces in contact and on real fatigue cracks constitutes the overall objective of experimental part.

This research project provides also an important educational opportunity in the field of Ultrasonics and Nondestructive Evaluation by means of ultrasonic waves.

Results in 2003

Parametric studies conducted with a newly developed model predicting the linear and nonlinear scattering of both surface and bulk waves from a surface-breaking crack with faces in partial contact have lead, among the others, to

i. upper estimates of the generation of the second harmonic component (up to -20 dB below the amplitude of the incident wave (see Fig. 1)),
ii. the spatial distribution of both the fundamental and second harmonic, and
iii. the optimization of the experimental set-up with respect to the generation and detection of the second harmonic.

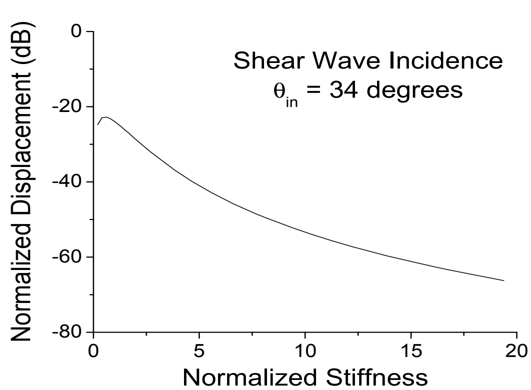


Figure 1: Horizontal displacement of the second harmonics versus the stiffness of the partially closed crack

In the course of this investigation, we confirmed that the current inspection practices, which prescribe the use of SV waves at 45 degree incidence in isotropic materials, can and should be improved substantially. As explained in a research proposal recently submitted to SKI, SJ, and to the British Safety and Standard Board, both theoretically and with the aid of preliminary experimental results, a configuration in which a SV wave impinges upon the cracked surface at an angle just above the critical angle for the longitudinal wave displays a sensitivity that is at least 10 dB higher than that achieved today with the current technique (Fig. 2).

On the experimental front, effort has been made on the optimization of currently the available set-up configuration. In particular, the abatement of the signal generated by the instrumentation at twice the fundamental frequency from an original level of -40 dB below the fundamental to a new value of -60 dB generation has been achieved. With this improvement, the second harmonic wave generated by an interface between rough surfaces in contact has been measured as a function of the externally applied load during both loading and unloading. Figure 2 illustrates sample results obtained on a steel-steel interface. Note the considerable level (nearly 20 dB above the background noise) of the second harmonic wave generated by the nonlinear interface. Several options are under consideration in order to further improve the signal-to-noise ratio.

Personnel and Collaborations

The project is lead by Claudio Pecorari, a Docent in Ultrasonics at the Marcus Wallenberg Laboratory, KTH. Pecorari is supported for 80 percent of his time by SKI. In this project, C. P. also supervises Milan Poznić, who is working towards a PhD degree in Technical Acoustics at the same institution. Poznić is supported by SKC for 80 percent of his time. SKC has also provided financial support for the acquisition of the relevant instrumentation to carry out this research.

Reference Group

The following are the members of the reference group supervising this project: Lars Skånberg, Peter Merck (SKI), Bengt Bengtsson (OKG), Claes Sandelin (Ringhals and Barsebäck), Alf Jonsson (Forsmark). The representative from Westinghouse is still to be named.

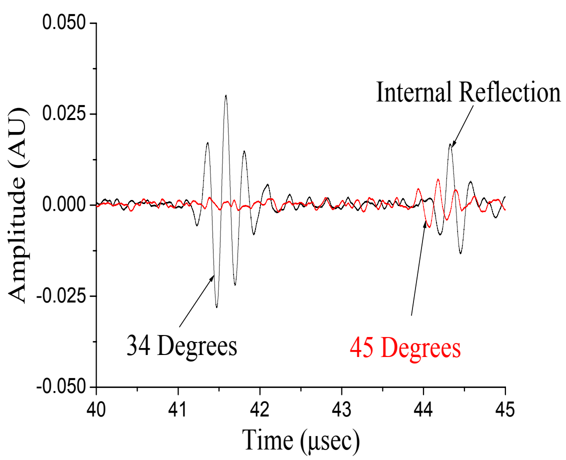


Figure 1. Linear signals backscattered by a surface-breaking defect with depth of 0.3 mm.
-----: SV incidence at 34degrees;
-----: SV incidence at 45 degrees.
The signal marked as 'Internal Reflection' is an artifact.

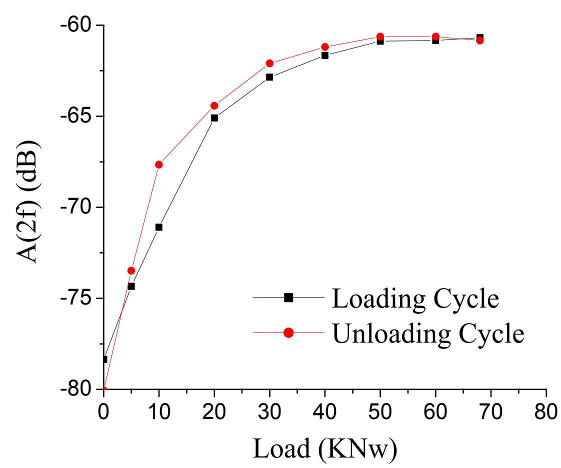


Figure 2. Second harmonic component (f = 10 MHz) generated by two rough steel surfaces in contact as a function of the load applied to the interface. The signal was measured in reflection mode using the emitting transducer working at the nominal frequency of 5 MHz

Radiation Chemistry in Nuclear Technology

Research leaders Hilbert Christensen Studsvik Nuclear, Professor Anders Lund, Dept. of Physics and Measurement Technology, University of Linköping, Scientist Tim Lundström Studsvik Nuclear

The specific aim of this project has been to educate a Ph. D. student in Radiation Chemistry relevant to Nuclear Technology. In a wider perspective the aim has been to contribute to maintaining competence within the nuclear industry of Sweden.

The project started Sept.1, 1998 with the employment of the Ph. D. student Tim Lundström and ended successfully Sept. 30, 2003. Sept. 15, 2003 Tim Lundström defended his Thesis: "Radiation Chemistry of Aqueous Solutions Related to Nuclear Reactor Systems and Spent Fuel Management" (1) at the Department of Physics and Measurement Technology, Biology and Chemistry at Linköping´s University. The faculty opponent was Mats Jonsson, Royal Institute of Stockholm. Tim Lundström was employed by Linköping´s University with Anders Lund as his professor. The work was carried out mainly in Studsvik with Hilbert Christensen as his tutor.

The project was sponsored by the Swedish Center for Nuclear Technology (SKC), Svensk Kärnbränslehantering (SKB) and Studsvik Nuclear AB. The effective study time was 4 years but the total time was extended to 5 years due to teaching at Linköping´s University and project work at Studsvik Nuclear. The progress of the work was continuously followed by a special reference group with members from all Swedish nuclear power plants, Westinghouse Atom, SKB, SKT and the Swedish Nuclear Power Inspectorate(SKI). The reference group met twice every year.

The main interest for Radiation Chemistry within the Nuclear Technology is in the following two areas:

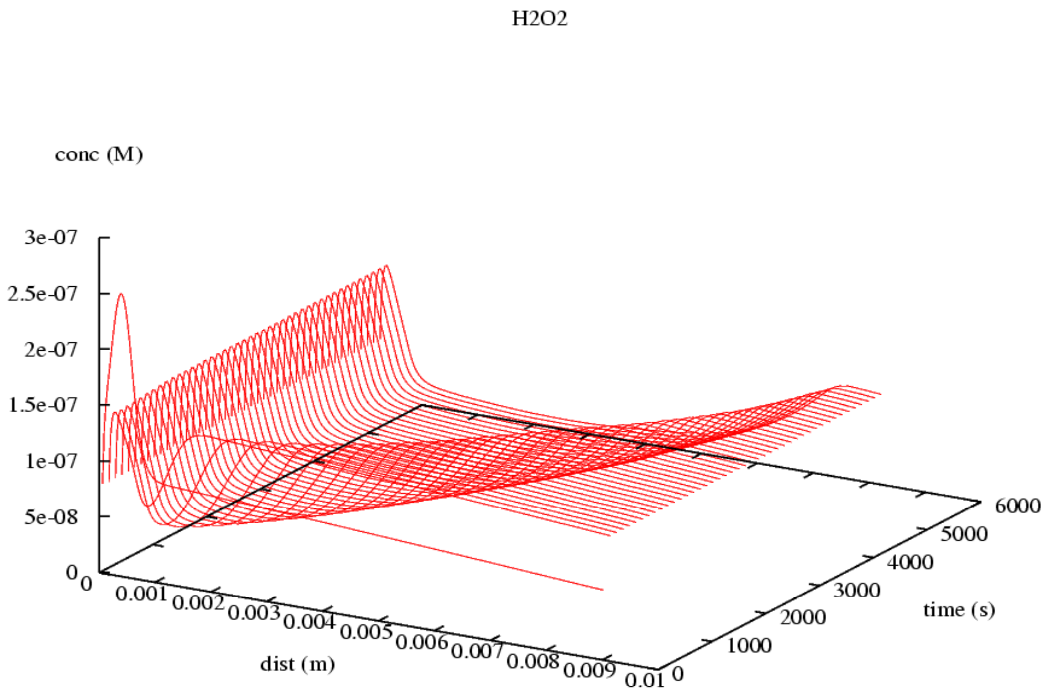
1. Radiation Chemistry in connection with the operation of Nuclear Power Reactors.

