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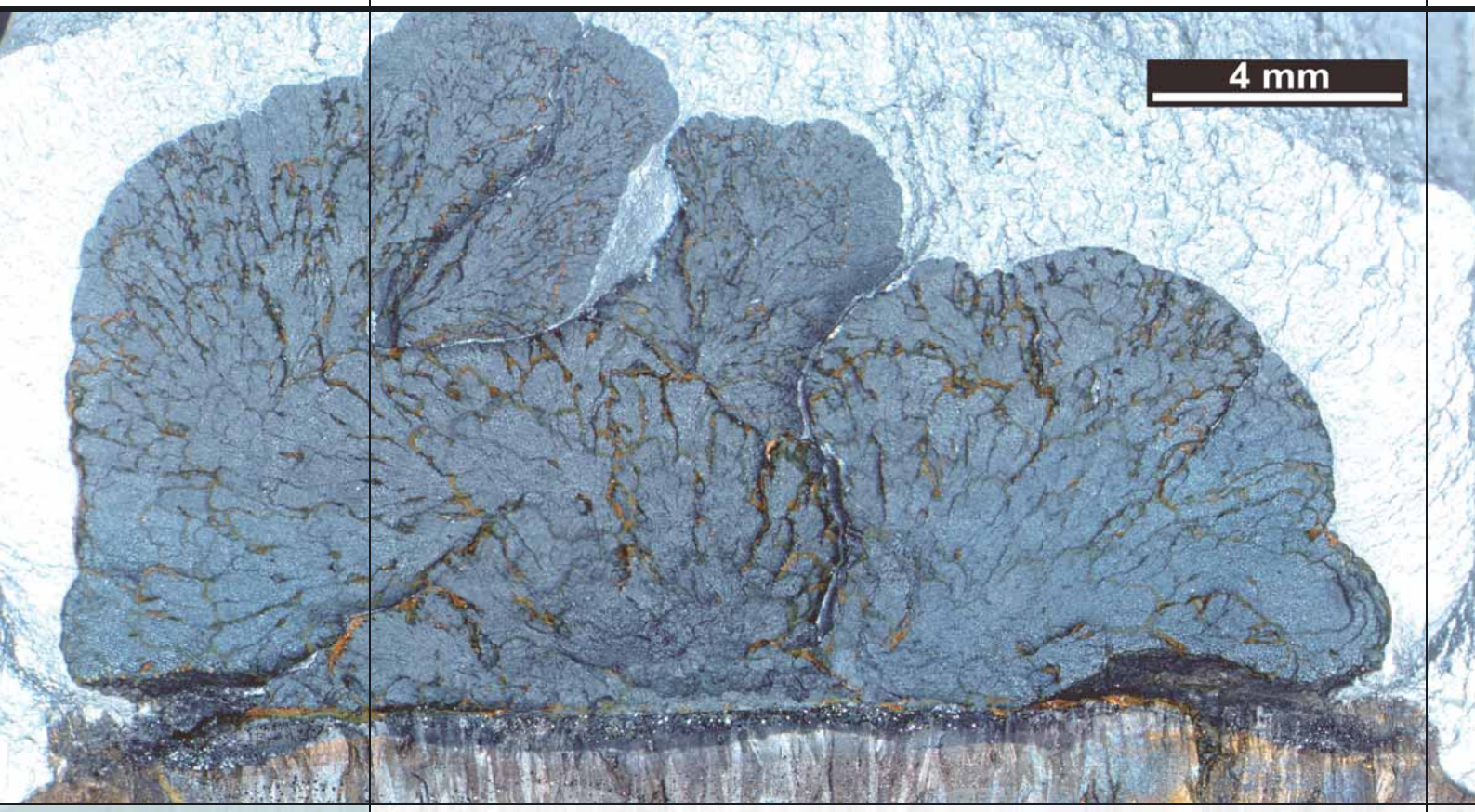
Scientific Highlights 2009

Nuclear Energy and Safety

Cover photo:

A stress corrosion crack in a dissimilar metal weld, growing from the Inconel 182 weld metal into the low-alloy Reactor Pressure Vessel steel, as seen during a constant load test using a compact tension specimen in a Boiling Water Reactor environment.



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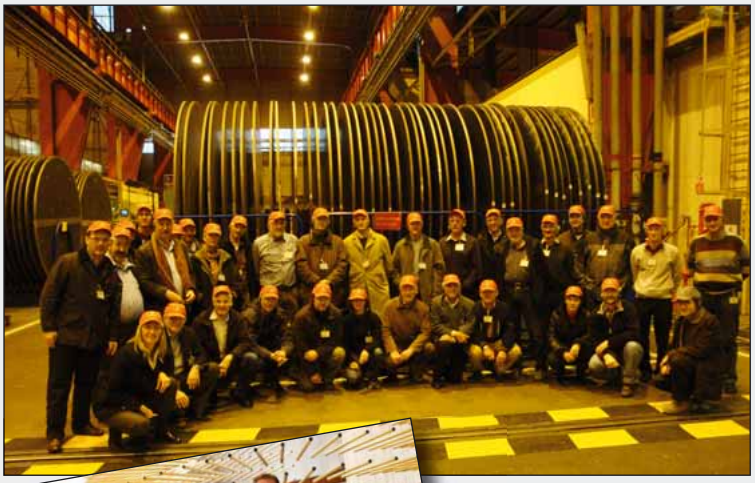


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Nuclear Energy and Safety Research Department (NES) 5

The strategic areas of activity within NES comprise the following:

- contributions to the safe and economic operation of the existing NPPs in Switzerland and proof of the safe geological storage of radioactive waste by reinforcing the scientific bases of the technologies in the appropriate areas;
- support to the reactor operators and safety authority in Switzerland, as well as the securing of stand-by functionality in key areas, particularly those requiring the services of a Hot Lab;
- preparation of inputs to 'stakeholders' for decision-making purposes;
- promotion of nuclear energy by means of R&D in terms of increased sustainability, safety and economy;
- training of young nuclear specialists, including those with experience in other energy systems, over a broad spectrum of disciplines;
- support and participation in the worldwide 'renaissance' of nuclear energy, and of its relevance to the current needs within Switzerland.

NES is structured into five research laboratories according to its specific scientific and technical areas of competence. It operates the only Hot Lab in the country, and the Reactor School offers education and training programmes for present and future reactor operators. In strong partnership with the two Federal Institutes of Technology, ETHZ and EPFL, NES contributes to the newly launched education programme: the Swiss Master in Nuclear Engineering.

◀ **Jean-Marc Cavedon (top right), Head of the Nuclear Energy and Safety Research Department (NES), and snapshots of selected group events taking place during 2009: *Klausur* (NES conclave), NES PhD Day, Newcomers' Day.**

Nuclear energy research and its complete toolbox

Jean-Marc Cavedon
Nuclear Energy and Safety Research Department, PSI

The need to understand nuclear energy production systems 'from the atom to the reactor' comes somewhat closer to operational reality every year. Such a comprehensive philosophy calls for a multitude of levels of research, and a broad spectrum of research tools to be available. This year's selection of scientific highlights from the Nuclear Energy and Safety Department have been chosen specifically to illustrate the variety of tools belonging to the nuclear energy researcher's toolbox, from an ab *initio* description of materials, to fluid mechanics, and on to plant-scale energy models.

Nuclear energy originates by nature from subatomic events: i.e. nuclear fissions, which deliver energy to complex-engineered power units in the gigawatt range. This inherent duality between the microscopic and the macroscopic worlds has served to shape the various research areas in nuclear energy, and to define the numerous, and complementary, experimental and numerical tools needed. The research topics from 2009 are representative of the full range of tools NES uses to obtain quality results, and to report its state-of-the-art research accomplishments.

Experiment, theory and simulation

The exponential increase in computing power brings numerical simulation on par with traditional experimental approaches in developing understanding of the basic physical phenomena important to nuclear energy and safety. M. Krack reports on the computer-simulated 'heating' of an UO_2 crystal up to 1500K, based on solid theoretical foundations (in this case quantum physics). This work could be described as an *in silico* experiment on a (virtual) radioactive sample. The neologism makes even more sense if one assigns the term *in vitro* to experiments in which all parameters are well-controlled, while *in vivo* would point to full-scale experiments in which the complexities of a completely engineered system (for reactors), or of the natural environment (for geological repositories), are preserved.

High performance computing

The next illustration of recent developments consuming hundreds of thousands of CPU-hours per year has to do with the behaviour of structural materials under nuclear conditions, in this instance the Fe-Cr-C system as a simplified model for steel, and ultimately for high-temperature steels, such as the oxide-dispersed-strengthened (ODS) family. A.C. Uldry *et al.* show that calculations based on Density Functional Theory already bring insights into how Cr atoms are clustered (or, conversely, soluted) in an Fe matrix according to the Cr content. Magnetism is believed to be the microscopic origin of the newly emerging properties, such as atom clustering.

High-accuracy / high-resolution measurements

An interdisciplinary team at PSI has been involved in a new estimate of the half-life ($t_{1/2}$) of ^{60}Fe (I. Günther *et al.*). Separation chemists, analytical chemists, radiation physicists and astrophysicists have all combined to determine the half-life by installing a known number of ^{60}Fe isotopes in a low-radiation background environment and measuring the absolute number of gamma rays emitted by their daughter ^{60}Co isotopes. The accuracy of the measurement is an improvement by a factor 12 over previous estimates. Surprisingly, this notable step forward in accuracy has revealed a value for $t_{1/2}$ somewhat higher (by 75%) than that previously accepted. This finding will force astrophysicists and cosmologists, i.e. the modellers of the Solar System and Universe, to revise their present models. Also noteworthy is the fact that the

large collection of 10^{15} or more isotopes of ^{60}Fe was made possible by transmutation reactions created during the bombardment of a copper block by the very high current of high-energy protons at PSI in the SINQ facility.
Safe underground storage is also a topic that benefits from high-resolution measurements. D. Popov *et al.* show that crystallography with present-day, high brilliance X-ray beams can yield precise identification of the structure and composition of micron-sized crystals in a highly heterogeneous environment. To help understand how the cements used today for packaging radioactive waste will look in 100 millennia, the team of geochemists have studied 100 000 year old natural cements, and have identified in them tiny tobermorite crystals. The micrometric spatial resolution of the micro-XAS beam line at SLS was crucial in extracting a clear signal for analysis from a very heterogeneous sample.

Full-scale and small-scale facilities

Present-day studies of the safety of nuclear reactors do not rely solely on atomic-scale calculations, and this by a long way. Large-scale phenomena are essential in describing real-life configurations. This year's example is given by D. Paladino *et al.,* who have studied the mixing of hydrogen, steam and air that would be found in a nuclear reactor containment after a (hypothetical) core overheating incident. Gas stratification could lead to the formation of hydrogen-rich layers, with the risk of hydrogen deflagration or detonation. The numerous mass and heat sources/sinks generated by the operation of various safety devices tend to destroy these layers by turbulent mixing. The dynamic interplay between the build-up and destruction of such layers will ultimately give rise (or not) to a hydrogen-risk situation.
Nothing less than full-height experiments (i.e. tens of metres) in highly-instrumented vessels, such as exist in the PANDA facility at PSI, can deliver the basic data needed for evaluating and mitigating the risks of such rare gas-mix configurations. The data collected are also essential for calibrating the complex Computational Fluid Dynamics (CFD) calculations used today, including any three-dimensional effects.
In contrast, there is still a crucial role to be played by small-scale experiments, or separate-effect tests, in which specially developed instruments provide the local measurements needed to further improve the CFD codes, and for thorough training of students in the field.

Nuclear energy as a part of the sustainable energy mix

The reliable and safe operation of nuclear power plants, together with the safe, long-term disposal of nuclear waste, are essential ingredients for the social acceptance of this energy source. A clean ecological record, and economic competitiveness, are the two principal criteria to be satisfied for nuclear energy to be regarded as a sustainable option. Plant-scale energy scenarios, like the ones devised by H. Turton et al., provide understanding of the position and trends of the share of nuclear energy in the sustainable energy mix. The results extracted from the ADAM project (co-funded by the EU) stress what stringent CO_2 atmospheric concentration targets would mean in terms of the technology development needed to meet these targets, and at what cost. The targets range from none, or 'business as usual', to a very stringent 400 ppm at the end of the century, barely higher than today's 380 ppm.
Focusing on the nuclear share of the supply mix, it appears that in all scenarios the nuclear fleet must at least double by 2050, but then decrease almost to the present level if uranium resources are consumed using today's technology (Light Water Reactors). If a more resource-sparing reactor technology is assumed, i.e. utilising fast-breeder reactors, the nuclear share soars to 30% of the world's electricity supply, while simultaneously reducing the cost of CO_2 mitigation measures by just a few percent in terms of world GDP.

Conclusions

The list of 'tools' used to obtain the results presented in the following pages includes computers, samples of nuclear waste or geological cements, detectors, mass spectrometers, X-ray beams, and full-size instrumented vessels, together with a global and accurate description of all technology sources.

NES facts and figures for 2009

Peter Hardegger
Nuclear Energy and Safety Research Department, PSI

Federal funds for nuclear research have remained stable, and the small growth seen last year in third-party funding has continued during 2009. Compared to 2007 and 2008, the turnover rate of personnel within NES was somewhat reduced. The economic crisis may have relieved some of the pressure on NES arising from the industrial sector, but nevertheless, from the NES standpoint, the recruitment market was still difficult in some research areas. With a total of 35 new staff members, most of the vacancies could be filled, and we could also compensate for those leaving during the year.

General Situation

After the steep decline in federal funds for nuclear research in the 1990s, and the efforts to compensate this decline as much as possible by third-party financing, the funding situation stabilised after the year 2000. Since 2005, a small growth could even be sustained, and, with an accelerating trend after 2007, this growth has continued during 2009. As before, this is based solely on the acquisition of additional third-party funding during the year.

The positive overall climate for nuclear research has continued, in sharp contrast to the current economic crisis. The employment situation in 2009 for NES improved substantially because the job market became more relaxed, which greatly helped NES consolidate its staffing levels.