2. Radiation Chemistry in connection with the storage of High-Level-Waste (HLW).

In both cases the work was concentrated on radiolysis of water and aqueous solutions.

The first part of the study was concentrated on determination of rate constants at high temperatures for reactions which are important for the radiolysis in the coolant of a power reactor. The experiments were carried out at the Danish National Research Laboratory at Risö in cooperation with Knud Sehested. Solutions were irradiated at various temperature in a special high-temperature, high-pressure cell, made of a high-purity synthetic quartz (inner cell) and stainless steel (outer cell). The cell was irradiated with 10 MeV electrons from a linear accelerator.

The second part related to the storage of HLW was carried out in cooperation with Bernd Grambow at Ecole des Mines de Nantes during a one year stay cthere. During his stay there, Tim Lundström developed a model for calculation of oxidation and dissolution of spent fuel caused by water radiolysis products. A previously developed radiolysis model was improved by introduction of simultaneous transport and radiolysis. The water was divided into an arbitrary number of small compartments and the time was divided into an arbitrary number of time steps. A radiolysis calculation was then carried out in each compartment for each time step. The model allows for combination of three different radiation types with different LET (Linear Energy Transfer). This study is under publication (4).



Variation of the concentration of H2O2 with the distance from a UO2-pellet and with time. Data calculated with TraRaMo.

References.

1. T. Lundström, Radiation chemistry of aqueous solutions related to nuclear reactor systems and spent fuel management, Linköping Studies in Science and Technology, Dissertation No 840, Linköping´s University 2003.
2. T. Lundström, H. Christensen and K. Sehested, The reaction of hydrogen atoms with hydrogen peroxide as a function of temperature, Rad. Phys. Chem. 2001, 61, p 109-113.
3. T. Lundström, H. Christensen and K. Sehested, The reaction of OH with H at elevated temperatures, Rad. Phys. Chem. 2002, 64, p 29-33.
4. T. Lundström, H Christensen and K. Sehested, Reactions of the HO2 radical with OH, H, Fe(2+) and Cu(2+), Radiation Physics and Chemistry, 69, (2004), 211-216
5. T. Lundström, H. Christensen and B. Grambow, A combined transport and radiolysis model, to be published in Nucl. Technol.

Advanced analysis methods for non-stationary processes in reactor cores

Research Leaders Professor Imre Pázsit, Department of Reactor Physics, Chalmers University of Technology, Göteborg, Docent Ninos Garis, Swedish Nuclear Power Inspectorate, Stockholm, Scientist Carl Sunde, Department of Reactor Physics, Chalmers University of Technology, Göteborg

1. Background

Diagnostics of reactor cores with noise methods is usually performed with FFT based spectral analysis, such as auto and cross spectral power densities. Such an analysis nevertheless makes an implicit use of the fact that the system is stationary, at least during the measurement period on which the spectral analysis is made. In other words the status of the system is assumed to be unchanged over several tens of thousends of the periods of the characteristic frequencies of the system.

Neverheless, the system status often changes during a much shorter period. Such non-stationary processes and even transients are in fact quite common in reactor systems. Examples are the occurrence and development of local and global core instabilities in BWRs, the short-term changes of vibration properties (core-barrel, fuel assembly etc) in PWRs, and the various phenomena in two-phase flow (vortex shedding, slug flow etc). Apart from temporal transients, spatial transients or non-stationarities may also occur, such as in the spatial structure of two-phase flow.

Spectral analysis is, by definition, unable to handle and diagnose such processes. However, powerful mathematical methods have been developed and applied lately for the analysis of such processes, out of which wavelet analysis is one of the most promising.

2. Goals

The purpose of the project is to introduce the use of analysis methods of non-stationary processes, and primarily wavelet analysis, into the noise diagnostic work of our Department and to explore their possibilities for diagnosing non-stationary processes. We expect to elaborate new methods for understanding the mechanism, and even predicting or early detection of the occurrence and intermittence of non-stationary processes and instabilities, and to elaborate reliable methods of parameter estimation under non-stationary circumstances. The methods will be tested on measurements taken in Swedish power plants.

3. Organisation

The reactor diagnostic group is headed by Prof. Imre Pázsit, who is also the leader of this SKC – supported PhD project. During 2003 he was assisted by Dr. Christophe Demaziere, and until August 2003 by Dr. Vasiliy Arzhanov, who worked together with the PhD student, Carl Sunde, on several aspects of the project. There is one more PhD student working in the field of reactor diagnostics and noise analysis, Johanna Wright. Also her project is supported by SKC. In the last three months of 2003 we had a visiting postdoc form Tuzla, Bosnia, Dr. Senada Avdic, who worked primarily on safeguard questions but also did joint work with Kalle on a particular application of wavelet analysis.
The members of the reference group are: Pär Lansåker Forsmark, Henrik Eisenberg OKG, Henrik Nylen Barsebäck, Ninos Garis SKI, Johan Larsson Ringhals

Camilla Rotander, Westinghouse

4. Methodology

The methodology is similar to traditional noise analysis work, which consists of both evaluation of measurements, and elaborating models of the reactor and its processes to expedite the interpretation of the measurement analysis. Hence both theoretical model development and analysis of measurements is involved. In the analysis part, in contrast to the FFT tool, used in the traditional methods, continuous (CWT) or discrete fast wavelet transform (DWT) is used. Just as with FFT methods, there are software tools available for the fast CWT and DWT transforms, e.g. in Matlab, around which one can build his or her own analysis application packages.

One difference between spectral and wavelet methods is that with the latter, there are a very large number of waveforms available with a number of free parameters (e.g. the order of the filter). Finding the most effective transform for each application requires extensive investigations, often in an empirical way. The usage of the different functions (de-noising, multiresolution analysis) also has several options. Often the transform coefficients themselves have a significant diagnostic value, e.g. in case of pattern recognition, hence the application packages often need to be extended by adding own modules to solve a particular problem.