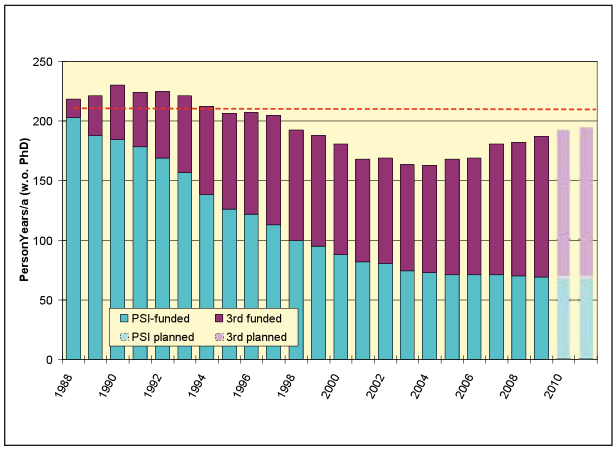


Figure 1: **History of NES funding resources.**

Personnel

With 35 new staff members, 2009 was still a year which can be regarded as one with a very high recruitment rate. This was the third year in a row in which more than 30 people had been recruited. In 2009, not only could the 16 staff members who left PSI be replaced, but most of the existing open positions could also be filled, resulting in a very low number of vacancies still outstanding by the end of the year. As a result

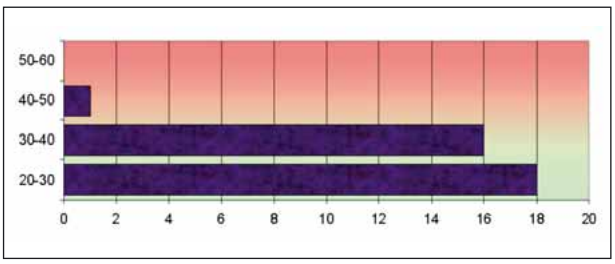


Figure 2: **Age structure of the 2009 recruitments.**

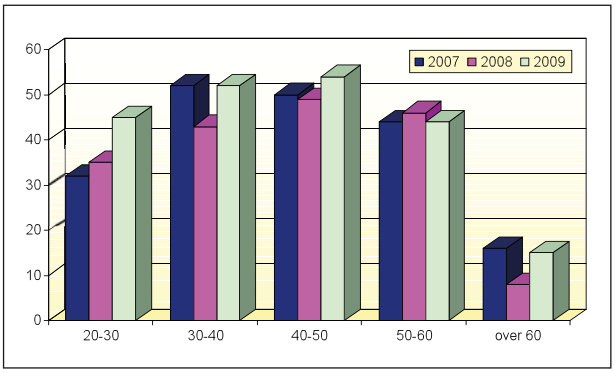


Figure 3: **NES age structure 2007–2009.**

of the continuing recruitment of young people, the trend in the overall average age of NES staff continued downwards. After the departure of many senior management staff in the preceding few years, the situation was much more stable during 2009, which has given the younger replacement staff room to consolidate their responsibilities and positions.
The number of open positions, which peaked at over 30 during 2008, but which could be reduced to 15 by the end of that year, was reduced further to 6 by the end of 2009.
In total, 16 NES staff left during 2009, out of which 4 were doctoral students who had successfully completed their course of studies. Simultaneously, over the year, the number of doctoral students increased, and now stands at 28.

Finances

The PSI resources, meaning the money made available through direct ETH-domain funding, remained constant during 2009. The funds made available for consumables and expenses were back to normal, having been at a reduced level the previous year.
A number of existing contracts could be renewed during the year, and adjusted to take into account increased costs. Several new contracts, with both existing and new partners, came into force, which supplied the increase of third-party funding necessary to sustain the overall growth of the department.
In total, 7 M CHF were available for investments and maintenance, made up of 1.7 M and 5.3 M CHF from PSI and third-party funds, respectively.

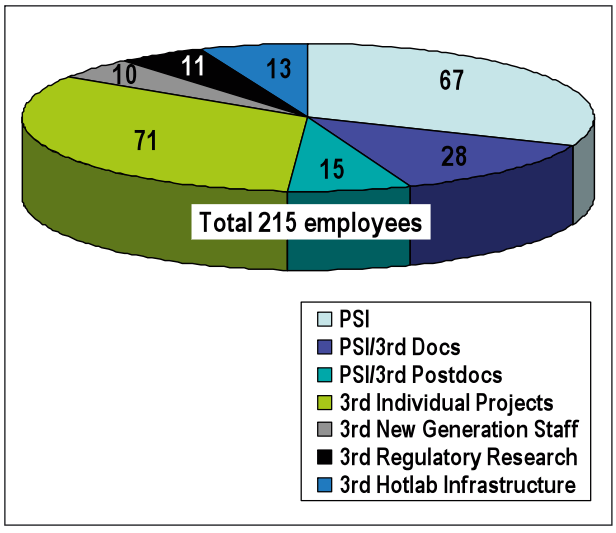


Figure 4: **How NES staff salaries are paid, showing the breakdown into PSI, third-party and joint funding.**

Partners / Contracts

Traditionally, the main emphasis of the research within NES (39%) is on safety issues relating to the existing Nuclear Power Plants (NPPs) within Switzerland. This also reflects the political responsibility of NES to support the safe operation of the Swiss NPPs. These activities are mainly supported by *Swissnuclear* (the association of operators of the Swiss NPPs) and ENSI (the Swiss Nuclear Safety Inspectorate), which are two of the largest third-party funding partners of NES, while research on existing safety systems and future reactor concepts (17%) is mainly funded from international collaborations (e.g. EU and OECD projects).
Waste management research is the third largest single activity within NES (13%). It is principally funded by Nagra (the National Cooperative for the Disposal of Radioactive Waste), which is itself the third of the largest third-party funding sources for the department.

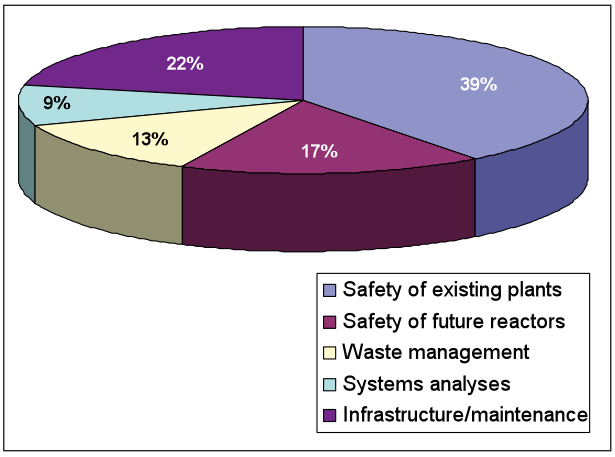


Figure 5: **Distribution of resources for 2009.**

Research in the field of Energy Systems Analysis is also an important fraction (9%) of the research conducted in NES, and one that has a very high visibility. The effort here is a common venture with the General Energy Department, and is financed from various sources.
The costs associated with the operation of the large nuclear facilities, the Hot Laboratory and PROTEUS, amounted to about 22% of the available funds in 2009.
During the year, several important new contracts were finalised. With ENSI, contracts for MELCOR, PISA, STARS, STARS-on-call and PASSPORT were signed, and Nagra is funding additional infrastructure at PSI for waste management research. Two new EU contracts were also signed (GETMAT, CP-ESFR), and the infrastructure cooperation with AREVA has been extended.
Within the framework of our existing contracts, 17 work statements/orders were signed (2 on HRA, 2 on STARS, 8 for the Hot Laboratory, and 5 with *Swissnuclear)*. In addition, several general funding agreements were renewed.

The Swiss Master in Nuclear Engineering: an EPFL / ETHZ / PSI / Industry collaboration

Rakesh Chawla[1], Horst-Michael Prasser[2]
[1] *EPFL and Nuclear Energy and Safety Department, PSI*
[2] *ETHZ and Laboratory for Thermal Hydraulics, PSI*

The Swiss Master of Science in Nuclear Engineering (NE) represents the first-ever common degree offered jointly by the two Swiss Federal Institutes of Technology, EPFL and ETHZ. Another unique aspect is that PSI – as the national research centre where most of the country's fission-related R&D is conducted – has a crucial role to play in this new educational programme. The main features and experience acquired to date with the running of the NE Master are described here, and a brief glimpse is given of future prospects.

The Swiss Federal Institutes of Technology at Lausanne (EPFL) and at Zurich (ETHZ) – in their capacities as the only two national technical universities in Switzerland – have a rich and long tradition in nuclear technology education. Student research, particularly at the doctoral level, has usually been conducted in collaboration with PSI, where almost all of the country's fission-related R&D is presently carried out.

Bologna and the nuclear renaissance

Since September 2008, a new dimension has been added to nuclear education in the country: the establishment of a Swiss Master of Science in Nuclear Engineering (NE) degree [1]. This advancement is due mainly to two important factors: the widespread implementation of the Bologna Process for European University Education on the one hand, and the worldwide nuclear renaissance (being felt currently) on the other. The realisation of this first-ever joint EPFL-ETHZ degree is in fact very much in line with similar developments being undertaken in other European countries, notably Belgium and Finland, where universities are collaborating to respond to the need for Master-level education in this highly multidisciplinary area [2].

The overall goals of the NE Master's programme are diverse, and have formed the main basis for establishing its curriculum structure and contents. These are: (i) to provide in-depth knowledge of the fundamentals and technology in harnessing the power of nuclear fission for safe and reliable energy supply, (ii) to provide complementary knowledge on nuclear fusion, (iii) to provide knowledge on nuclear techniques in medicine, research and industry, (iv) to provide a view of the entire nuclear energy conversion system, and (v) to underline the positioning of nuclear energy as part of a global sustainable energy mix.

Curriculum and organisation

The NE Master – which is taught entirely in English – is currently a programme of 90 ECTS[1] credits, i.e. extending over three semesters. The first two semesters are spent on course work, the final semester being devoted to an 8-week industrial internship, followed by a 17-week research project. The basis for implementation of the programme, as detailed below, has been provided by the close collaboration, not only between EPFL and ETHZ, but also with PSI and *Swissnuclear*. Thus, the students spend their first semester at EPFL, the second at ETHZ, while the third is spent mainly at PSI on the selected research project.

There are seven compulsory courses in the NE Master, corresponding to 28 ECTS credits in total. These are: Neutronics, Reactor Experiments, Reactor Technology, Nuclear Fuels & Materials, Nuclear Safety, Special Topics in Reactor Physics, and Nuclear Energy Systems (relating to the nuclear fuel cycle). An additional 20 ECTS credits of course work, which the students need to complete, correspond to five NE *core electives*. These are chosen from 12 optional courses offered in the following three *tracks:* Energy Systems, Physics and Materials, and Thermal Hydraulics. The remaining ECTS

[1] European Credit Transfer System

credits are acquired from a free elective course (4 credits), a course in entrepreneurship (2 credits), a semester project (6 credits), and finally the combination of industrial internship and Master-level thesis (30 credits).

The semester project is aimed at introducing the students to R&D in nuclear engineering. The topic is chosen by the student himself/herself, largely on the basis of a 1-day technical visit to PSI, arranged towards the end of the first semester. Here, the principal on-going NES research activities are presented, along with an indication of possible Master-level thesis topics. This constitutes an important criterion for the student's choice of laboratory in which to work, since the semester project is usually considered as a preparatory phase for the thesis. As illustration, Table 1 lists the different R&D activities presented during the students' visit to PSI in December 2009.

	R&D Activity	Responsible Laboratory
1.	Experimental Reactor Physics	Reactor Physics and Systems Behaviour
2.	LWR Core & Transient Analysis	
3.	Gen. IV Fast Reactor Studies	
4.	Thermal-Hydraulics Phenomena	Thermal Hydraulics
5.	Severe Accident Phenomena	
6.	Nuclear Fuels R&D	Nuclear Materials
7.	Reactor Component Safety	
8.	High Temperature Materials	
9.	Analytical Techniques (Fuels)	Hot Lab
10.	Waste Management	Waste Management
11.	Technology Assessment	Energy Systems
12.	Risk & Human Reliability	
13.	Materials for Nuclear Fusion	Centre for Research in Plasma Physics (EPFL)
14.	Magnets for Nuclear Fusion	

Table 1: **NES presentations made to the 2009 batch.**

As regards organisational aspects, the NE Master is conducted under the supervision of a *core group,* composed of professors from the two universities, the head of NES, and a representative of *Swissnuclear*. Applicants to the programme hold Bachelor degrees in various fields, physics and mechanical engineering being the most common; selection of the best candidates for admission to the NE Master is one of the principal functions of the core group.

Although many of the NE courses are taught by EPFL and ETHZ professors, a key challenge has been finding the additional lecturers needed to meet the demanding requirements of the full Master curriculum. Here again, the PSI contribution has been crucial, the supplementary academic personnel needed having been recruited largely from senior NES staff.

The first batch of NE Master students will receive their degrees in October 2010. These will carry the title of "Master of Science in Nuclear Engineering EPF Lausanne – ETH Zürich" and will bear the emblems of both universities.

Experience to date and prospects

As of the end of 2009, there are 25 students carrying out the NE Master programme – 12 from the 2008 batch and 13 from 2009. Only about 30% of these are students originating from Swiss universities. As such, the programme, although naturally addressing Switzerland's needs, is clearly to be viewed in an international context: namely, that of the Bologna Process. This is further evidenced by the fact that, during the last semester at Lausanne, there were several exchange students in Nuclear Engineering from other European countries.

The general feedback from the NE Master students themselves has been very positive. Those of the first batch – the ones who have completed the two semesters of course work at EPFL and ETHZ – report that attending classes in two different universities has indeed been an enriching experience. In spite of the diversity of their technical backgrounds at the Bachelor level, all the students have found the courses both interesting and challenging. Moreover, the wide range of R&D topics made available for the research work undertaken at PSI has been seen as a noteworthy strength of the programme.

The experience acquired to date with running the NE Master has, however, also brought out the need for upgrading the programme from 90 to 120 ECTS credits. On the basis of detailed deliberations conducted during 2009, it has accordingly been decided to introduce – starting September 2010 – an additional semester. This will be spent largely at PSI, and will involve the integration of new courses, as well as allowing an increase in the time available for the industrial internship and for research. It is expected that this forthcoming change will not only strengthen the programme as a whole, but also serve to further enhance its compatibility with other major nuclear engineering programmes in Europe.

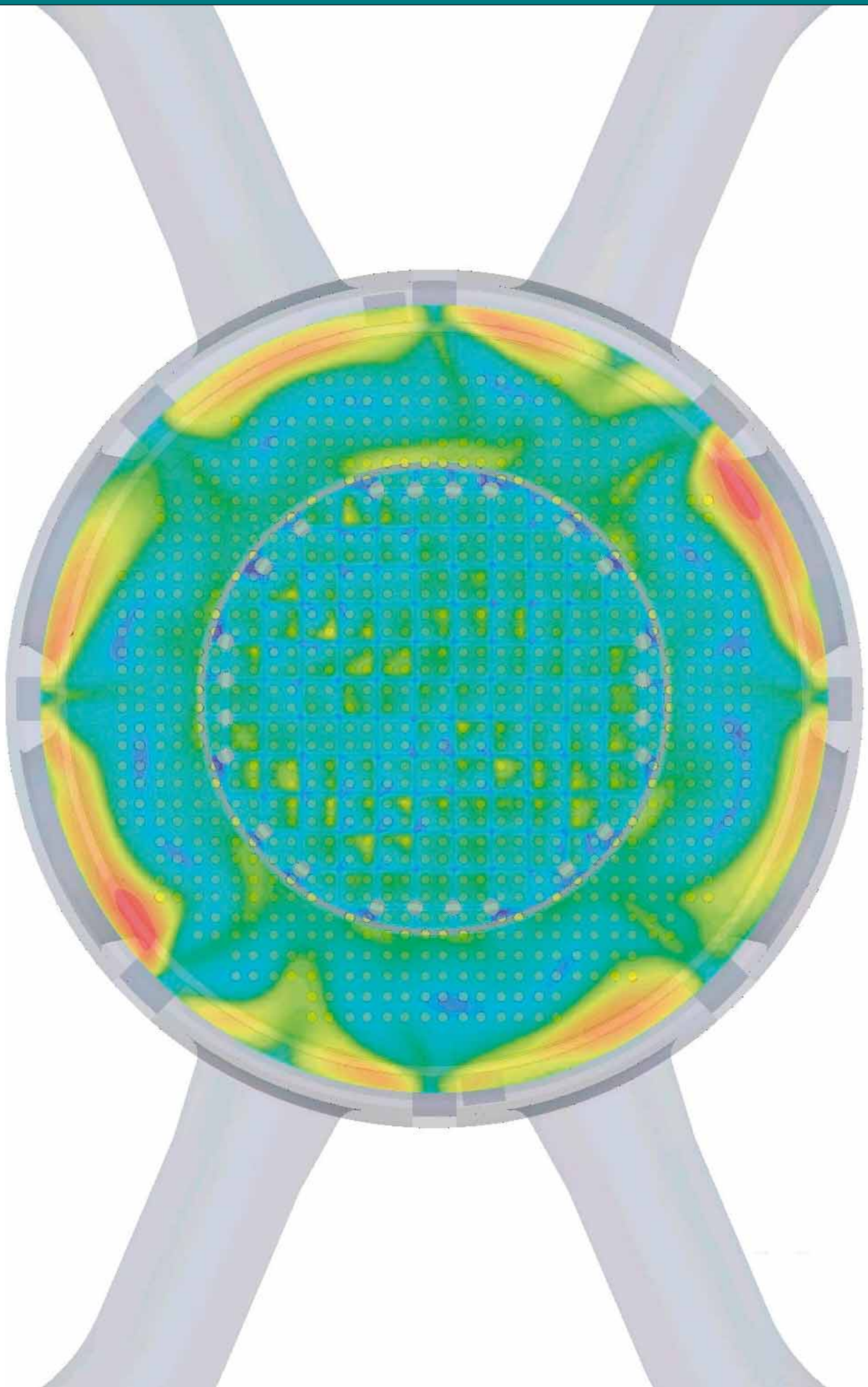
Acknowledgements

The authors would like to acknowledge the invaluable assistance received from staff of EPFL, ETHZ, PSI and the Swiss nuclear industry who have contributed to the success of the NE Master programme.

References

[1] http://www.master-nuclear.ch/

[2] http://www.enen-assoc.org/



Laboratory for Reactor Physics and Systems Behaviour (LRS) 13

Current activities within LRS are centred around four principal project areas:

LIFE@PROTEUS

This project aims at improving measurements of fission-rate distributions across the interface between fresh and highly burnt fuel. The data will serve to validate modern reactor analysis codes, especially in regard to detailed pin-power calculations.

PROTEUS-UPGRADE

This project is concerned with the upgrading of the PROTEUS zero-power reactor to contain significant amounts of radio-activity, as a pre-requisite for the measurement of large quantities of highly burnt fuel. At the same time, requirements by the regulator with respect to I&C and earthquake resistance are being addressed.

STARS

The STARS project aims at the development, maintenance and application of a comprehensive code system, together with the necessary input database, to enable a safety assessment of the Swiss nuclear reactors from "the pellet to the turbine" to be made. Focus areas include neutronics analysis of the reactor cores (including fast-fluence evaluations and criticality safety assessments), coupled (neutronics-TH) transient analysis of plant systems, and uncertainty analysis for TH and neutronics problems, and fuel behaviour modelling. This project cultivates the multi-physics aspects of plant safety assessment for LWRs.

FAST

This project is aimed at the development and implementation of a code system representing state-of-the-art safety analyses of nuclear systems with fast neutron spectra (Gen IV reactors). Its specialities are the comparative analysis of gas-cooled, lead-cooled and sodium-cooled fast reactor systems, and the evaluation of iso-breeding equilibrium cores.

Education

The research projects within LRS additionally provide motivation and subject material for doctoral and MSc theses in support of training in nuclear technology at EPFL, and are strongly coupled with the joint EPFL-ETHZ Nuclear Masters Programme. It also includes teaching assignements of senior collaborators.

◀ **Computed velocity field in the EPR reactor pressure vessel below the lower plenum mixing device.**

Approaching uranium dioxide from first principles

Matthias Krack, *Laboratory for Reactor Physics and Systems Behaviour, PSI*

Numerical simulation based on first principles has matured to become a third pillar of equal importance in research to the two classical pillars of experiment and theory. Accurate and reliable simulation methods, based on the fundamental laws of physics, are now available for chemical reactions using supercomputers, thus opening a new era in materials research. The behaviour of nuclear fuel, such as uranium dioxide, can now be determined numerically, thereby reducing the need for difficult, costly and hazardous experiments. The properties thus determined can be used as input parameters to the macroscopic fuel performance codes employed for safety evaluations.

In recent decades, numerical simulation has become, alongside experiment and theory, the third major component in research, and fundamental research in particular is driven nowadays by the strong interplay between these three basic ingredients (Fig. 1).

Advances in the use of simulation techniques is due to the rapid growth in computing power. The development of accurate and reliable simulation methods has opened the door to a new quality of research in, for example, biology, chemistry and materials technology. For instance, chemical reactions are now performed in the computer (*in silico* biology) using first-principles simulation methods. In this way, computers have become virtual laboratories, and supercomputers can now be regarded as a new kind of high-performance research facility, complementary to experimentation.

First-principles methods

First-principles, or *ab initio,* methods are directly derived from an accurate description of the established laws of physics, involving no *ad hoc* assumptions or fitting parameters. Their predictive power originates from this basic concept. Prominent examples are electronic structure methods, which solve the Schrödinger equation of quantum mechanics to obtain the wavefunction of a system. Once this is known, then, in principle, all kinds of physical properties can be derived from it. However, it is difficult to solve the Schrödinger equation, since the electrons behave as non-classical particles, and exhibit complicated, correlated motions with respect to the nuclei. A straightforward, 'brute-force' solution is already computationally too demanding, even for systems with just a few atoms. Controlled approximations that can be physically justified are required.

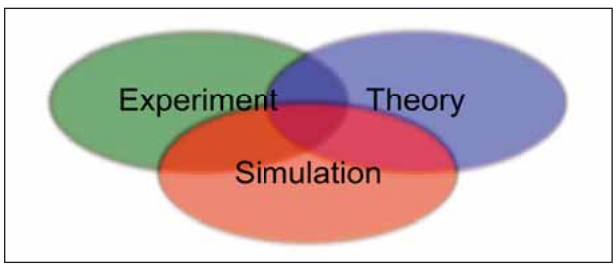


Figure 1: **Interplay of major research ingredients.**

For instance, an important approximation that is commonly being applied is the adiabatic separation of the motion of nuclei and electrons, also known as the Born-Oppenheimer approximation. The separation is physically justified because of the large mass difference between nuclei and electrons. However, to determine the correlated motion of the electron alone still remains a challenging problem, and many advanced techniques are employed for its solution.

Density Functional Theory (DFT) has become a very popular and efficient approach to tackle the problem. Hohenberg and Kohn [1] showed in their seminal work in 1964 that there is a one-to-one correspondence between the electron density and the energy of a system. The advantage of dealing with the electron density rather than the wavefunction becomes immediately obvious if one notes that the wavefunction of an N-electron system depends of 3N coordinates (or even 4N if spin is included). In contrast, the electron density is given by the square of the wavefunction integrated over N-1 electron coordinates, which only depends on the 3 spatial coordinates, independently of the number of electrons. Within the framework of DFT, the electronic interactions are described by a functional that provides a direct mapping between electron density and energy. Though the exact functional is

not known, functionals derived from the physical properties of the electron gas have been derived. The results obtained are surprisingly accurate and reliable, even though one would not intuitively expect that the electrons in a crystal or a molecule to bear any resemblance to an electron gas. Consequently, strongly correlated electrons, like the *d*-electrons of the first-row transition metals, or the *f*-electrons of the lanthanide and actinide elements, are challenging for DFT methods, and require special treatment. Moreover, for the heavy actinide elements like uranium, appropriate consideration of the relativistic effects is also needed.

Ab initio molecular dynamics

Nowadays, using a supercomputer, it is possible to solve the electronic structure problem for an atomic configuration consisting of about 100 atoms in less than a minute with advanced implementations of the DFT method [2]. The actual potential of the system is calculated 'on-the-fly', based on first principles. The energy and the forces on all the atoms are computed, which allows propagation of the system in time by integrating Newton's equation of motion. An integrator time-step of the order of a femtosecond (10^{-15} s) is needed, due to the fast motion of the atoms. This is a very short interval, but many chemical reactions take place on a femtosecond time-scale, and simulation times of a few tens of picoseconds (10^{-12} s) are often sufficient to simulate a reaction, thus enabling insights to be gained at the atomistic level into the elementary chemical processes. The upcoming SwissFEL experiments will enable comparisons between experiment and simulation to be carried out on the same time-scale. In this way, further validation of the applied simulation techniques and their underlying theoretical methods can be achieved.

Simulation of nuclear fuels

Nuclear fuels consist of actinide materials. Experiments with such materials are difficult, and are often very expensive, especially if irradiated material is to be examined. Computer simulations using DFT methods provide an alternative way to obtain reliable data for these materials, which can then be used as input parameters for fuel-performance codes. In this way, a direct link from the atomistic scale to the macroscopic simulation methods employed for safety evaluations of nuclear facilities may be established. Accordingly, the development, validation and application of new computational tools that exploit the performance of modern supercomputing facilities are required. This is the main goal of the materials simulation group, which is a new activity within the STARS project at PSI. The CP2K program package [3] for atomistic simulations is being developed in the framework of an open-source project with a focus on the application to actinide materials, such as uranium dioxide (UO_2). This is technologically one of the most important actinide materials, since it is the main component of the nuclear fuels currently employed in power reactors. Figure 2 shows the fluorite structure of pristine UO_2.

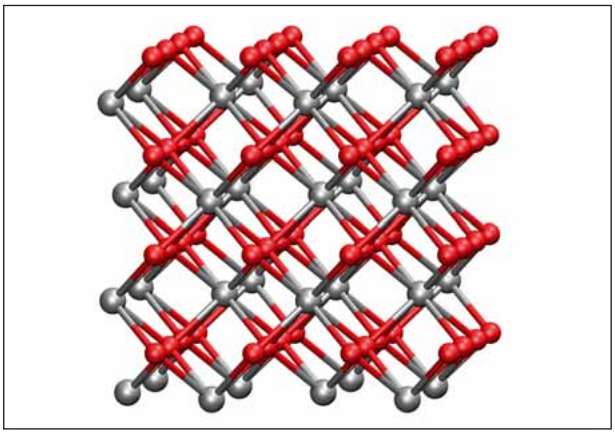


Figure 2: **UO_2 (U grey, O red) fluorite structure at 0 K.**

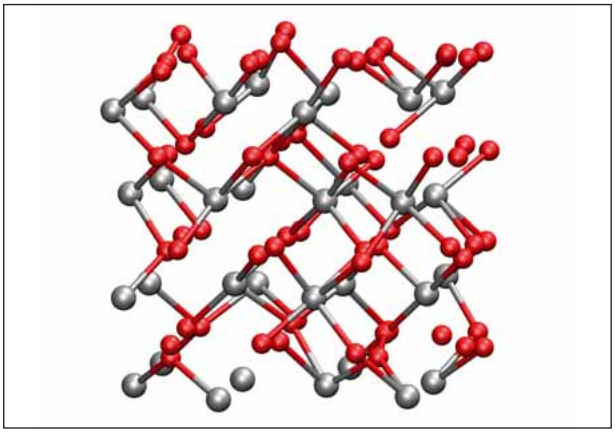


Figure 3: **Snapshot from a molecular dynamics simulation of pristine UO_2 at 1 bar and 1500 K.**

This sample was computationally 'heated' to 1500 K at 1 bar pressure using the *ab initio* molecular dynamics scheme implemented in CP2K. As seen in Fig. 3, the oxygen sublattice already exhibits a much higher disorder than the uranium sublattice at this temperature.

The work described here has been undertaken within the EU FP7 project F-BRIDGE [4].

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Gamma-ray and delayed-neutron measurements of fission-rate distributions in burnt fuel

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Laboratory for Reactor Physics and System Behaviour, PSI

The LIFE@PROTEUS programme is being undertaken at PSI to characterise the interfaces between burnt and fresh fuel assemblies in modern Light Water Reactors (LWRs). In this context, new techniques to measure fission rates in burnt fuel are currently being developed by the PROTEUS reactor team. Following irradiation in PROTEUS, the induced fission rates for fresh- and burnt-fuel samples are estimated through the detection of both the high-energy gamma rays (i.e. above 2200 keV) emitted by short-lived fission products freshly produced in the fuel, and by delayed neutrons. Experimental results using both techniques have successfully demonstrated the feasibility of such measurements in burnt fuel.

Higher initial fuel enrichments and discharge burn-ups have led to increasingly heterogeneous core power distributions in modern nuclear power plants. In the light of these trends, PSI has launched, in collaboration with *Swissnuclear,* an experimental programme called LIFE@PROTEUS [1], which necessitates an upgrade of the PROTEUS reactor at PSI. One of the goals of the programme is to accurately measure the pin power distributions across the interfaces between fresh and spent fuel in the PROTEUS test zone. As a consequence, novel experimental techniques are needed to determine the fission rates in both fresh and spent fuel pins. Two new techniques are currently being evaluated. One utilises the high-energy γ-rays (above 2200 keV) emitted by short-lived fission products freshly produced in the fuel [2], and the other makes use of the output of delayed neutrons following irradiation [3].