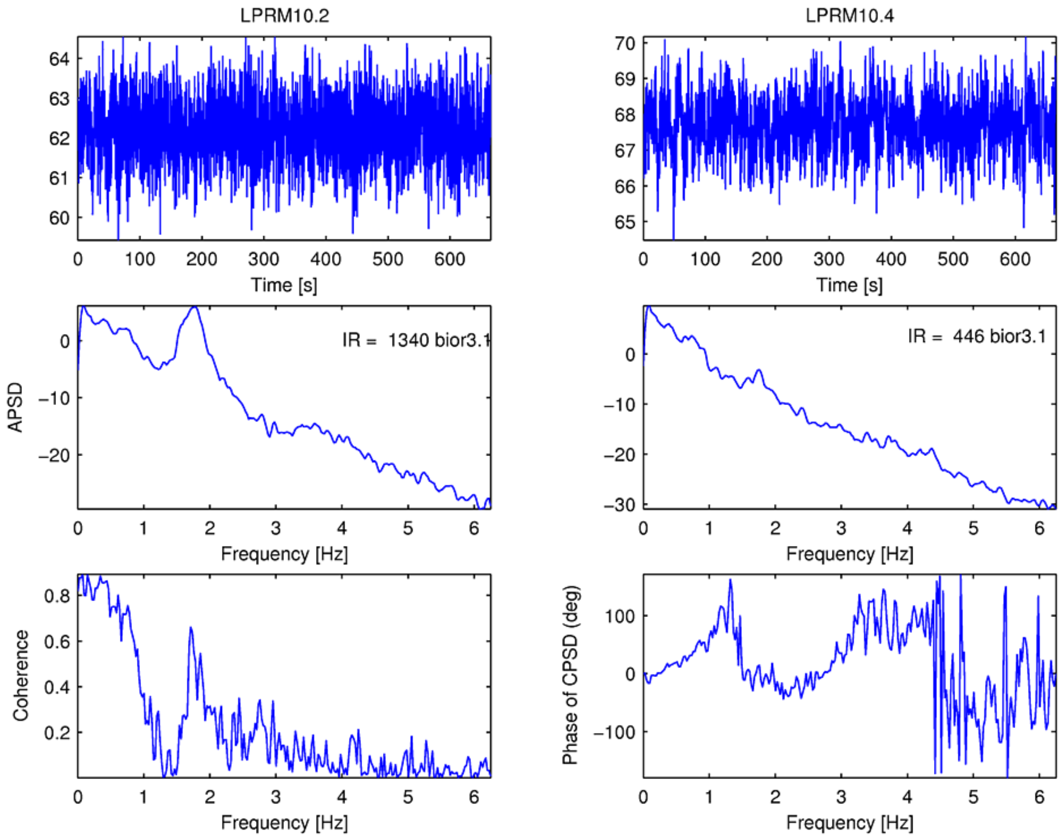


Fig 1 *LPRM signals from a detector string in Ringhals-1, which is suspected to vibrate and impact with the fuel assemblies (September 2002). The reasons for being suspicious of this string are the broad peak in the APSD and the high coherence and zero-phase at the same frequency. The IR number in the APSD plots is a so-called Impact Rate number, calculated with a wavelet method developed at the Department.*

5. Results-with focus on 2003

- a two-dimensional two-group model of core barrel vibrations was developed, and used for the interpretation of Ringhals measurements (Ref. [1]);
- analysis of measurements made in Ringhals-1 for the detection of detector string impacting with traditional and wavelet techniques (Ref. [2]])
- analysis of neutron radiography measurements for identification of two-phase flow by wavelet techniques and neural networks (Ref. [3]).

6. References

1. C. Sunde and V. Arzhanov, Calculation of the neutron noise induced by shell-mode core-barrel vibrations in a 1-D 2-group 2-region slab reactor. CTH-RF-173 (2003)

2. C. Demazière, C. Sunde, V. Arzhanov and I. Pázsit, Final Report on the Research Project Ringhals Diagnostics and Monitoring,Stage 8. CTH-RF-177 (2003)

3. C. Sunde and S. Avdic, Analysis of two-phase flow using soft computing methods. Manuscript, to be submitted. (2003)

Development of the Cf-252 method for reactivity measurements during core loading

Research Leader: Professor Imre Pázsit, Scientist: Johanna Wright, Department of Reactor Physics, Chalmers University of Technology, Göteborg

1. Background

Measurement and monitoring of reactivity during the loading of a power reactor has a clear safety relevance. The methods currently available for this purpose are not satisfactory. The question of monitoring reactivity has received inceased actuality in connection with a few recent incidents and accidents such as the criticality accident in Tokaimura in 1999, the erroneous loading of the French PWR Dampierre-4 in 2002, and lately the cooling accident in a fuel cleaning facility at Paks-2, Hungary. Methods of measuring reactivity in a subcritical system with a source are all based on the statistics of the subcritical chains, induced by the source neutrons. Such methods are the variance-to-mean or Feynman-alpha, the correlation or Rossi-alpha method, the source modulation and the break frequency method. The first two have been tested and used extensively at research and zero power reactors. None of the methods have been tested or used extensively at power reactors.

An alternative method was proposed some time ago by Mihalczo at Oak Ridge, which is based on the so-called Cf-252 method (Refs [1]-[3]). The essence is to use a Cf-252 neutron source, which is built together with an ionisation chamber (the Cf is put electrochemically on one of the plates of a parallel-plate ionisation chamber). Such an arrangement is called a "Cf-252 detector". The detector detects each spontaneous fission event, leading to neutron emission, through the ionised fission products, but without absorbing any neutron. Using two more ordinary neutron detectors in the system, and combining various auto- and cross-spectra between the CF-detector and the neutron detectors, the multiplication constant can be extracted in absolute values, without knowlegde of the delayed neutron fraction.

2. Goals

The purpose of the project is to get acquainted with the principles and the theory of the method, and develop it further. In the derivations of the formula used in the method that are found in the literature, several simplyfing assumptions are made. One objective of the project is to reduce the dependence of the method on these simplifiations. Comparison with experiments is possible, because our Dept will have access to such Cf-252 detectors. Test and study of other methods, such as the break frequency method, is also planned. The project will be performed in collaboration with CEA France, Nagoya University and KURRI (Japan), and KFKI Budapest. Other fluctuation-based reactivity measurement methods will also be investigated and developed further, partly in order to have alternative methods available, and partly because the formalism is similar for all methods. The understanding the importance and significance of the space-dependent effects due to the localised source is one important partial objective of the project.

3. Organisation

The reactor diagnostic group is headed by Prof. Imre Pázsit, who is also the leader of this SKC–supported PhD project. During 2003 he was assisted by Dr. Christophe Demaziere. There is another PhD student in noise diagnostics, Carl Sunde, whose project is also supported by SKC. The leader of the experimental activity at the Department is docent Anders Nordlund. There are two technicians who support the experimental part of the project.
The members of the reference group during 2003 were: Tell Andersson Ringhals, Ninos Garis SKI, Jan Hanberg Forsmark, Kjell Adielsson OKG, Marie Nilsson Westinghouse

4. Methodology

The methodology is based on the so-called master equation technique. The master equation (or Kolmogoroff-Chapman equation) is a balance equation for the temporal and spatial evolution of the probability distribution of the neutrons, neutron precursors and detector counts in a multiplying medium. From the master equation one can derive equations for the moments, out of which the first two, the mean and the variance are used, or some functions of those, such as temporal correlations or power spectra. An analytic expression of some measured quantity, such as the time dependence of the relative variance of the detector counts (Feynman-alpha) or the auto- and cross spectra of the detectors in the Cf-252 method, is then used for fitting the experimental data and extracting the reactivity (through the prompt neutron time constant).

5. Results so far

The theory of the deterministically pulsed Feynman alpha method was elaborated and the corresponding equations solved for both square and Gaussian-shaped pulses. A quantitative analysis of the dependence of the Feynman-alpha function on the pulse repetition frequency, the pulse width and the pulse shape was made. It was investigated both on simulated signals as well as real measurements how the method can be used for extracting the reactivity from pulsed Feynman-alpha measurements. It was seen that the reactivity could be determined with good accuracy (Ref. [1]). The results were presented at a project meeting of the 6th Framework EU-program MUSE.

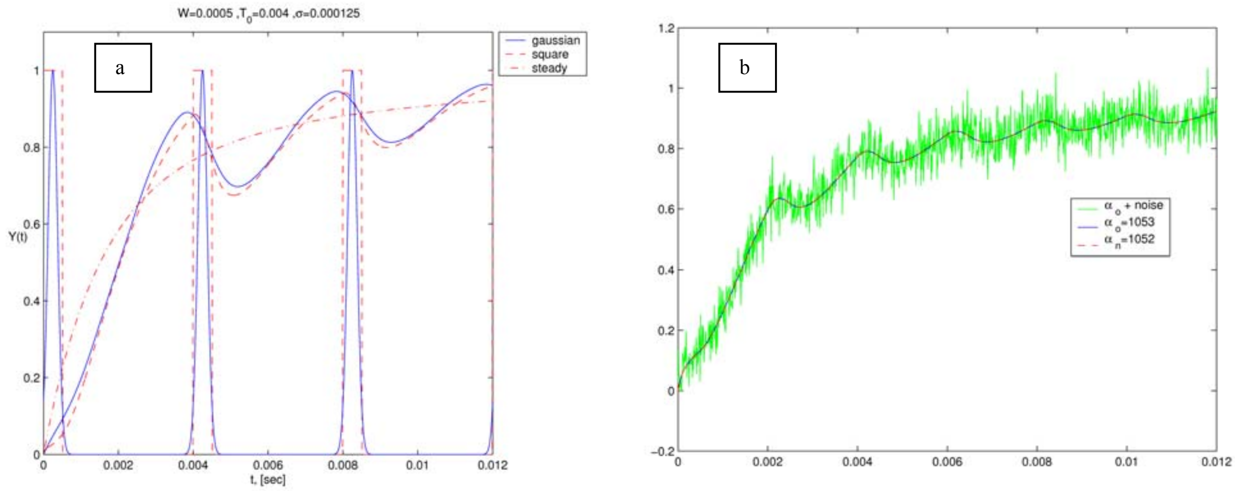


Fig. 1. Deterministically pulsed Feynman-Y curves. a): calculated curves for square and Gaussian-shaped pulses; b) a simulated experiment with added noise (green) and the result of the fitted curve (red). The true and unfolded alpha values are given in the box in the figure.