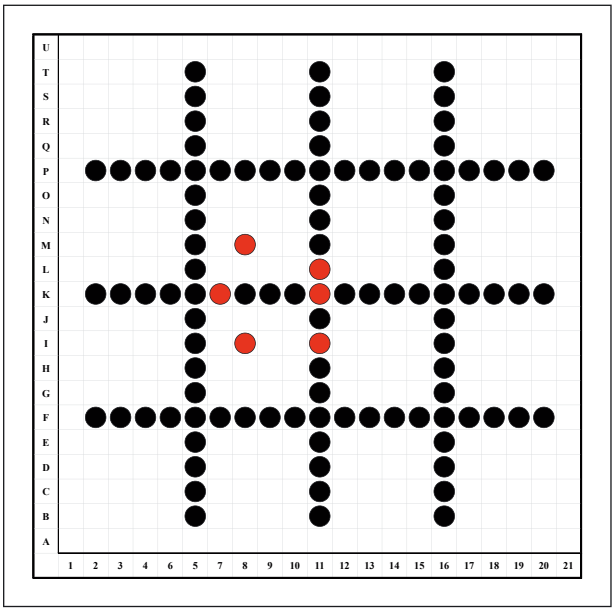

Figure 1: **Layout of the lattice mock-up in the PROTEUS test zone. The 5%-enriched fresh UO_2 fuel pins are marked in black, while the positions available for insertion of fresh and burnt fuel samples are marked in red.**

Experiment

To demonstrate the feasibility of such techniques, fresh- and burnt-fuel samples, with nominal burn-ups of 0 (fresh), 36, 46 and 64 GWd/t, have been irradiated in the PROTEUS test zone, and, in separate experiments, their γ-ray and neutron emissions after irradiation recorded. The mock-up lattice, in which the samples were irradiated, is shown in Fig. 1. The irradiation positions I8, I11, K7, K11, L11 and M8 are highlighted in red.

An example of the γ-ray spectra obtained for the 36 GWd/t sample before and after irradiation is shown in Fig. 2. For the first time in a zero-power reactor like PROTEUS, it has been possible to detect the high-energy, freshly-induced γ-ray activity in burnt fuel, despite the high intrinsic activity (with energies of up to 2200 keV).

Based on γ-ray lines above 2200 keV from four short-lived fission products with half-lives of 10–90 min. (^{142}La (2542 keV), ^{89}Rb (2570 keV), ^{138}Cs (2640 keV), and ^{95}Y (3576 keV)), four estimates of the relative fission rates could be derived by comparing the same samples irradiated in different lattice positions. At the current state of analysis, in which the four separate estimates were combined to a single estimate by

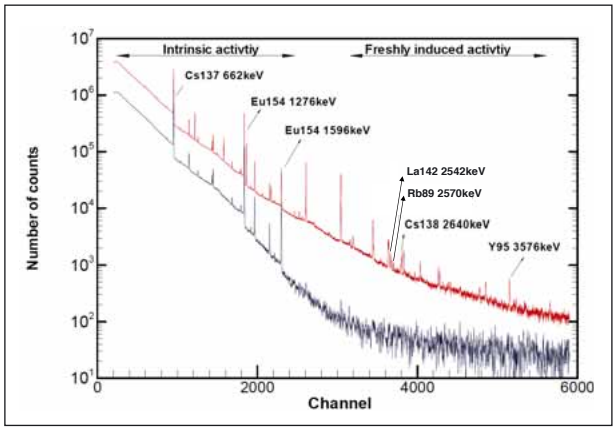

Figure 2: **Spectra of γ-ray activity from the 36 GWd/t burnt sample before irradiation (blue) and directly after irradiation (red).**

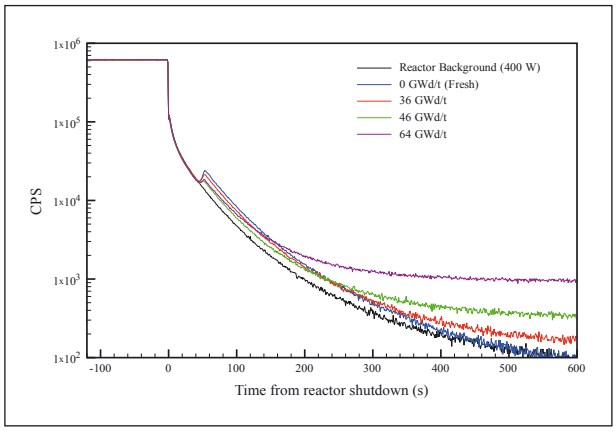

Figure 3: **Detector counts after irradiation of different fuel samples for a reactor flux of 2×10^9 n/cm²s, corresponding to a power of 400 W.**

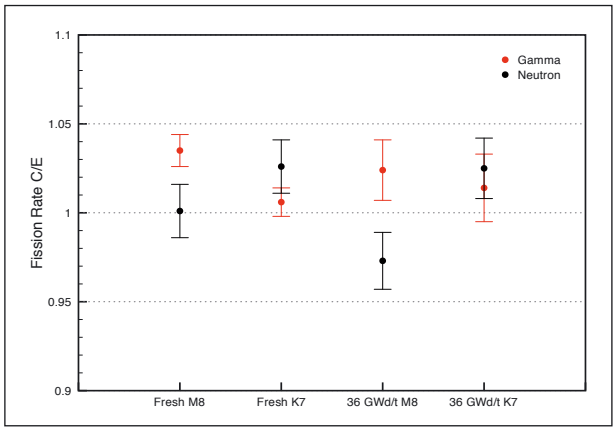

Figure 4: **Comparison of C/Es for the gamma-ray and delayed-neutron techniques.**

taking a weighted mean, it appears that discrepancies between the measured fission-rate ratios may be attributed primarily to the underlying statistical uncertainties.
With regard to the delayed-neutron approach for fission-rate measurements in burnt fuel, the present method has the advantage that, by this means, it is much easier to identify the intrinsic neutron activity (mainly due to ^{244}Cm). Sample neutron outputs are shown in Fig. 3. Accurate fission-rate estimation requires a precise model of the delayed-neutron source for each fuel sample, with the proper proportions of neutrons in each delayed group.

Results

Comparison between the MCNPX-calculated and the experimentally-derived fission-rate ratios (Calculated/ Experimental, C/Es) for both techniques are given in Fig. 4. The ratios were measured for the given lattice positions (M8 and K7) and a reference lattice position (L11) for fresh and 36 GWd/t burnt fuel. The perspective for the future is to reduce the statistical uncertainties of both γ-ray and neutron measurements by a method that increases signal data, such as repeat measurements, irradiation at higher reactor power, or alteration of the detector system to increase count-rate and efficiency.

Conclusions

Both the γ-ray and delayed-neutron techniques show good agreement with the MCNPX predicted values, and represent an important first step in the validation of two novel experimental techniques for the determination of fission rates in both burnt and fresh fuel. As a result of this analysis, work may proceed on comparing fresh-to-burnt fission rates ahead of designing an advanced measurement station for the upgraded PROTEUS reactor.

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Comparison of neutronic and safety parameters of Gen-IV fast-spectrum cores

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The advanced Gen-IV fast reactors should be capable of breeding their own fuel from low-fissile ^{238}U, and to recycle the actinides from their own spent fuel. This recycling, or more specifically the fuel-cycle closure, can significantly reduce the amount of long-lived radioactive waste for ultimate disposal, and increase the sustainability of uranium-fuelled reactors, albeit with a negative impact on safety. The numerical tool EQL3D has recently been developed at PSI to study the equilibrium fuel-cycle procedure for fast reactors, to examine the closed-fuel-cycle concept, and to generally compare the equilibrium safety-related parameters of Gen-IV reactors.

The advanced Gen-IV fast reactors should be capable of utilising ^{238}U as a fissile fuel, and to operate in an iso-breeding mode with a closed fuel-cycle. This concept implies equal production and consumption of ^{239}Pu, and the complete recycling of spent fuel. Each long-term simulation of an iso-breeder reactor of this type converges to an equilibrium condition.

The recently developed EQL3D numerical procedure [1] can be used to provide a quantitative description of the two basic situations: (i) an open-cycle equilibrium – the result of periodic operation with fresh fuel without recycling; and (ii) a closed-cycle equilibrium – the asymptotic state resulting from operation with fixed fuel management, and with recycling of its own fuel. In both cases, EQL3D calculates explicit cycle-by-cycle reactor operation under specified periodic fuel management until an equilibrium state has been achieved.

Three Gen-IV fast reactors: namely, the Gas-Cooled Fast Reactor (GFR), the Sodium-Cooled Fast Reactor (SFR), and the Lead-Cooled Fast Reactor (LFR), have been compared in terms of equilibrium-cycle safety and performance parameters [2]. The design-specific, fuel-cycle parameters have been accounted for, and a ring-wise reloading pattern developed [3-5] for all three cores (see Fig. 1).

Results

It was found that the iso-breeding capability of the initial core depends principally on the ^{239}Pu/^{238}U mass ratio in the fresh fuel. Furthermore, since this ratio tends to equalise in equilibrium for all three cores, its initial value also determines the time-dependency of the reactivity curve.

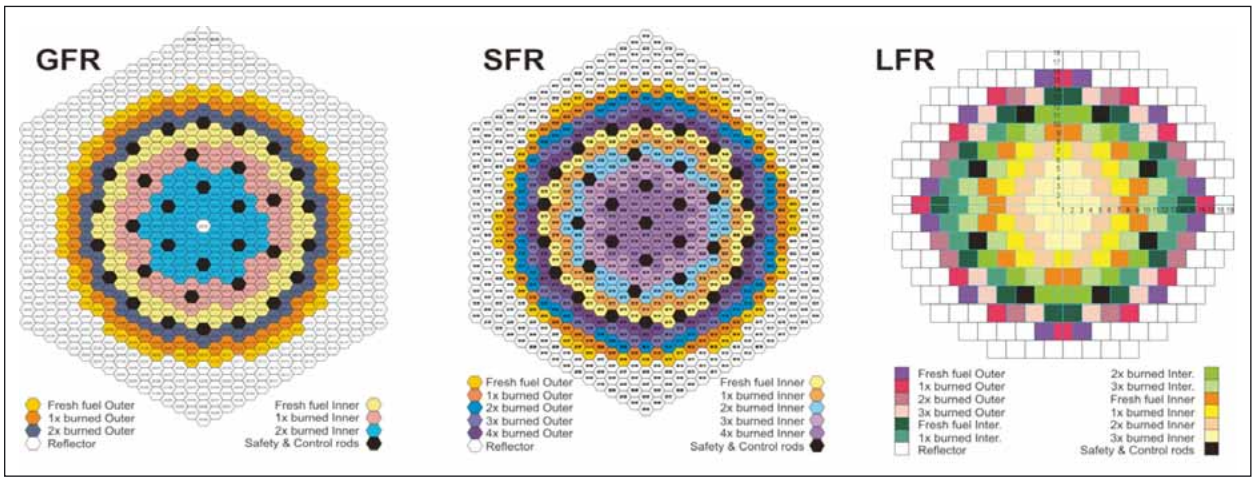

Figure 1: **Multi-batch reloading pattern for three Gen-IV cores.**

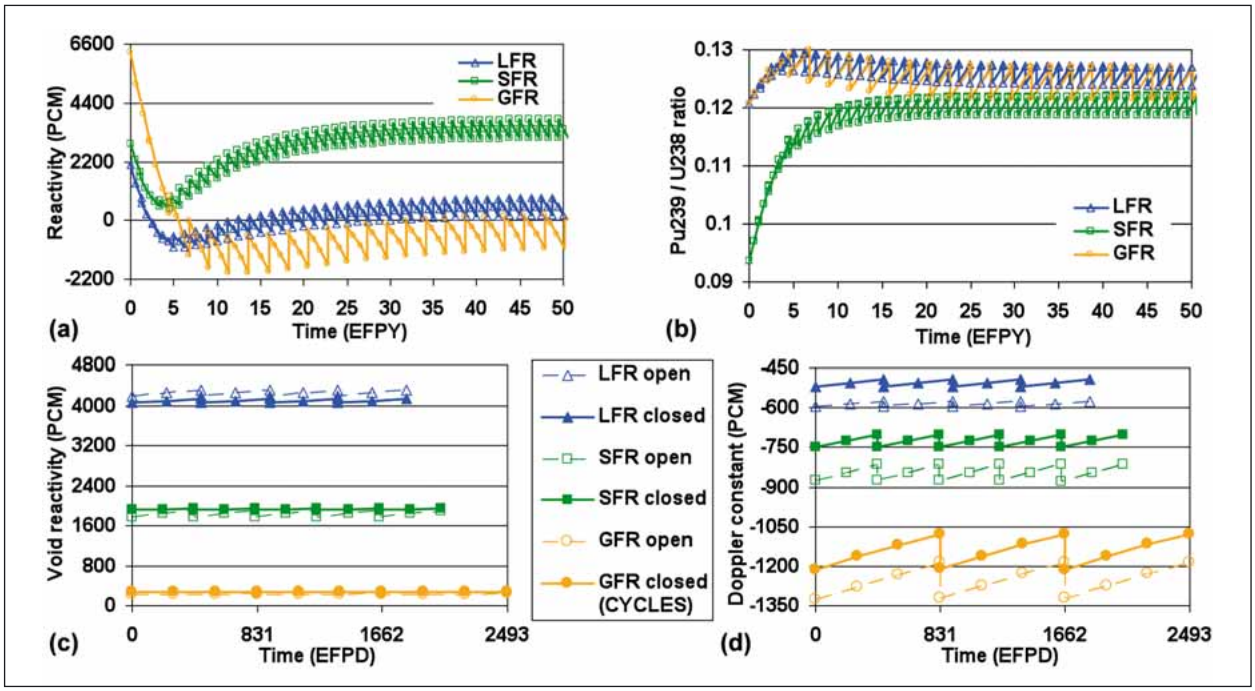

Figure 2: **Evolution of (a) reactivity; (b) 239Pu / 238U ratio during the first 50 Effective Full Power Years (EFPY); (c) equilibrium void reactivity; and (d) Doppler constant for open and closed fuel cycles.**

As can be seen from Fig. 2a, the reactivity curves for all three cores decrease during the first cycle, due mainly to the build-up of fission products. The later evolution is influenced by the variation of the $^{239}Pu/^{238}U$ ratio. In the SFR case, the ratio grows strongly towards equilibrium (Fig. 2b), inducing an increase in reactivity. Therefore, the SFR reactivity curve is always positive.

For the other two cores, the initial and equilibrium ratios are comparable, and so do not provoke strong reactivity increases. As a consequence, the corresponding reactivity curves are partly negative after the build-up of fission products. This situation can be avoided by enlarging the initial ^{238}U inventory, which increases the actinide load to the core, and simultaneously decreases the initial $^{239}Pu/^{238}U$ ratio, thus improving the reactivity curve evolution [3].

The EQL3D procedure also enables safety-related parameters to be directly compared. As an example, void reactivity and Doppler constant [2] are also shown for equilibrium open and closed cycles. The void reactivity (Fig. 2c) depends predominantly on the type of coolant voided in the core. For example, the void reactivity is around 300 PCM (Per Centum Mille = 10^{-5}) for the GFR core, 1800 PCM for the SFR core, and more than 4000 PCM for the LFR core. The SFR and LFR cores have relatively high void reactivity, but the difference between open and closed cycles remains below 10% for these two cases.

The second important parameter is the Doppler constant, which is only indirectly influenced by the type of coolant, through the neutron spectrum. However, the differences between the cores are very noticeable (Fig. 2d). Since the equilibrium $^{239}Pu/^{238}U$ ratio is almost the same for all three reactors, the differences between the Doppler constants may be attributed to their different spectra. Nonetheless, also in this case, the values for open- and closed-equilibrium cycles are in the same range (with a 15% variation). Similar results were also found for the other safety-related parameters.

Conclusions

In spite of the similar equilibrium $^{239}Pu/^{238}U$ mass ratio, the safety-related parameters for the GFR, SFR and LFR reactors are seen to differ strongly as a consequence of the different coolants and spectra. Nevertheless, the results for open- and closed-fuel cycles seem to be comparable. Thus, from a neutronics point of view, once optimised, all three cores could serve as sustainable (i.e. iso-breeding) and clean (in terms of fuel recycling) energy sources.

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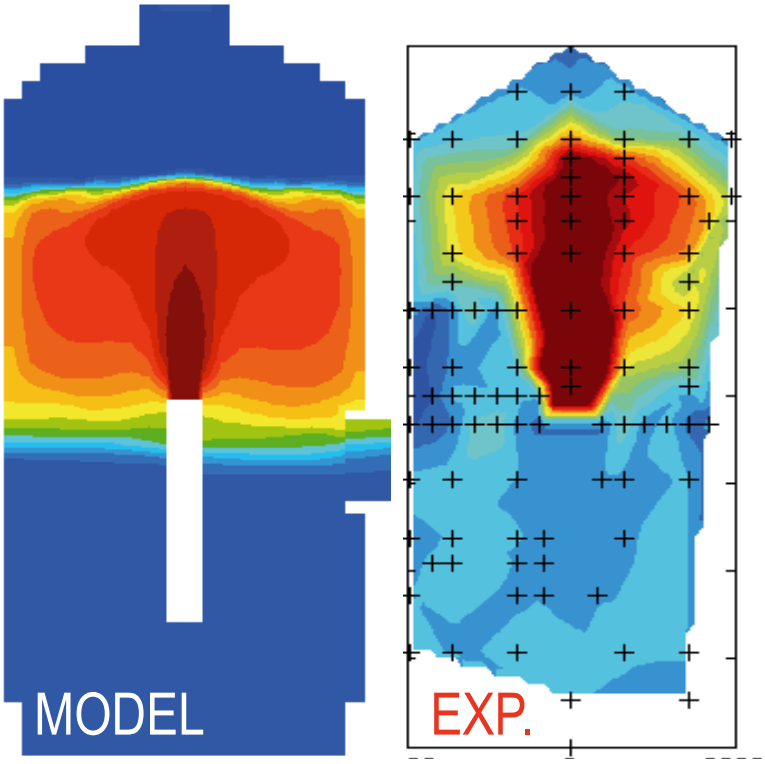
MODEL
EXP.

Laboratory for Thermal Hydraulics (LTH) 21

The Laboratory develops, validates and applies simulation tools at the cutting edge of modelling technology, with a focus on multi-phase and multi-component flows in nuclear reactors and containments, flow boiling and condensation heat transfer, turbulent mixing, aerosol physics and iodine chemistry. The work is oriented towards a stepwise transition from empirical to fundamental modelling on the basis of a multi-scale approach to the issues under investigation.

Efforts fall broadly into two main project areas.

ALPHA

The project addresses safety-relevant, thermal-hydraulic issues common to Generation II, III and IV Nuclear Power Plants (NPPs) concerning accident situations, efficiency and plant life-time management. Originally, the work was focused on the passive safety systems of innovative Light Water Reactors (LWRs). More recently, the experimental base has been broadened to encompass fundamental phenomena in both the primary circuit and containment of NPPs. The unique, large-scale containment test facility PANDA, which is the experimental backbone of this work, has evolved into one of the best instrumented and most versatile containment test facilities in the world. A number of new small-scale tests, equipped with high-resolution, multi-phase measuring instruments, complement the large-scale facility, providing the parallel Computational Fluid Dynamics (CFD) activity with its essential experimental database.

Source Term Evaluation

Activities here are centred around the ARTIST test facility, which provides unique data on aerosol transport and retention during a severe accident involving a Steam Generator Tube Rupture (SGTR) event. The particular focus on iodine chemistry has resulted in novel, highly efficient methods for filtered venting of the containment to be constructed. Findings from the tests have been incorporated in state-of-art, severe-accident analysis codes, such as MELCOR. LTH is an internationally recognised competence centre in the field of beyond-design-basis accidents and source-term analyses.

◀ **Advanced experiments for nuclear safety: large-scale containment tests on hydrogen behaviour (top), liquid films in BWR fuel rod spacers (bottom left), aerosol deposition in a PWR steam generator tube bundle (bottom right).**

Turbulent mixing of stratified fluid layers within and beyond the OECD/SETH-2 project

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Hydrogen may be released into the containment of a Light Water Reactor (LWR) during a (postulated) severe accident. With the presence of hydrogen, there is always the risk of deflagration and/or detonation, so accurate prediction of the actual hydrogen distribution in the containment volume becomes an important consideration in assessing the overall risk. Mixing and stratification are key elements in determining the hydrogen distribution, and the PANDA tests within the OECD/SETH-2 project address these issues. In addition to the large-scale PANDA tests, complementary, dedicated, small-scale experiments, featuring innovative measuring techniques, are also being performed, focusing on the fundamental aspects of turbulent mixing phenomena in the presence of strong density gradients.

Mixing and stratification are important phenomena in nuclear safety assessment: mixing of coolant streams in T-junctions in parts of the primary reactor circuit during Emergency Core Cooling (ECC) water injection, and in the outlet duct of High Temperature Reactors (HTRs), are two examples. The same phenomena also occur in a reactor containment during a (postulated) accident involving core overheating, in which hydrogen, steam and air are all present. Stratification, due to the different densities of the gases, can lead to a local increase in hydrogen concentration, and to the formation of mixtures which could result in deflagration and/or detonation.

The steam released from the primary circuit during a Loss of Coolant Accident (LOCA), water injection by the spray system, the heat release due to the functioning of the catalytic hydrogen recombiners, and the heat removed by containment coolers, all induce turbulent flow conditions in the containment, promoting mixing and the subsequent destruction of any potentially dangerous hydrogen-rich mixtures. Prediction of the exact flow dynamics is a challenging task for both advanced reactor system and 3D Computational Fluid Dynamics (CFD) codes.

Experiments in the PANDA facility in the framework of the OECD/SETH-2 project [1] are designed to increase understanding of the mixing processes taking place in the initially stratified gases making up the containment atmosphere, and to quantify them by the creation of a database suitable for the assessment and validation of the associated computational tools. The added value of the large-scale, multi-compartment PANDA facility [1] is its ability for tests to be performed at a scale approaching those of the compartments of an actual LWR containment using CFD-grade instrumentation.

PANDA experiments and simulations

The operating conditions reproduced in the SETH-2 tests (injection geometry, extent of the helium/steam stratification layer, temperatures, pressures, etc.) are all designed to be representative of possible accident conditions in an actual LWR containment, and so represent a relevant experimental database for the accompanying numerical analyses.

An example is shown in Fig. 1, in which 2D/3D results obtained using the GOTHIC code are compared with measured data for one of the tests, named 'Vertical Fluid Release', in which a vertical steam jet released into a PANDA dry-well vessel impinges upon an overlying helium-steam layer, inducing mixing. A 2D, fine-mesh representation predicts the destruction of the stratification layer to occur after about 1400s, while according to a 3D coarse-mesh simulation the stratification persists up to 1800s.

Participants in the SETH-2 project (regulatory authorities, industry and national research institutes) have also used the test results for their own validation exercises, using codes such as FLUENT, CFX, GASFLOW, ASTEC, TONUS and CAST-3M. Other tests in the series focus on the influence of horizontal jet release, containment sprays, containment coolers, hydrogen/oxygen recombiners, rupture disks, and the Integral Passive Containment Cooling system on the hydrogen distribution.

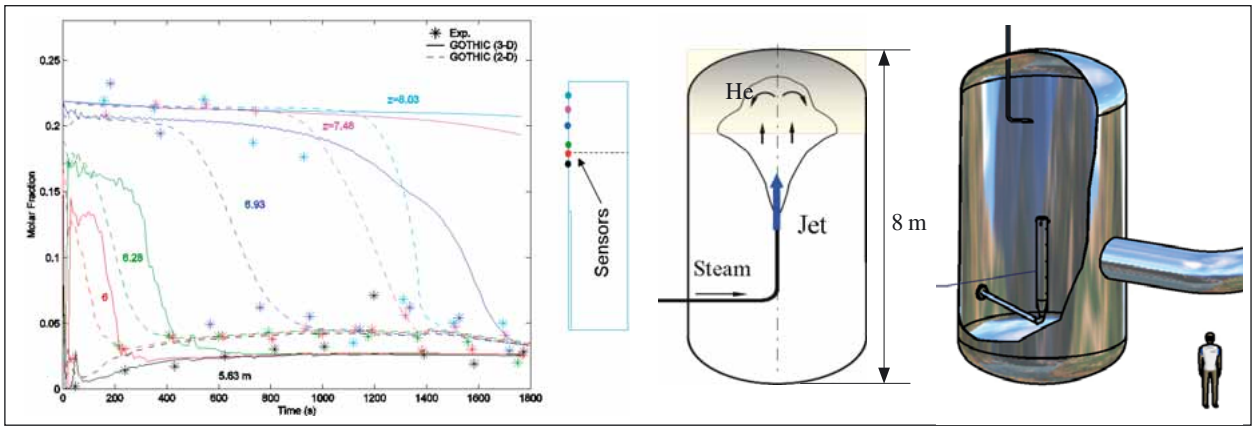

Figure 1: **Simulation of a PANDA test with the GOTHIC code.**

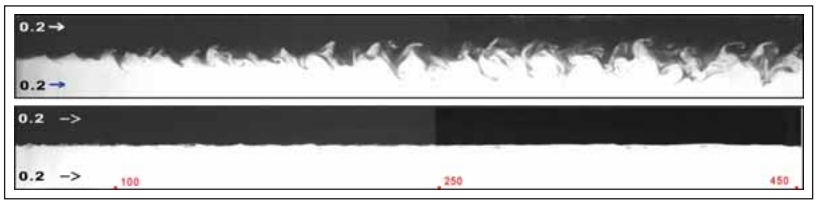

Figure 2: **Isokinetic mixing in the GEMIX facility.**

Stratified layer tests in GEMIX

Complementary to the PANDA tests, simplified, small-scale experiments are also being performed. The data obtained are more detailed than is possible in a large-scale facility, and so are better suited to address the fundamentals of mixing, and for the improvement of the underlying numerical models, particularly those representing turbulent mixing.

The GEMIX (GEneric MIXing) facility consists of a horizontal channel of square cross-section in which two liquid streams of different densities mix downstream of a splitter plate separating the upper and lower halves of the channel in the inlet section. In the channel, a combination of different, high-resolution measuring techniques is employed [2]. Local liquid velocities are measured using Particle Imaging Velocimetry (PIV) and Laser Induced Fluorescence (LIF), and additional measurements are provided by wire-mesh and wall sensors. All the measured data together are aimed at characterising the flow field, and quantifying the transport scalar describing the progress of the mixing with a resolution sufficient to capture the details of the turbulent structures close to the stratified layers. Of particular importance is accurate visualisation and parametric characterisation of the turbulent mixing layer itself, especially the effect of the density gradient on the enhancement and/or suppression of the turbulence intensity. The statistical processing of such experimental data, coupled with the accompanying fundamental numerical turbulence modelling techniques, such as Direct Numerical Simulation (DNS) and Large Eddy Simulation (LES), is primarily directed towards the improvement of the turbulence models used in CFD codes, and in the pseudo-3D system codes currently used for integral containment analysis.

Figure 2 contrasts the mixing process for iso-kinetic streams under unstably-stratified (i.e. heavy fluid above light fluid, upper image) and stably-stratified (i.e. light fluid above heavy fluid, lower image) conditions in GEMIX. The mixing region grows with distance downstream in the non-stratified case, while this growth is almost completely suppressed in the presence of stratification. That is, turbulent mixing in the vertical direction (and consequently entrainment) is effectively suppressed for the stratified case.

An important spin-off benefit is the fact that the small-scale tests are especially rich sources of research for student projects. In particular, students enrolled in the new Masters Degree in Nuclear Engineering course, recently launched jointly by ETHZ and EPFL, are actively involved in the project.

Summary

Mixing and stratification (of both liquids and gases) are phenomena occurring in different parts of a nuclear power plant, and in many other industrial-scale installations. Consequently, the research activities reported here have a broad range of application.

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Reynolds-Averaged and Large-Eddy-Simulation studies of turbulent mixing in a square channel

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The quantification of turbulent mixing is of fundamental importance in many engineering applications, including chemical processing, environmental flow studies, and nuclear reactor operation and safety. It is essential therefore, to develop a detailed understanding of the relevant phenomena, and to validate the accepted numerical models in current use. In the present study, Reynolds-Averaged Navier Stokes (RANS) turbulence models and Large Eddy Simulations (LES) have been applied to the mixing process of two iso-kinetic water streams of similar densities flowing in a square channel.