6. References

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Use of intelligent computing methods (”soft computing”)" for flow measurements and two-phase flow diagnostics

Research Leaders Professor Imre Pázsit, Docent Anders Nordlund, Scientist Håkan Mattsson, Department of Reactor Physics, Chalmers University of Technology, Göteborg

1. Background

The general goal of the project is to elaborate and use soft computing tools for novel methods of flow measurements. Correlation methods, in combination with neural network and other unfolding methods will be employed. The actual measurement data are produced with pulsed neutron activation, and the simulation data for the training of the network is produced by computational fluid dynamics (CFD) methods.

Pulsed Neutron Activation (PNA) is a method for activation of e.g. ^{16}O to^{16}N using neutron pulses from a neutron generator. In this way can radioactivity be produced at a suitable place in a water flow in a pipe. The signal from a detector downstream from the activation point can be used to make an accurate determination of the water flow.

The detector signal is measured as a function of time after the neutron pulse. One problem with the project is that extraction of data from this curve is not trivial. The main reason for the problems is thought to be that the activity in the pipe is not homogeneously distributed in the pipe. This, in combination with that there is a velocity profile in the pipe, will make the velocity of the activity change with the distance from the neutron generator. Another problem is that the velocity of the activity will not be the same as that of the water. These factors will affect the shape of the detector signal.

2. Goals

The objective of the project is the development and the use of intelligent computing methods ("soft computing") for flow measurements and two-phase flow diagnostics. Intelligent or soft computing is a terminology which refers to several new methods that have appeared in the area of signal analysis (neural networks, wavelets, fuzzy algorithms, neuro-fuzzy methods, fractal methods, genetic algorithms etc.). These methods open new possibilities of signal analysis and diagnostics, and they make improved and more effective applications possible.

The ultimate goal of the project is to develop a flowmeter that can measure the velocity of water in pipes.

3. Organisation

The Department of Reactor Physics is headed by Prof. Imre Pázsit, who is also the co-leader of this SKC–supported PhD project. The leader of the experimental activity at the Department is docent Anders Nordlund, and he is also the advisor of Håkan Mattsson.

The reference group is not yet complete. The person representing Halden is Davide Roverso. Further members so far are: Pär Lansåker Forsmark, Sven Andersson OKG, Ninos Garis SKI,
Nils Erik Nilsson Ringhals.

4. Methodology

The PNA method can be said to consist of four parts. activation of the water, transport and mixing of the activity, detection of the activity and analysis of experimental data. All of these four part have been studied within this project.

Monte Carlo calculation has been used to simulate the distribution of the acitvity in the pipe. These calculations were used as a starting point of CFD calculations where the transport and mixing of the activity in the pipe was investigated. The commercially availale CFD code FLUENT was used for these calculations. Monte Carlo calculations will be used to calculate the detector response from activity in different parts of the pipe. The results from these calculations will be used for a comparison of simulated and experimental data.

However, to make such a comparison, adequate treatment of the experimenal data must be made. The background in the experimental data has long been a problem since the origin of the background has not been known. A method was therefore developed which identifies the origin of the background as well as a method to subtract from the experimental data.

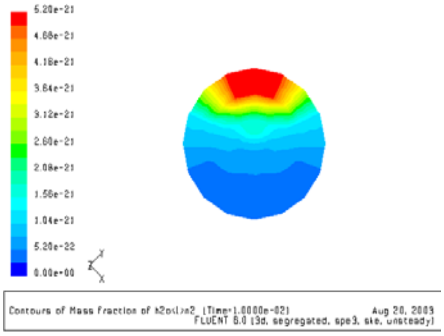

Figure 1: The initial distribution of activity as calculated from Monte Carlo simulations.

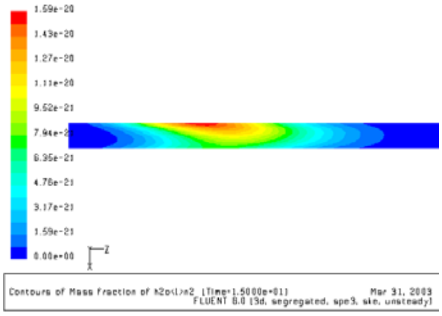

Figure 2: The activity distribution in a pipe calculated with a CFD code.

5. Results-with focus on 2003

- The origin of the background and a method to subtract it from experimental data has been developed [1]
- Simulation of the activity distribution after a neutron pulse using Monte Carlo calculations [2]
- The mixing of the activity with the water has been simulated with a CFD code [2]
- A Licentiate thesis has been written [3]

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Positron techniques for investigation of radiation damage in materials

Research Leader Docent Anders Nordlund, Scientist Elisabeth Tengborn, Department of Reactor Physics, Chalmers University of Technology, Göteborg

1. Background

Positron annihilation spectroscopy is a set of established techniques in the study of vacancy on open volume defects in materials. Due to its positive charge, the positrons can be trapped in such defects, resulting in a longer lifetime before annihilation. By measuring both the annihilation rate and the positron lifetime information about the defect concentration and type can be derived.
At the Department of Reactor Physics, Chalmers University of Technology, a beam with pulsed positron with variable energy is under construction. This will be one of only a few such facilities in the world. The pulsing of the positrons, in combination with a fast scintillator for annihilation gamma detection, enables direct lifetime measurements, while the variable energy of the beam facilitates depth scanning of material defects.

2. Goals

The objective of the project is the finalizing of the pulsed positron beam and the optimization of the beam parameters to achieve a measurement system well suited for positron lifetime spectroscopy in a wide range of materials. The PhD project will be much focussed on the properties of the beam and also on measurements on materials with different radiation induced vacancy concentration.

3. Organisation

The Department of Reactor Physics is headed by Prof. Imre Pázsit. The leader of the experimental activity at the Department is docent Anders Nordlund, and he is also the advisor of Elisabeth Tengborn.
Much of the beam construction is carried out in close collaboration with the University of Ghent, Belgium.

The reference group is not yet complete.

4. Methodology

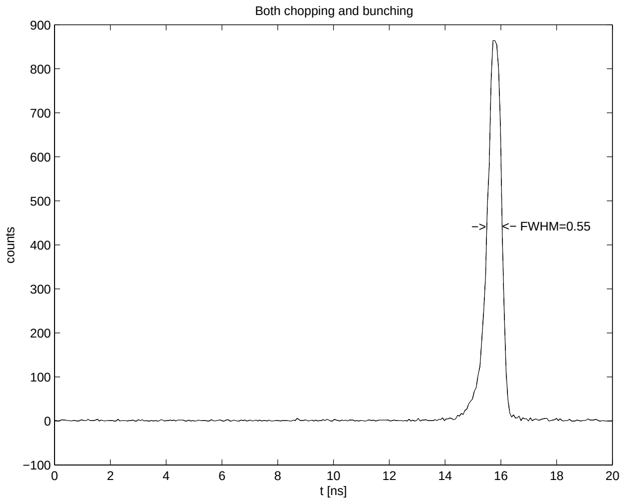
The development of the positron annihilation spectroscopy facility requires the following:

- Finalizing the physical beam by adding an acceleration stage and a sample chamber. This will be done in collaboration with Ghent University, Belgium.
- Optimizing the beam parameters such as parameters for pulsing (chopping, bunching systems), transmission (magnetic field, drift acceleration potential), main acceleration and detection system and data acquisition.
- Measurements on irradiated materials.
- Modelling and interpretation of results.

5. Results with focus on 2003

Since the project has only recently started (nov 2003), not many results have yet been produced. The beam is, with the exception of main acceleration stage and sample chamber, operational, and optimization of the chopper/buncher systems has so far resulted in a pulsed positron beam with a pulse width of about 0.5 ns.

The Department has also entered the EU-collaboration PERFECT, an integrated project within the sixth framework. This project regards irradiation damage effects in reactor components, mainly steel.



Left: The pulsed positron beam at Chalmers University of Technology. The positron timing is measured by a multi channel plate positioned at the end of the beam line, at the bottom of the picture. Right: Time spectrum recorded with both chopper and buncher operating at 50 MHz, and positron energy is 250 eV. The width of the positron pulse is about 0.5 ns.

The ORCCA – project

Research leader adjunct professor Carl Rollenhagen, Mälardalens högskola
Scientist Irene Eriksson

The ORCCA project (**O**rganisation, **R**isk, **C**ommunication, **C**ulture, **A**nalysis) is focused on describing and understanding interaction among subcultures in nuclear organisations and how change management is interacting with cultural elements. ORCCA is based on a cultural approach. The cultural perspective focuses on principles guiding the behaviour of organisations and its personnel with an interest in the meanings attributed to the organisation and the generation of these meanings. Especially interesting are those meanings that relate to the demands of work. The value of a cultural approach is that it enables a generic view of the social dynamics in a complex and diverse domain.

The first part of the project was conducted in close cooperation with researchers in Finland (Teemu Reiman and Pia Oedewald, VTT Industrial Systems) in the context of a specific project about maintenance culture. This study aimed to characterise, assess and develop the organisational cultures of participating nuclear power companies' maintenance departments. Assessment was made by means of maintenance core task modelling (Oedewald & Reiman 2003). The theoretical core task model was used to assess the characteristics of the organisational culture. The study also aimed to validate the methodology for contextual assessment of organisational culture (Reiman & Oedewald 2002).

Main findings
The study contains many interesting observations about two maintenance organisations in two different Nordic countries. Olkiluoto and Forsmark had rather different organisational cultures, but they were also sharing a set of dimensions. Common to both plants, perceived at a general level, was that the goals of maintenance tasks were clear - maintenance is a prerequisite for the reliable production of electricity. The personnel saw their work as highly important, even though the plants differed significantly on how the personnel perceived how their work contributed to the overall goals of the organisation. Data can be understood from different angles. A major issue is to what extent the obtained data really say something specific about maintenance cultures, or if they better should be interpreted as general observation about work in complex organisations (regardless if it is maintenance, operation etc). Taking the latter point of departure, some of the structures obtained from the factor analysis are of much interest. As a hypothesis, we propose that work activities and their context, with a generalisation from the present data, may be characterised in at least the following important general dimensions:

- Meaningfulness
- Communication climate
- Experienced control
- *Structure.*

These dimensions are complex dimensions and affect each other. Experienced control, for example, is dependent on meaningfulness, but also on communication climate and structure. Meaningfulness is a complex cognitive variable presumably resulting from several other, more specific, factors such as the content and variation of the tasks and the feeling that the task is important and leads to personal development. Meaningfulness as a dimension was in the present study found to exhibit significant positive correlation's with job motivation and job satisfaction (which both may be assumed to be output variables resulting from more specific factors). Good communication climate as a dimension of the work context was also found to correlate positively with motivation and well-being. Introduction of complex and large matrix organisations also makes it difficult to structure the communication. In fact, the more "matrix" used, the more communication seems to be important to support then functioning of the matrix. To some extent this increased need seem to counteract the efficiency benefits looked for in the matrix arrangement.

Structure is a general term with many meanings. In this context we define structure as the degree to which people feel that goals, tasks, responsibilities etc are well defined. Judging from specific correlation's among some of the items measuring what we here call structure it was found that structure correlated positively with safety related items. This is perhaps an expected but nevertheless interesting observation that evokes general issues about how structure and flexibility interact in safety related activities.

It is interesting to speculate to what extent these general dimensions are affected by different management innovations and how they correlate to various structural arrangements (matrix organisations, line organisations etc). Different organisational changes probably affect different dimensions. It could it meaningful to inspect these dimensions when doing organisational changes, and especially when conducting risk analyses before these changes are made. This area needs more research. It can be hypothesised that outsourcing for example could affect the meaningfulness and communication climate in the company.

The ORCCA project will continue to work together with VTT to further explore cultural dimensions in NPP:s. For the coming project period, more emphasis will be invested upon dimensions of change management at NPP:s. Due to unforeseen circumstances the graduate student Irene Eriksson will bee replaced by another graduate student (Ulf Kahlbom) in the future work.

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Mechanistic Modelling of Dryout in Fuel Assemblies

Research leader Senior lecturer Henryk Anglart, Divison of Nuclear Reactor Technology, Department of Energy Technology, KTH, Scientist Mattias Hemlin, Vattenfall Bränsle AB

Background

In boiling water reactors (BWR), one of the most important limitations for core design and core operation is the critical power ratio (CPR), which is a measure of how far from dryout you operate. Today, empirical correlations are used to calculate CPR, and these correlations are based on very expensive measurements. The advantage of the correlations is that the agreement to the test data is often very good because of the small number of data used to build the correlations, but the disadvantages are bigger. First of all the correlations are of no use in developing of new fuel constructions and the ability of the correlations to predict transient behaviour is questioned. The correlations are used to predict one single critical power for the whole bundle, which can lead to very conservative correlations, which in turn can lead to economical penalties. Because of this, the need of better methods to predict dryout is desirable.

Objectives

The object of this work is to improve the calculation of dryout in a BWR fuel assembly, by developing more physical models, compared to the correlations that are used today. There has been much work done in this area, but there are many different questions unanswered. Under BWR flow conditions, annular flow is the dominant flow regime, where the liquid is flowing as a thin film along the wall. One of the main difficulties is to calculate the entrainment of droplets from the liquid film to the gas core in vertical co-currant annular two-phase flow. Of that reason the focus has been at improving entrainment rate models, by investigation of hydrodynamics and stability of liquid films in annular.

Results in 2003

Starting with the continuity and the Navier-Stokes's equations, an evolution equation of the liquid film thickness, (h in the figure below) in adiabatic annular co-current two-phase flow in a channel was derived. In the derivation, the boundary layer approximation was used, by assuming that the wavelength of the waves on the liquid film surface is much larger than the film thickness

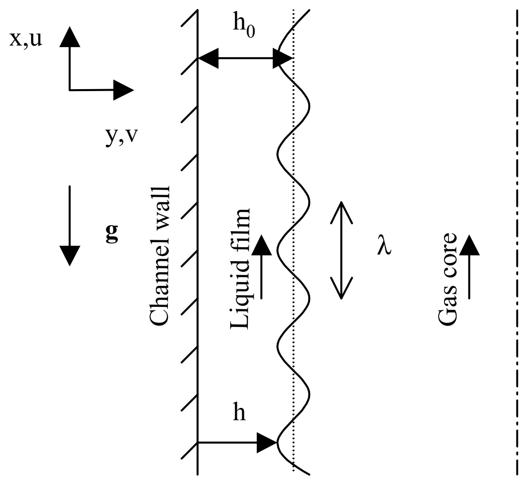


Figure 4 co-current annular two-phase flow

By introducing disturbances into the evolution equation a weakly non-linear disturbance equation for the disturbed liquid film thickness was derived. By weakly non-linear is meant that all terms of degree three or higher in the disturbances are rejected. By using the neutral stability condition and by introducing linear disturbances, a critical wavelength was found. This critical wavelength will be used in the derivation of the entrainment of droplets from the liquid film to the gas core.

Under 2003, Mattias Hemlin also participated in one course in Turbulence and one course in Experimental Methods in Fluid Mechanics at KTH.

About the project

The project started in December 2001 and the members are PhD. student Mattias Hemlin and supervisor Henryk Anglart (replacing Wiktor Frid as the supervisor). Mattias Hemlin, who is working 80% of his time in the project, is employed at Vattenfall Bränsle AB.

Reference Group

The members of the reference group supervising this project are: Oddbjörn Sandervåg (SKI), Jan Hanberg (Forsmark), Tell Andersson (Ringhals), Fredrik Winge (Barsebäck), Bo Söderqvist (OKG), Rolf Eklund (Westinghouse), Marek Kosinski (Vattenfall Bränsle).

Experimental and Theoretical Investigation of Air-Steam-Hydrogen Distribution in Reactor Containments with Focus on Steam Condensation Effects

Research leader Senior lecturer Henryk Anglart, cientist Krzysztof Karkoszka, Division of Nuclear Reactor Technology, Department of Energy Technology, KTH

Background

A steam condensation in presence of non – condensable gases plays very important role in nuclear power safety analysis. During Loss of Coolant Accident (LOCA) conditions large amount of steam and hydrogen mixture can be realized into the reactor containment. The presence of air and hydrogen reduces the heat transfer coefficient significantly. Also the direct-contact condensation phenomena on a water film surface and condensation on the water droplets (condensation on a fog) can occur during such conditions. Both of them also influence the heat transfer coefficient and decrease the condensation rate.