Turbulent processes play an important role in many engineering applications involving the rapid and effective mixing of fluids. Reliable prediction of mixing using numerical methods is highly desired, but is computationally challenging, since the mixing process takes place over a wide spectrum of turbulent scales, necessitating the validation of different turbulence models against experimental data. In this work, the results of RANS and LES models are compared against measured data from laboratory-scale experiments dealing with basic mechanisms of turbulent mixing. The standard *k-ε* turbulence model and the Reynolds Stress Model (RSM) are employed for the RANS modelling, and a number of subgrid-scale (SGS) models for the LES approach. The effects of using different spatial discretisation schemes are also discussed.

Experimental set-up

The experimental facility GEMIX (Generic Mixing Experiment) consists of a square channel of dimensions 50×50 mm, constructed of acrylic glass, with the upper and lower inlets separated by a splitter plate of 2 mm thickness (see Fig. 1). Two co-current water streams at 20 °C, but with different electrical conductivities, are introduced into the upper and lower sections of the channel, and allowed to develop separately over the splitter plate for 1000 mm before mixing.

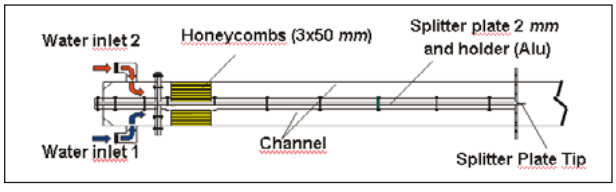

Figure 1: **Schematic of the PSI EXTREM facility.**

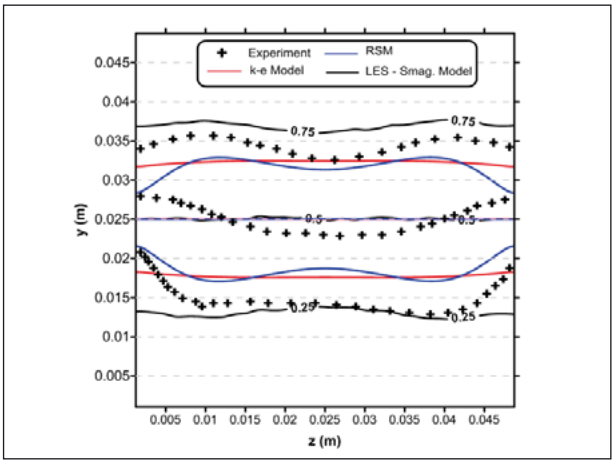

Figure 2: **Comparison of concentration isolines for the RANS (k-ε) and LES (Smagorinsky) models.**

Electrical conductivity measurements are performed using a Wire-Mesh Sensor (WMS) [1] at channel cross-sections varying from 596 mm to 949 mm downstream of the splitter plate trailing edge.

Calculations

The Fluent 6.3 CFD code [2] has been used for the simulations performed in this study, with the standard *k-ε* and RSM turbulence models being employed, the latter being specifically applied to predict the secondary flows. In addition, the Large Eddy Simulation (LES) approach has been employed with four SGS models: Smagorinsky [3], Dynamic-Lilly [4,5], WALE [6] and the turbulent SGS transport model [2]. All calculations have been performed using the wall-function approach to avoid excessive mesh concentrations near boundaries.

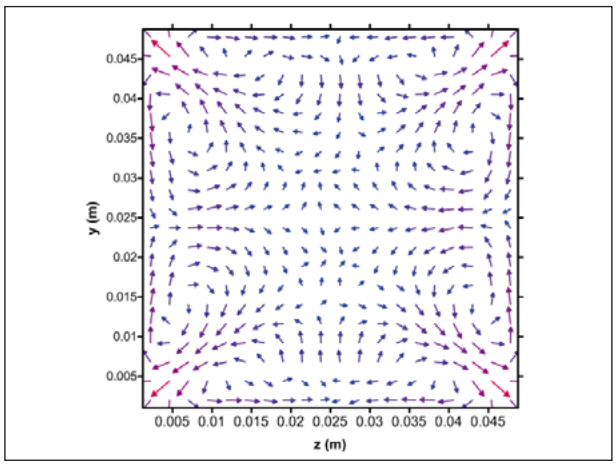

Figure 3: **Secondary flow structures, as predicted by the LES models.**

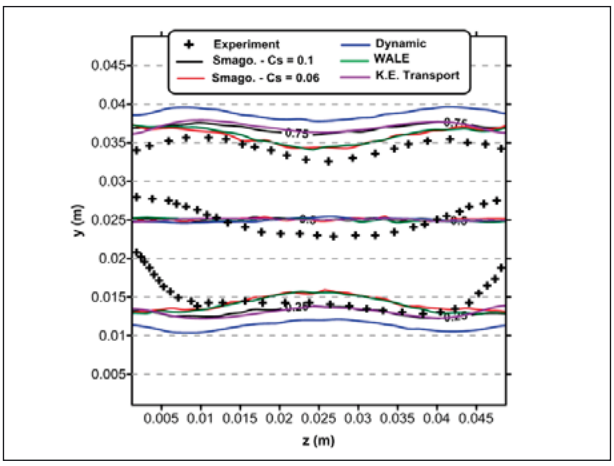

Figure 4: **Comparison of concentration isolines obtained using LES with different SGS models.**

The entire channel, including the developing regions over the plate, was discretised using around 500K hexahedral meshes. The mesh resolution was $\Delta y^+ = \Delta z^+ \cong 90$ and $\Delta x^+ \cong 160$. The time-step used in the LES calculations is constrained by the time-scale of the smallest resolved scales of motion and the maximum allowable Courant number. The simulations were continued for 35 large-eddy turnover times, of which the first 10 were used to achieve fully-developed turbulent flow conditions. In addition, a further 25 turnover times (i.e. 60 overall) were simulated to ensure that asymptotic conditions had been achieved.

Results

All the results shown below refer to the cross-section 949 mm downstream of the splitter plate tip. In Fig. 2, it can be seen that the standard k-ε model gives an almost flat profile, while the RSM and LES models are both able to predict the qualitative behaviour of the concentration isolines measured in the experiment; in addition, LES gives good quantitative comparisons. One merit of the latter two models is their ability to predict the secondary flow structures shown in Fig. 3. These have a significant influence on the mixing process, since they transport low-momentum fluid from the corners of the channel to the centre, and high-momentum fluid from the centre to the corners. Comparing the different SGS models (Fig. 4), it is seen that the kinetic energy SGS model, in which a further transport equation (that for the SGS turbulent kinetic energy) is used to determine the SGS eddy viscosity, gives the best results. Figure 5 illustrates that all the SGS models give similar results if the bounded central difference (BCD) scheme (a blending of central and upwind differencing) is employed, and seems to imply that the associated numerical diffusion has masked the influence of the very low SGS turbulent diffusivity predicted by the models.

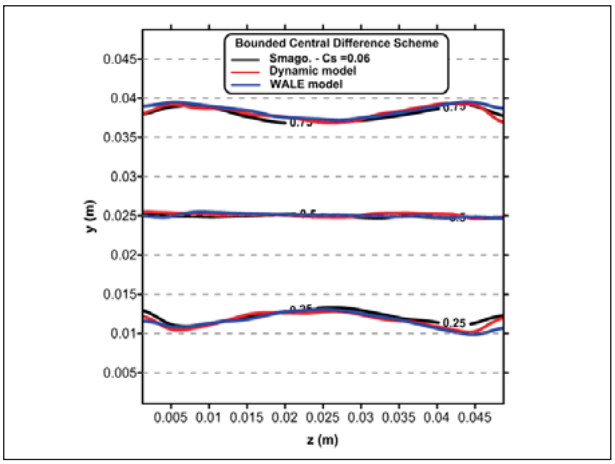

Figure 5: **Comparison of concentration isolines obtained using LES with different SGS models (each employing the BCD scheme).**

Conclusions

RANS and LES turbulence models have been applied to simulate the mixing of two iso-kinetic water streams in a square channel. Best comparisons against experimental data are obtained using LES with the turbulent kinetic energy SGS model. In addition, the bounded central difference scheme appears to be over-diffusive, influencing the results more than the SGS models themselves.

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Accelerated fuel cladding oxidation under air ingress

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Air ingress, which can occur as a consequence of rupture of a reactor pressure vessel during a postulated severe accident (SA), can lead to accelerated oxidation, fuel degradation and enhanced release of fission products, especially of highly radiotoxic ruthenium. Existing oxidation models in SA codes do not represent all the relevant physical processes, and are not guaranteed to be conservative. A new model has been developed at PSI which attempts to capture the essential features of the oxidation kinetics. The model has undergone assessment against data from separate-effects tests carried out at the Karlsruhe Institute of Technology (KIT). Implementation into MELCOR, the principal code used in Switzerland for analysis of SAs in Light Water Reactors (LWRs), and assessment against integral data are currently underway.

The safety impacts of air ingress on nuclear fuel elements at high temperature have been investigated over many years in severe-accident analyses involving failure of a Reactor Pressure Vessel (RPV) lower head [1], or in Spent Fuel Ponds (SFPs), following accidental loss of coolant. Possible situations that could occur are illustrated in Fig. 1.

The presence of air can lead to accelerated oxidation of the Zircaloy cladding compared to that occurring in steam alone, due to the faster kinetics, and the 85% higher heat-of-reaction drives this process further. Air ingress is also characteristically associated with poor heat transfer. The combined effect of these two factors can give rise to an increased rate of core degradation.

Figure 2 shows the percentage mass loss with air compared to pure oxygen, demonstrating the faster kinetics after a slower initial period. Nitrogen alone remains comparatively unreactive, and acts mainly as a catalyst. (Note that rig limitations often require that oxygen be used as a substitute for steam; separate experiments have demonstrated that the gases behave similarly.)

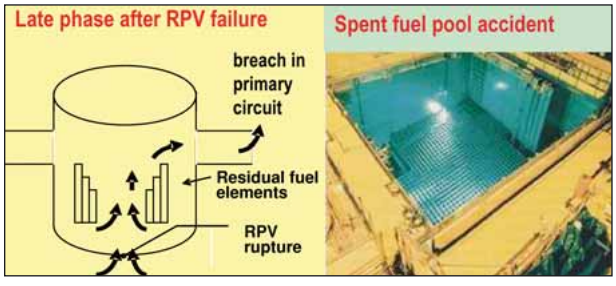

Figure 1: **Examples of air ingress situations.**

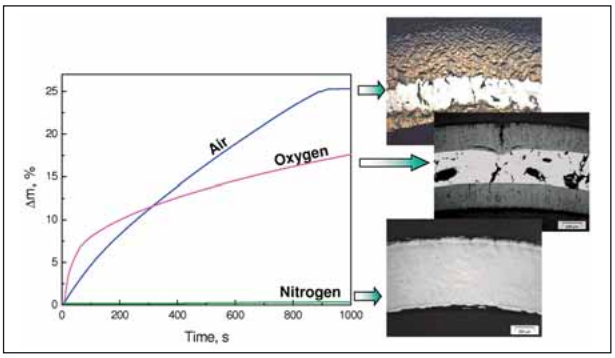

Figure 2: **Effect of nitrogen during air oxidation.**

Also shown in Fig. 2 is the formation of zirconium nitride inclusions, these causing the oxide scale to break away, thus reducing both the resistance to further oxidation and the effectiveness of the oxidised cladding as a barrier to fission product release. Furthermore, the exposure of uranium dioxide to oxygen at high temperatures can lead to increased volatility of some fission products, in particular ruthenium, which is highly radiotoxic.

MELCOR [2] is the principal numerical tool in use in Switzerland for analysis of severe accidents in LWRs, from initiating events through to potential release of radionuclide fission products into the environment. MELCOR is supported by the SCDAP-based codes, which offer more detailed treatment of thermal hydraulics and core degradation. However, neither code adequately models all of the important aspects of air oxidation – particularly the transition to breakaway oxidation – and cannot be guaranteed to be conservative. A new model is required to redress this deficiency.

Model development

Models for cladding oxidation are typically based on the principle that the oxide forms a protective layer, which retains its integrity, thus reducing the rate of further oxidation (in proportion to its thickness). The evolving kinetic rate is referred to as 'parabolic'. Experimental data support this model over a wide range of accident conditions in which steam is the principal oxidising agent. Air oxidation experiments reveal an initial (pre-breakaway) parabolic trend, followed by a transition to post-breakaway linear kinetics once further oxidation fails to increase the protectiveness of the oxide layer. The transition from one state to the other is often accompanied by accelerated oxidation.

The transition to breakaway kinetics is represented explicitly in a new model [3] developed recently at PSI. A central feature of the model is the introduction of two values for the oxide thickness: one related to the criterion for the onset of transition, $\delta_{crit,}$ and the other an effective protective thickness corresponding to the fully-established, post-breakaway state, δ^* (typically somewhat less than δ_{crit}). A timescale, θ, for the transition is also defined, to reflect the observed behaviour. The values of δ_{crit}, δ^* and θ are determined empirically from experimental data. The model is shown schematically in Fig. 3.

The model is conceptually simple, but does take into account a number of additional features not used hitherto. First, transition is observed experimentally to depend on temperature, and the values must reflect this dependence, particularly during a thermal transient. Second, air ingress is typically preceded by a period of oxidation in steam, so a protective oxide layer may already exist. In fact, there may be a mixture of steam and air (or steam and nitrogen, if the oxygen is fully consumed). Finally, oxidation by steam occurs only in the absence of oxygen, while steam-nitrogen mixtures exhibit similar kinetics to air. The model includes features to capture all these characteristics.