Objectives

The objective of this project is to investigate simplified model of the condensation phenomena during LOCA conditions. The air – hydrogen (or helium) – steam mixture condensation on a water film (water droplets) is investigated. The physics of such phenomena needs to be deeply understood and mathematical model has to be implemented into CFD software (CFX – 4) and validate against available empirical experiments. This project also gives a good opportunity to elucidate the governing phenomena and to develop theoretical models to describe the condensation processes during LOCA conditions.

Results in 2003

1. Two months spent in Paul Scherrer Institut (PSI) in Switzerland where simple condensation model on horizontal flat surface with constant temperature has been implemented into CFX – 4. For the prediction of condensation mass flow rate the following correlation has been used:

$$j = -k\Delta Y_s \qquad (1)$$

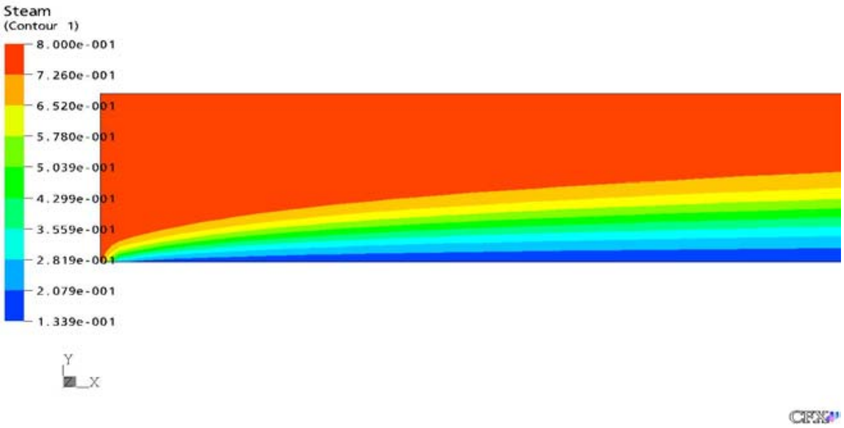
where: j - condensation mass flux,
k - mass transfer coefficient (set artificially)
Y_s - mass fraction of steam.

2. The Implementation of condensation model for the same geometry (at KTH) into CFX – 4. This time for the prediction of condensation flow rate Fick's law has been implemented in the following form:

$$j_i = -\rho D_{SA} \frac{\partial Y_s}{\partial z_i}, \qquad (2)$$

where: D_{SA} - diffusivity coefficient.

One of the examples of steam distribution received from this calculation is shown on the plot below:



Personnel and collaborations
The scientist is Krzysztof Karkoszka and the supervisor (from 2004) is Henryk Anglart (previous supervisor was Wiktor Frid). There is also collaboration with PSI.

Reference group
The reference group of this project consists of the following persons:
Anders Henoch – Ringhals, Farid Alavyoon – Forsmark, Lilly Burel – Barsebäck
Oddbjorn Sandervag – SKI, Henryk Anglart – Westinghouse, Claes Halldin – OKG.

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Measurements and Analysis of Dryout and Film Thickness in a Tube with Various Axial Power Distributions.

Research leader Senior lecturer Henryk Anglart, Divison of Nuclear Reactor Technology, Department of Energy Technology, KTH, Scientist Carl Adamsson Westinghouse Electric Sweden

Background

In high performance heat exchangers, such as nuclear reactors, the critical heat flux gives the most important design boundary. In a BWR nuclear reactor the critical heat flux occurs through the process of dryout, i.e the disappearance of liquid film from the fuel rod surface. At the transition to dryout the heat conduction between the fuel and the coolant is vastly reduced, leading to a sharp increase in fuel temperature and possible fuel damage. It is obvious that accurate methods to predict the dryout limit under various conditions are needed. However, dryout has turned out to be an utterly complicated multi-physics phenomenon and the success of the mechanistic models developed so far has been limited. Today the industry relies on empirically tuned correlations, which require extensive full-scale experiments. Moreover, since the correlations used today are not well founded in physical reasoning they cannot be trusted if used outside the parameter range of the underlying experiment. In some cases this can be a severe limitation; e.g. there has recently been an increasing interest in the influence of the axial power distribution on the dryout power. For practical reasons it is only possible the perform experiments for a very limited set of power distributions. It is thus questionable if empirical correlations can be trusted to predict the quit large effect of the power distribution in an adequate way. This and the high costs of large series of full-scale experiments are the background to the need for mechanistic models to predict dryout.

Previous Work

Several researches have, for several decades, put a lot of theoretical and experimental work into the task of finding an accurate mechanistic model for dryout. Most models developed are built on the assumption that the annular steam-water flow can be described as a balance between a gas-field, a liquid droplet-field and a liquid film-field. Dryout is then postulated to occur when the liquid film thickness becomes zero, or sometimes a small positive value (a critical film thickness). The challenge is then to formulate the equations for the mass transfer between these three fields. Many attempts have been made, but so far none has proved general and accurate enough for practical use. One problem is that experiments designed for development of empirical dryout correlations usually focus only on the dryout power. To develop and validate mechanistic models however, experimental data on the film thickness and film flow rate are much more useful. Such experiments have been performed by several researchers under various conditions and a lot of published data are available today. Most of this data however do not focus on the axial power distribution, which today is one of the main challenges. In the cases when the axial power distribution has been varied, the film thickness has been measured only at one point at the outlet. A notable exception is Hewitt’s measurements with a moveable “cold patch”. The results of these experiments are very interesting and calls for further investigation with more realistic power distributions.

Experimental Program

In short the experimental program in the present project will be aimed at measuring the liquid film flow for various axial power distributions at several axial locations. The method for film flow measurements has been used by several researchers before; the film will be sucked of the tube wall and gas content in the sample will be measured through a heat balance calculation. The results will be valuable to validate existing models for mass transfer between the film- and the droplet fields and if necessary develop new ones. Hopefully they will also shed light on the question if there is a critical film thickness larger than zero.

Theoretical Work

The theoretical part of the project will be to investigate the deposition of liquid droplets onto the liquid film by Computation Fluid Dynamics (CFD) methods. To predict the dynamic behavior of the liquid droplets, there are plans to use both Lagangeian particle tracking and the Eularian description of the droplet field. The work is needed since there are strong indications that the most common correlations used to calculate the deposition rate today cannot be generally valid.

Results During 2003

The project started in July 2003. The construction of the experimental equipment has begun.

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Development of a Thermodynamic Database for Zirconium alloys

Research leader Professor Bo Sundman, Scientist Rosa Jerlerud Pérez
Department of Materials Science and Engineering, Division of Computational Thermodynamic KTH

Background

The aim is to reduce the amount of experimental work necessary to design Zr alloys with a new compositions. This can be achieved by using a thermodynamic approach to create a thermodynamic database, for calculating the stable phases. In the database the Gibbs energy of all the components and all phases of the system are described as functions of temperature and composition. With this thermodynamic description the equilibrium state is calculated by minimizing the total Gibbs energy of the system. Thus, the database will provide the materials designer with a powerful tool to perform thermodynamic equilibrium calculations in multicomponent and multiphase system.
Elements included in the database: C, Cr, Fe, Mo, Nb, Ni, O, Si, Sn, Zr.

Method

The main technique is to use experimental information on phase diagram and thermo-chemistry and analyse it using mathematical models which describe the properties of the phases, this is also referred to as the Calphad technique (www.calphad.org). Consistent models must be used for the pure elements and for the phases (binary ternary or higher order) in order to combine results from independent assessments in a common database. Those models are able to describe a large amount of experimental information by small amount of model parameters. All the calculations are performed using ThermoCalc software (www.thermocalc.se).
The Gibbs energy of the pure constituents *i* at any temperature and physical state of interest is given relative to the enthalpy of the element in its stable state at 298.15 K, mathematically described as follows.

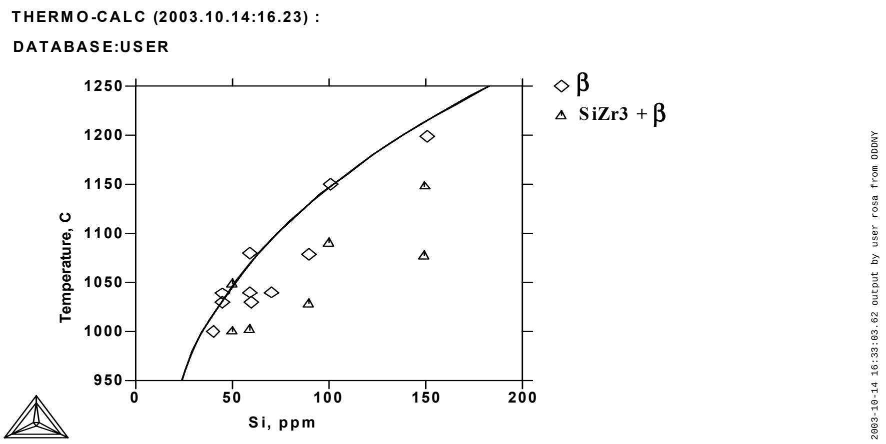
$$^{o}G_i - H_i^{SER} = a + bT + cT \ln T + \sum_n d_n T^n$$

These data have been evaluated by the Scientific Group Thermodata Europe SGTE [91Din] (www.sgte.org).
More detail concerning the description of phases with composition variation (non-stoichiometric) can be find in [01Per] and [03Per].

Results 2003

The lack of experimental information regarding the ternary systems make it necessary to select the most relevant ternary systems to perform experimental work . Considering the fact that zirconium alloys interact strongly with oxygen both during manufacturing of the alloys and *in-reactor* performance, the O-Sn-Zr can be considered as an important system.

Fig 1. Solubility limit of Si in β phase vs transformation temperature in



In the fig it is shown the calculated phase boundary β / β +SiZr3 vs experimental values by Charquet and Alberitiere Zirconium in the Nuclear Industry, 7th Symposium,(1997).

The intermetallic compounds (SPP) present in Zr alloys: $(Fe,Ni)Zr_2$_C16 (tetragonal C16) and $(Cr,Fe)_2Zr$ (laves c14 or c15) in Zircaly-2 and Zircaloy-4 and $(Zr,Nb)Fe_2$ laves_c14 and $(Zr,Nb)_2Fe$ (cubic c16) in Zirlo, provide a guide for selection of the important ternary systems: Fe-Nb-Zr, Cr-Fe-Zr, Fe-Sn-Zr, O-Sn-Zr.

The database contains the following binary systems:

Metallic systems

C-Zr [95Fer], Cr-Zr [94Zen], Fe-Zr [95Ser], Cr-Fe, [87And, 93Lee], Cr-Ni[86Din] Fe-Ni [86Cha, 93Lee], Mo-Zr [03Per], Nb-Zr [91Fer], Ni-Zr [94Gho], Si-Zr [94Gue], Sn-Zr [99Dup], Cr-Nb [93Cos], Fe-Nb [00Tof], Fe-Sn [96Kum], Nb-Sn [02Tof], Cr-Sn [01Per]

Oxide and others important systems

Cr-O [90Tay, 95Kow], Fe-O [91Sun, 95Kow], Nb-O [00Dup], Ni-O [90Tay,95Kow], O-Sn [00Dup],
O-Zr [01Lia], H-Zr [00Dup].

Ternaries

Cr-Ni-O [90Tay], Cr-Fe-Ni [91Lee], Fe-Ni-O [95Luo]
In the Table 1 important intermetallic compounds and their respective structures described in the database are listed.

Table 1. Most Important Intermetallic Phases in the Database

	Prototype structure	**System**	**Phase in the ally**
A15	Cr_3Si (Cubic)	Nb-Sn Sn-Zr	Nb_3Sn $SnZr_4$
	NaCl (Cubic)	C-Zr	CZr_x (Fcc_A1)
C1	CaF_2	H-Zr O-Zr	H_2Zr-δ ZrO_2 . (Fcc_C1)
C14	$MgZr_2$ (Hexagonal laves)	Cr-Nb, Cr-Zr, Fe-Nb, Fe-Nb-Zr , zirlo, Cr-Fe-Zr, zircaloy-2,4	$(Nb,Fe)_2Zr$ " $(Cr,Fe)_2Fe$
C15	Cu_2Mg (Cubic laves)	Cr-Nb, Fe-Zr, Mo-Zr, Cr-Fe-Zr ,zircaloy-4	$(Cr,Fe)_2Zr$
	$NiTi_2$ (Cubic)	Fe-Nb-Zr zirlo	$Fe(Nb,Zr)_2$
C16	Al_2Cu (Tetragonal)	Fe-Zr , Fe-Sn, Ni-Zr, Si-Zr Fe-Ni-Zr, zircaloy-2	$(Fe,Ni)Zr_2$
C43	O_2Zr	O-Zr	O_2Zr (Baddeleyite)
E1A	BRe_3 (orthorhombic)	Fe-Zr	$FeZr_3$

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01Per R. J. Pérez, Calphad, 25,1 (2001), 59-66.
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Modelling of radiation effects on mechanical properties of ferritic steels.

Research leader: Assoc. professor Jan Wallenius, Scientist Christina Lagerstedt, Department of Physics, Division of Nuclear- and reactor physics, KTH

Background
Mechanical properties of steels used as components in reactors are degraded due to effects of radiation, thermal ageing and thermo-chemical environment. Often threshold behaviours are observed, meaning that a component may have served without problem for many years, or even decades, before an abrupt change in ductility or volume takes place. These phenomena are further known to be dose rate dependent, meaning that accelerated irradiation tests often will give wrong predictions of limits to service life in a real reactor environment. This is especially trouble-some in light water reactors, where the threshold time for embrittlement or swelling to become significant is of the order of decades.
Therefore, it becomes important to obtain a basic understanding of the mechanisms responsible for the irradiation degradation of mechanical properties. Today this can be achieved for pure metals by means of computer modelling, using a multi-scale approach ranging from solutions of the Schrödinger equation to elasticity theory for macroscopic bodies.

Goals of the project
In the present project, existing empirical models for pure elements like Fe are extended to the Fe-Cr-C system, which may serve as an idealised model of ferritic steels actually used for reactor components. By the end of the project, a so called ”Embedded atom method”, or EAM model for this system will have been developed, that is able to correctly reproduce elastic, thermo-physical and point defect properties of this material out of pile, as function of Cr and C content. This model will be used for predicting the change of mechanical properties as function of irradiation dose, dose rate and temperature. Comparison with relevant experimental data will then be made, to check the predictive power of the model. Finally, an evaluation of the applicability of the results with respect to real industrial ferritic steels will be attempted.

Organisation
The work is performed by PhD student Christina Lagerstedt and Associate Professor Janne Wallenius at the department of Reactor Physics. Collaborations with Uppsala University, the institute of Chemical Metallurgy in Paris and the Belgian Nuclear Research Centre in Mol are providing essential input and feedback to the project. The results are presented at international conferences and published in refereed journals.
The contact reference group consists of Behnaz Aghili, SKI, Magnus Limbäck, Westinghouse, Mats Molin, Forsmark, Pål Efsing, Ringahls/Barsebäck and Bengt Bengtsson OKG.

Methodology
In the EAM formalism, the total energy of a system is written as the sum of pair-wise interactions and a many-body term given as function of electron density. Historically, EAM potentials describing the effective interaction between atoms of the same kind have been fitted to reproduce experimental data for lattice parameters, elastic constants, crystal structure and vacancy formation energies. In order to include information relevant for defect production in irradiated materials, the short range of the pair-potential has been fitted to threshold energies for Frenkel pair production in electron irradiated speciments.
Several potentials for iron have been reported in the literature, which reasonably well reproduce the properties they were fitted to. However, none of them provides correct values for thermal expansion. In addition, only short-range potentials, excluding the FCC lattice second nearest neighbour, could reproduce the relative stability of self-interstitials in different lattice directions. In order to obtain a better potential for iron, our group started out by fitting a long-range pair potential to the measured thermal expansion coefficients of iron. Interestingly, it was found that the stability of the <110> interstitial was improved by this procedure, at the expense of increasing the absolute formation energy of the defect.
Chromium is anti-ferromagnetic and highly anisotropic at room temperature. Hence it was believed to be impossible for EAM potentials to reproduce its elastic properties. The latter fact has been considered to be a major obstacle for the applicability of the embedded atom method to simulation of

Cr bearing steels. Examining the temperature dependence of the elastic constants, we however found that at higher temperatures, where chromium is paramagnetic, that the so-called Cauchy pressure becomes positive, meaning that the EAM formalism may be applied. By thus fitting the Cr potential to the elastic constants of its paramagnetic state, we were able to obtain a potential reproducing elastic properties at T > 450 K. Since reactor components typically operate at even higher temperatures, we believe that results obtained in simulations using this potential should be relevant. Further, it is known that the addition of just a few percent of iron to chromium makes the alloy paramagnetic at room temperature. Hence our Cr potential should well describe the behaviour of Cr in the alloy at all temperatures of interest.
Mixed pair potentials, i.e. potentials describing the interaction between Fe and Cr atoms, have been fitted to reproduce the lattice parameter, the bulk modulus and the mixing enthalpy of the alloy, at Cr concentrations of 5 and 20%. The mixing enthalpy for the ferro-magnetic state was fitted to data calculated with Ab Initio methods in collaboration with Uppsala University [Olsson03]. These data show that the formation energy is negative for Cr concentrations below 6%, a fact that was not known in previous attempts to obtain EAM potentials for the alloy.