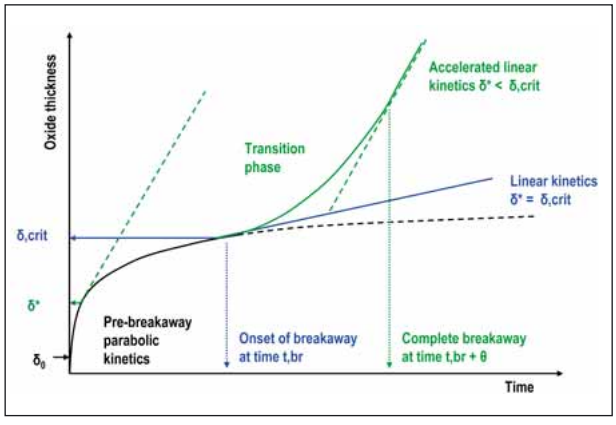

Figure 3: **Schematic of the air oxidation breakaway model.**

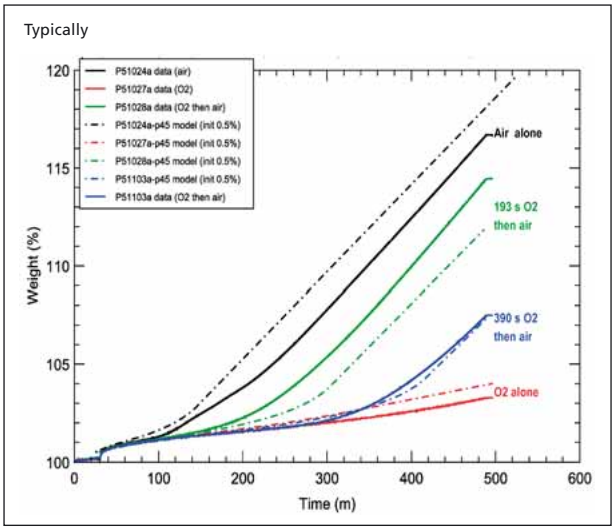

Figure 4: **Comparison with KIT data on oxidation in oxygen and air at 800°C.**

Assessment of the model has been undertaken by comparing model predictions against separate-effects data from experiments performed at KIT. Comparisons for four tests are shown in Fig. 4: for air alone, for oxygen alone, and for air following two different periods of pre-oxidation in oxygen. The results show similar post-transition kinetics (after a rather long pre-transition phase), despite only short periods of pre-oxidation in oxygen. It appears that even a shallow layer of (protective) oxide has a significant delaying effect on the breakaway.

The validation effort will continue with assessments against independent separate-effects data from other sources, such as MOZART, and against integral transient tests, such as QUENCH-10 and OECD SFP [4]. Integral simulations will be performed with the full MELCOR code to give confidence in the application of the model to reactor and SFP transients. Implementation of the model into MELCOR is in progress.

The separate-effects tests also show the oxidation kinetics to depend on cladding type. A worthwhile development would be to extend the model to Zirlo™ and M5® cladding, which are identified for new build.

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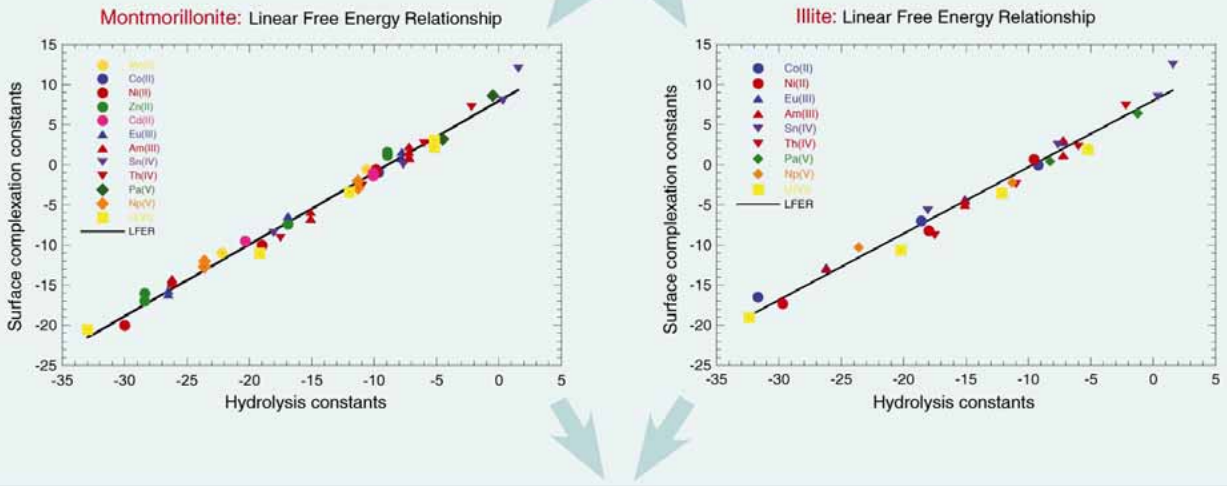
Mechanistic Sorption Model for Clay Minerals; 2SPNE SC/CE



Influence of Speciation/Sorption Competition

Thermodynamic Sorption Data Bases

Laboratory for Waste Management (LES) 29

The mission of the Laboratory for Waste Management (LES) is to carry out a comprehensive research and development (R&D) programme in support of Swiss radioactive waste disposal options. The Federal Government is responsible for radioactive wastes arising from medicine, industry and research in Switzerland, and on its behalf LES carries out a R&D programme in collaboration with the National Cooperative for the Disposal of Radioactive Waste (Nagra), the organization charged with the disposal of all Swiss radioactive waste. LES serves the national needs, present and future, in the safe disposal of radioactive waste in the fields of geochemistry and the transport mechanisms of radionuclides, including geochemical retardation and immobilisation.

LES makes use of some of the unique infrastructure within Switzerland available at PSI, in particular the A-Laboratory radioactive facilities, (micro-) X-Ray Adsorption and Fluorescence Spectroscopy (XAS, XFS) beam lines at the Swiss Light Source (SLS) and the Spallation Neutron Source. Research activities within LES are performed on very different spatial and temporal scales, to take advantage of all the information which can be obtained from the different facilities: i.e. from the nano-scale (molecular modelling) to the micro-scale (XAS), on to the cm scale (laboratory), and up to the field and regional scales (Mont Terri Rock Laboratory at St Ursanne, Switzerland).

A key point in the strategy of LES is that the Laboratory continues, and wherever possible and appropriate, intensifies its integration within the scientific and waste management communities through cooperations and joint projects, including participation in EU-Framework programmes. Also, an important aim of LES is to contribute to “educating the next generation” in the area of waste disposal, and our connections to universities enable us to provide PhD and Post-Doctoral positions within the Laboratory.

In 2008, the Federal Office of Energy (BFE) released approved guidelines for the site selection of radioactive waste repositories sited within Switzerland, as defined in a *Sectoral Plan* (Sachplan Geologische Tiefenlagerung). Participation in the safety analyses carried out by Nagra during the site selection process for SMA and HAA repositories, and the preparation of licensing applications (2014/2016), will be a central function of LES in the coming years.

◀ **The procedure towards the establishment of thermodynamic sorption data bases for performance assessment.**

X-ray micro-diffraction on 100 000 year old natural cementitious materials

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Daniel Grolimund, *Laboratory for Energy and Environment, PSI*;
Philip Pattison, *EPFL Lausanne and ESRF/SNBL, France*;
Urs Mäder, *University of Berne*

A key matrix for the safe disposal of radioactive waste is cement, which is used both to solidify the waste and to construct an engineered barrier system in deep, geological repositories. Investigations on natural analogue samples afford a unique opportunity to extend present knowledge of the long-term behaviour of a cementitious near-field (which is mainly based on laboratory and field studies carried out over a few years at most) to geological time-scales of more than 100 000 years. Recent improvements in X-ray optics and detectors make micro-diffraction a powerful tool for the investigation of such highly heterogeneous systems.

Cement-based materials play an important role in the multi-barrier concepts being developed worldwide for the safe disposal of radioactive waste. For example, ~95 wt% of the near field of the planned Swiss disposal cavern for low- and intermediate-level waste is comprised of cementitious materials. In a deep geological repository, very strong chemical gradients control mineral alterations at the interfaces between the cementitious near-field (pH>12.5) and the surrounding claystone formations (pH~7–8), due to the large differences in the respective chemical conditions. The interaction of the hyper-alkaline pore water of the cementitious near-field with the surrounding host rock changes the physical and geochemical properties at the interface between them. Unfortunately, experimental data relating to the chemical reactions taking place, and the minerals formed in the alteration zone, are almost completely lacking.

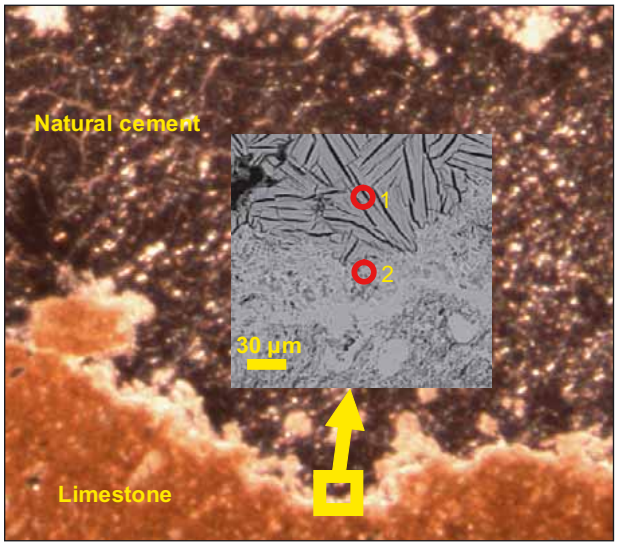

Figure 1: **Optical image of a more than 100 000 year old alteration zone formed between a natural cement and limestone, a sedimentary rock. The inset shows a scanning-electron-microscope (SEM) image of the interface, illustrating the length-scale and morphology of the different mineral phases analysed by X-ray micro-diffraction (micro-XRD).**

Laboratory experiments have been successful in following diffusion-controlled alteration zones, but the identity of the secondary minerals formed could be established to a limited extent only [1]. Complementary to the data from short-term laboratory and long-term field experiments, information can be gained on the nature of the alteration products at the interface between the cement and the surrounding rock from natural analogues that have developed naturally over time periods relevant to geological disposal.

The most important natural hyper-alkaline system was discovered at Maqarin (in Jordan), and has been studied for more than a decade [2,3]. In this case, the combination of the high-temperature and ambient-pressure conditions have led to the formation of clinker, and, following subsequent re-hydration, to the formation of cementitious phases. The use of U-Th disequilibrium series dating suggests the age of the cement mineralisation to be about 100 000 years. Continuous leaching along fracture-bound groundwater flow paths has formed cementitious in-fills, as well as interfaces to the adjacent clay-bearing limestone (Fig. 1).

The inset to Fig. 1 shows the SEM image of an alteration zone, of thickness about 30–50 µm. The aim of this study was to

determine the mineral composition and spatial heterogeneity of compact samples (thin sections) prepared from the cement/limestone interface. Micro-XRD was applied, because it is capable of providing basic structural information from selected micron-sized and submicron-sized crystals within complex matrices.

Micro-XRD investigations

Initial XRD characterisations were carried out using an unfocused beam (collimated down to 200×100 μm^2) at the CRISTAL beamline at SOLEIL, in France. The XRD images collected exhibit only a few, very weak diffraction lines (Fig. 2, top). This can be attributed to the presence of large amounts of amorphous components in the sample. A search in the PDF-2 database revealed that the diffraction lines observed matched the (100), (004), (008) and (0012) reflections of ettringite:
$(Ca_6Al_2(SO_4)_3(OH)_{12} \cdot 26H_2O)$.
Micro-XRD techniques were applied to improve the resolution of the XRD data, with the aim of performing a single-crystal refinement. The microXAS beamline at SLS delivers an intense X-ray beam with a spatial resolution down to 1×1 μm^2. The availability of state-of-the-art XRD detectors (such as PILATUS) made the use of the beamline crucial for this study. In contrast to measurements with the unfocused beam, micro-XRD patterns collected using the micro-beam exhibited strong diffraction spots of ettringite (Fig. 2) consistent with the hexagonal translation lattice (a=b=11.23 Å, c=21.48 Å).
SEM investigations of the interface between the limestone and the cement further showed small (~1 µm), platelet-like structures, consisting mainly of Ca, Si, Al, O (Fig. 3). The secondary phases formed at the interface (Spot No. 2 in Fig. 1) have been identified as 11 Å tobermorite, a crystalline calcium-silicate-hydrate (C-S-H) mineral (space group I2 mm, a=5.58 Å, b=3.69 Å, c=22.85 Å).
Previous studies on 11 Å tobermorite, which were performed on larger crystals, showed that the mineral exhibits significant ordering-disordering (OD) features [4]. Application of the OD approach to the micro-XRD data from micron-sized crystals revealed a strong stacking disorder of the 11 Å tobermorite. To the best of the authors' knowledge, this was the first in-situ study on naturally-formed, micron-sized tobermorite crystals, and was only feasible due to the use of a high-brilliance, highly-focused X-ray source, such as that available at the microXAS beamline of SLS.

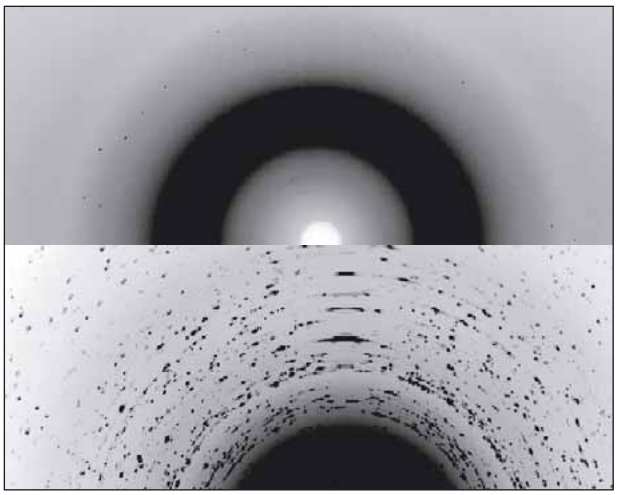

Figure 2: **Comparison of XRD data for ettringite (Spot No. 1 in Fig. 1) collected with beam sizes of 200×100 μm^2 (top) and 10×10 μm^2 (bottom).**

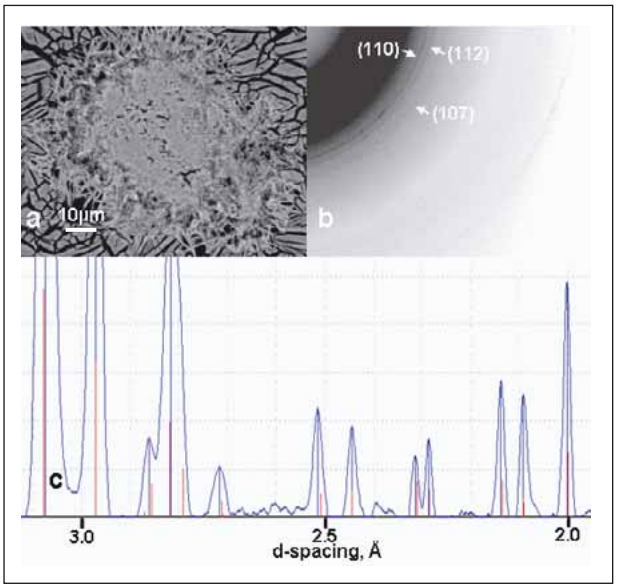

Figure 3: **Characterisation of a C-S-H area of the alteration zone: (a) SEM image; (b) micro-diffraction pattern; and (c) one-dimensional diffraction diagram of 11 Å tobermorite. Diffraction lines shown in red were predicted from the structure.**

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New solid solution models of C-S-H consistent with structural and spectroscopic information

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Simple aqueous-solid-solution (Aq-SS) models of C-S-H (Calcium Silicate Hydrate) are being used in studies of cement hydration and waste/cement interactions, though without a clear mechanistic basis. A newly developed sublattice SS approach is consistent with both the defect-tobermorite structure of C-S-H and the ^{29}Si NMR (Nuclear Magnetic Resonance) data. Effects of structural ordering are accounted for in a ternary CSH3T model, reproducing both solubility and polymerisation of the tobermorite-like C-S-H. Numerous solubility data sets can be fitted with the semi-empirical CSHQ model, and both SS models can be further extended by introducing other cationic species on the sublattice sites.