Results
A detailed account of our results has recently been published in Physical Review B [Wallenius04]. One may note that our set of potentials yield better values for vacancy activation energies than any other published potential. The relative stability of interstitials in iron is also in good agreement with measurements, while the absolute formation energy appears to be somewhat high. Using our alloy potentials in kinetic Monte Carlo (KMC) simulation of vacancy driven thermal ageing it was found that the potential fitted to the negative mixing enthalpy of Fe-5Cr predicted no precipitation of Cr at any temperature. The potential fitted to the positive mixing enthalpy of Fe-20Cr did however yield formation of Cr clusters, as seen in Figure 1. Cr-rich clusters are indeed observed in real alloys only for Cr concentrations above nine percent, being denoted as the alpha-prime phase. The calculated time and temperature dependence of the precipitation rate was found to be in good agreement with data for hardening of Fe-Cr alloys.

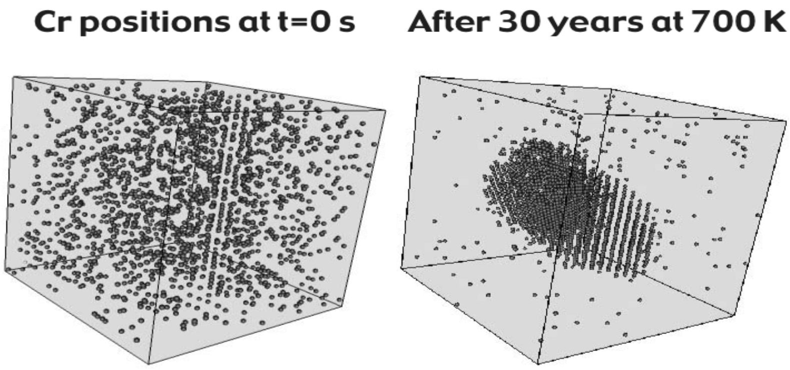

Figure 1: Simulated precipitation of Cr in Fe-20Cr.

The calculated sizes of the precipitates do however not agree with the measured size distribution (2-4 nm). This is due to the fact that the properties of Fe-20Cr no longer are relevant for describing a cluster containing 85% Cr, which is the measured Cr content in the alpha-prime phase. We will need to introduce a many-body potential into the EAM that is dependent on the local Cr concentration in order to predict a correct cluster size distribution. Such a work is foreseen to be performed in 2004. We are also preparing to construct potentials for Fe-C and Cr-C, with the purpose of simulating formation of metal-carbide precipitates, which are known to govern the mechanical properties of real steels.

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External Source Effects and Neutronics in Accelerator-driven Systems

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Department of Nuclear and Reactor Physics, KTH

Introduction

An important factor when designing an ADS is to optimize the beam power amplification, i.e. the core power over the accelerator power, given that the reactor is operating at a certain sub-critical reactivity level. Optimizing the source efficiency and thereby minimizing the proton beam requirements can have an important impact on the overall design of an ADS and on the economy of its operation. The neutron source efficiency parameter φ* is commonly used to study this quantity, since it is related to the number of fissions produced in the core (which is proportional to the total core power) by an average external source neutron.

However, calculating φ* for an ADS introduces some complications. Since the neutron source is generated by a proton beam/target simulation, the distribution of the source neutrons is dependent on the target properties and the proton beam properties. In order to determine φ*, the external neutron source first has to be defined and then the efficiency of this neutron source can be determined. The major drawback with using φ* is that the neutron source can be defined in several different ways, and the results are directly dependent on the choice of definition. Therefore, completely different values of φ* are often observed, due to different choices of external neutron source definition. Another complication associated with the neutron source efficiency is that, studying φ* as a function of a certain system parameter might change the neutron source distribution and the number of neutrons produced per source proton (*Z*). If a change in the studied system parameter changes the distribution of the neutron source, φ* has to be weighted by *Z*. With the target neutron leakage definition, examples of parameters affecting the source distribution are the target dimension, the proton beam energy and the axial proton beam impact position. Other system parameters, such as the core coolant material, the fuel composition and the core dimensions are independent of the target region and do not affect the neutron source. In contrast to the target neutron leakage source, it has been shown that using the energy cut-off definition, the neutron source distribution is rather insensitive to changes in the target radius. However, substituting the coolant material or changing the fuel composition in this case might affect the distribution of the neutron source.

Results

In the fist paper [1], numerical simulations have been performed with the Monte Carlo code MCNPX in order to study ψ* as a function of spallation target radius for different inert matrix fuels. It was found that, in order to maximize ψ*, and thereby minimizing the proton current needs, a target radius as small as possible should be chosen. A ZrN or an YN matrix, mixed with the plutonium and americium mixed nitride fuel, appears to be a slightly better choice than a HfN matrix, considering only the proton source efficiency (Fig. 1). It was also found that a power flattened double-zone core, compared to a single-zone core, decreases ψ* by about 5% for the ZrN matrix and by about 10% for the HfN matrix.

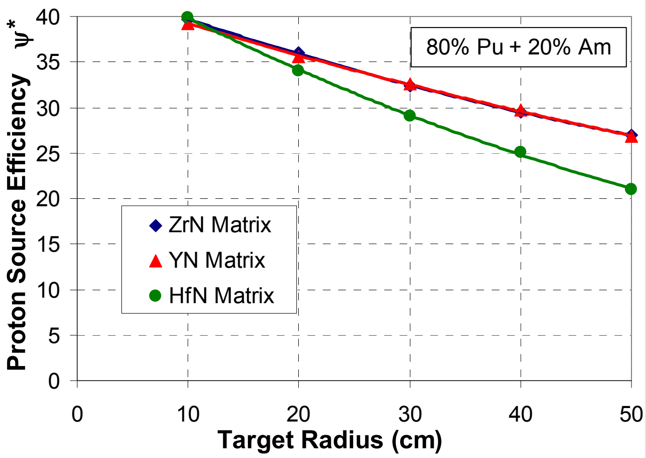

Fig. 1. ψ* versus target radius for different plutonium based matrix fuels (80% Pu + 20% Am).

In the second paper [2], the proton source efficiency (ψ*) was studied for homogeneous and heterogeneous distributions of minor actinides in a nitride-fuelled and lead-bismuth-cooled accelerator-driven system. The findings from the MCNPX simulations indicate that, compared to a homogeneous configuration, a gain in ψ* by up to 16% can be obtained by distributing the minor actinides heterogeneously, Cm being placed in the inner zone of the active core and Am in the outer zone (Fig. 2). The reason for this is the higher fission probability for neutrons for Cm than for Am in the energy range below 1.0 MeV.
Moreover, a comparative study of two different physics packages available in MCNPX, the Bertini and the CEM models, has been performed, focusing on the production of neutrons in the spallation target and on the proton source efficiency. The Bertini model was found to produce a higher number of neutrons in the low-energy range (below ~15 MeV) than the CEM model. Consequently, the Bertini model also over-estimates ψ* by about 10%, compared to the CEM model.

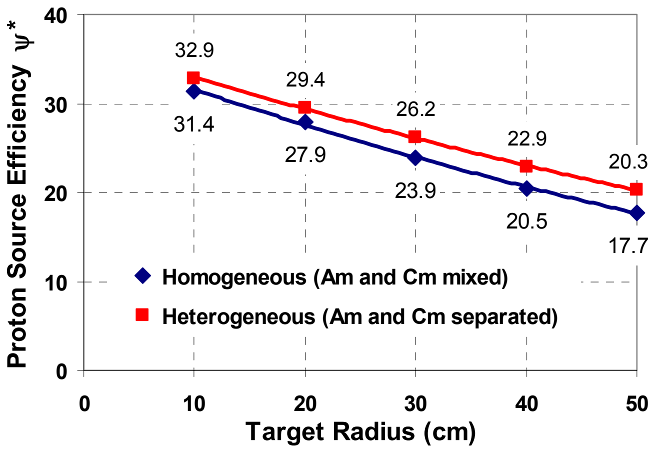

Fig. 2. Proton source efficiency ψ* for different target radii of the homogeneous and the heterogeneous configurations (1σ-error ~0.50%).

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