Knowledge of C-S-H phases is crucial in studying the hydration, strength and long-term behaviour of concrete, and for understanding the retention of (radio)toxic cations in a cementitious waste matrix. C-S-H has variable composition (0.7<C/S<1.7, where C/S is the molar Ca/Si ratio) and water content (C/S + x). Upon de-/re-calcification, carbonation and dilution, crypto-crystalline gel-like C-S-H dissolves rapidly, and then re-precipitates with different compositions. For the thermodynamic modelling of such systems, C-S-H Solid Solution (SS) models are needed.

The ideal, two-binary SS model of C-S-H [1] has been widely used, improved [2], and included into the Cemdata'07 database [3] for the GEMS-PSI package [4]. This SS model reproduces measured $[Ca]_{Aq}$ and pH values in the whole C/S range, and can be semi-empirically extended for the minor cations (Zn, Sr, Na, ...). The main shortcomings of simple SS models of C-S-H are: over-prediction of $[Si]_{Aq}$ at C/S>0.9 (seen on $[Ca]_{Aq}$–$[Si]_{Aq}$ diagrams); the absence of the structural background of end-member stoichiometries; and the lack of evidence for the existence of a solid solution between silica- and tobermorite-like end-members.

Recently, the structures of C-S-H mineral analogues (1.4 nm tobermorite and jennite) have been determined; ^{29}Si NMR data have been obtained for C-S-H samples of known C/S and solubility [5]; the defect-tobermorite model of C-S-H has been further corroborated [6]; the non-existence of C-S-H SS at C/S<0.6, and the structural ordering in C-S-H at C/S≥1.0, have both been proven [5]. A corresponding improvement in the C-S-H SS models is now required to make them more consistent with the structural and spectroscopic information.

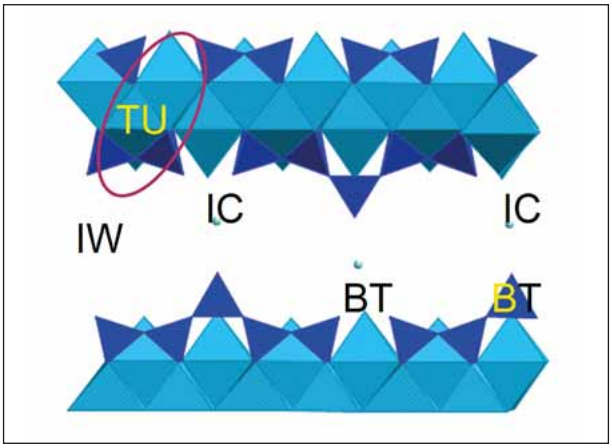

Figure 1: **Fragment of the defect-tobermorite structure of C-S-H with sublattice sites (see text for explanations).**

Sublattice models for C-S-H

In the defect-tobermorite model, the C-S-H structure is obtained from that of tobermorite by removing some bridging tetrahedra (BT in Fig. 1) from the silicate 'dreierketten' chains. A vacant BT site consists of two Si-O- bonds that can attract cations (H^+, Ca^{2+}, Na^+, ...) surrounded by H_2O molecules in the interlayer. The excess Ca can be incorporated as an additional octahedral $Ca(OH)_2$ sheet, or as fragments of jennite structure [3,4]. The concentration of BT defects can be estimated from ^{29}Si NMR spectra as the mean silicate chain length CL, where 2<CL< ∞.

Structure-composition relationships in C-S-H may be expressed in Richardson's formula [6], re-written in the present context (per *dreierkette*) as:

$[Ca(OH)_2]_{(u+y-2)/2} \cdot [(CaSiO_{3.5})_2 \cdot (SiO_2)_{1-v}] \cdot (H_u \cdot Ca_{1-u/2}) \cdot mH_2O$. Here, v is the fraction of vacant BTs ($0<v<1$); u is the degree of Si-O$^-$ groups protonation ($0<u<2$); y is the number of Ca^{2+} ions in the interlayer, or present as extra $Ca(OH)_2$ for $0<y<2$; and m is the number of interlayer H_2O molecules ($m \leq 5$).

Defining *sublattice* as the set of all structurally equivalent sites, the above formula is converted into a template $[CU^0]_2$:$[TU^-]_2$:$[BT^0]_1$:$[IC^+]_2$:$[IW^0]_5$, in which sublattices are separated by colons. Here, $[TU^-]_2$ stands for a main dimeric tobermorite unit $Ca_2Si_2O_7^{-2}$ in which no substitutions occur; CU^0 can be $Ca(OH)_2$ or a vacancy V_{CH}; BT^0 is either SiO_2 in the BT site, or a vacancy V_{BT}; IC^+ is an interlayer cation H^+ or $½Ca^{2+}$; and IW^0 is an interlayer H_2O or a vacancy V_{IW}. A one-by-one substitution of species or vacancies into the sublattice template will generate 16 end-members.

To make the SS model tractable, the number of interlayer H_2O molecules was fixed at 4 (representing full occupancy at water saturation), thereby reducing the number of end-members to 8. In a further simplification, the observations [5] of quasi-reversible relations between C-S-H solubility, C/S ratio and CL (which in general depend on C-S-H maturity and preparation method) were used. Since CL decreases as C/S increases, the substitutions in BT and IC sites can be coupled by merging them into a BTI sublattice $[CU^0]_2$:$[TU^-]_2$:$[BTI^+]_2$:$[IW^0]_4$, where BTI^+ is $Si_{0.5}OH^+$ or $HO_{0.5}Ca_{0.5}^+$. This yields an SS model with 4 end-members connected by the reciprocal reaction: JenH + TobD = TobH + JenD.

A semi-empirical way of further improving the model was to downscale end-members by a factor of 3, leading to an ideal CSHQ SS model (Table 1). Although this is less consistent with the C-S-H structure, it reproduces well various solubility data sets (Fig. 2), as well as the measured CL, H_2O content and C-S-H density.

Another way of improving the sublattice model is to use the evidence [7] of interlayer ordering in tobermorite-like C-S-H with $0.9<C/S<1.25$. In doing this, the CU sites were set vacant, and the BTI site was split into two sites ($[BTI1^+]_1$:$[BTI2^+]_1$:$[TU^-]_2$:$[IW^0]_4$) with substitutions of $Si_{0.5}OH^+$ by $HO_{0.5}Ca_{0.5}^+$, yielding a CSH3T SS model with end-members TobH ($C_2S_3H_5$), T5C ($C_{2.5}S_{2.5}H_5$), T2C ($C_3S_2H_5$), connected by an ordering reaction ½TobH + ½T2C = T5C.

The model has a built-in dependence of CL on composition, consistent with measured values for tobermorite-like C-S-H [5]. With $G°_{298}$(TobH)=−5121.92, $G°_{298}$(T2C)−4931.88, $G°_{298}$(T5C)=−5036.18 (in kJ/mol), the CSH3T model fits the C-S-H solubility data remarkably well (Fig. 3), and can be further extended for minor cations by substituting them on sublattice sites in appropriate structural environments.

End member	Formula	$G°_{298}$ kJ/mol	$G°_{298}$ range	
			+	−
TobH	$C_{2/3}SH_{1.433}$	−1668.56	1.2	2.3
TobD	$C_{5/6}S_{2/3}H_{1.433}$	−1570.89	1.2	3.4
JenH	$C_{4/3}SH_{2.4}$	−2273.99	2.9	1.7
JenD	$C_{3/2}S_{2/3}H_{2.4}$	−2169.56	2.3	1.7

C=CaO; S=SiO_2; H=H_2O; $G°_{298}$ is molar free energy at 25 C.

Table 1: **The down-scaled CSHQ simple ideal model.**

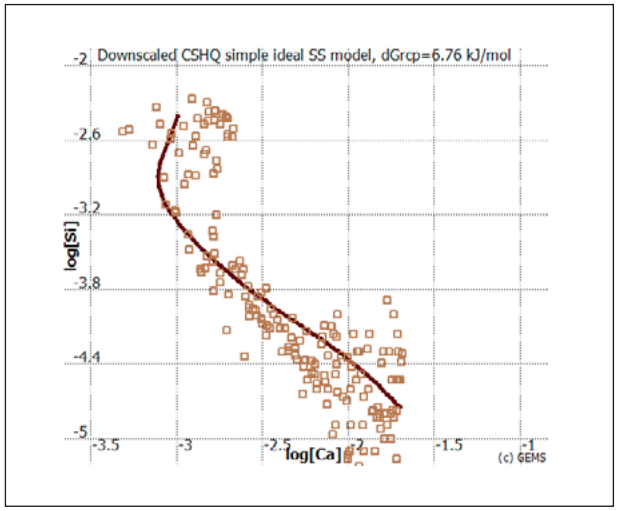

Figure 2: **Performance of the CSHQ model in $[Ca]_{Aq}$-$[Si]_{Aq}$ space vs reported C-S-H solubility data.**

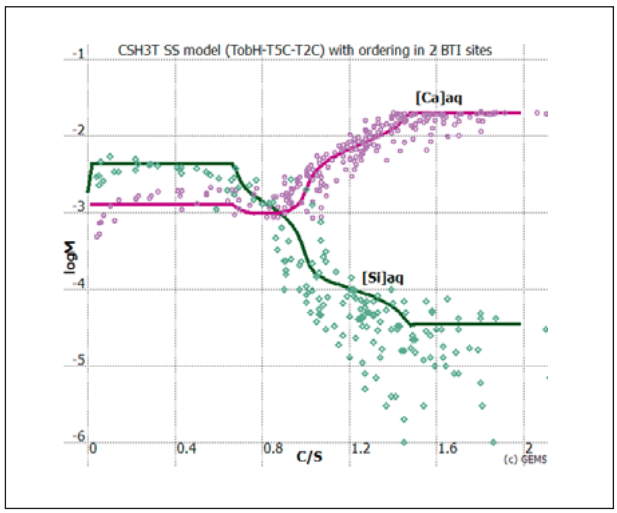

Figure 3: **Performance of the CSH3T model vs C/S ratio against reported C-S-H solubility data.**

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Effects of geochemistry and transport on the evolution of interfaces in a cementitious waste repository

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Laboratory for Waste Management, PSI

Understanding the geochemical interactions between the various natural and engineered barriers in a nuclear waste repository is essential for assessing the long-term safety of the facility. In this article, the interfaces between argillaceous and cementitious materials are discussed in the light of recently developed, state-of-the-art geochemical models, combined with advanced transport codes. These particular systems are of special interest, since numerical simulations all indicate a tendency towards system clogging, which could lead to self-sealing of the repository with time.

In Switzerland, deep geological disposal in clay-rich rocks is foreseen for not only the high-level radioactive waste, but also for intermediate-level and low-level waste. Typically, intermediate- and low-level waste repositories contain large quantities of cementitious materials, which are used for waste conditioning, confinement, and as backfill for the emplacement caverns. The interaction of this kind of repository construction with the surrounding clay rock and other clay materials, such as sand/bentonite mixtures, which are potential materials for backfilling the access tunnels, needs to be thoroughly investigated.

The interaction between clay and cementitious materials is of special interest, because they are very different materials from a geochemical point of view. In the long term, the interaction between these materials can lead to degradation of the cement, and to the development of zones of 'altered' clay rock. Such alterations may affect the functionality of the repository's engineered and natural barriers (Fig. 1).

With the help of a numerical reactive transport model, the evolution of cement/clay interfaces for different geochemical and transport conditions may be compared. The calculations are an aid to defining a geochemical base dataset of the unaltered and altered materials used in performance assessment calculations in exploring the spatial and temporal scales of the alterations, and for alternative repository design options to be compared.

The multi-component reactive transport code OpenGeoSys-GEMS, developed at PSI in collaboration with the Helmholtz Centre for Environmental Research (UFZ) in Leipzig, has been used to stimulate the transport of chemical components under isothermal conditions. Embodied in the code is a sequential, non-iterative approach for coupling the transport code OpenGeoSys [1] with the PSI geochemical Gibbs Energy Minimisation code GEMIPM2K [2]. Details regarding code development and verification can be found in [3].

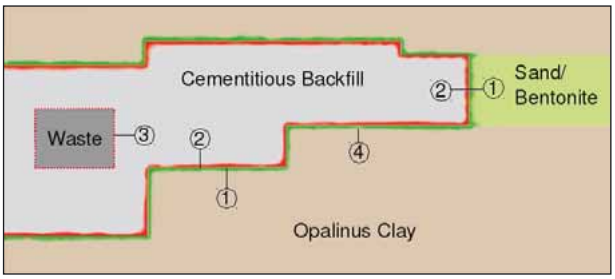

Figure 1: **Processes in a cementitious waste repository resulting from hydrochemical interactions: (1) reaction of cement pore water with clay; (2) reaction of clay pore water with cement; (3) interaction of waste with cement pore water; and (4) oxidation reactions in the partially saturated rock zone during construction and operation.**

Application

A typical application is the interaction between concrete and a 20/80wt% bentonite/sand mixture. Both materials are foreseen for backfilling of emplacement caverns and access tunnels. For the concrete, the mineral composition and pore solution of a CEM I 52.5 N HTS hydrated cement [4] were taken. For this, the most recent CEMDATA07 thermodynamic database was used, in conjunction with the Nagra/PSI thermodynamic database 01/01, including several ideal solid solutions for the hydrated cement minerals.

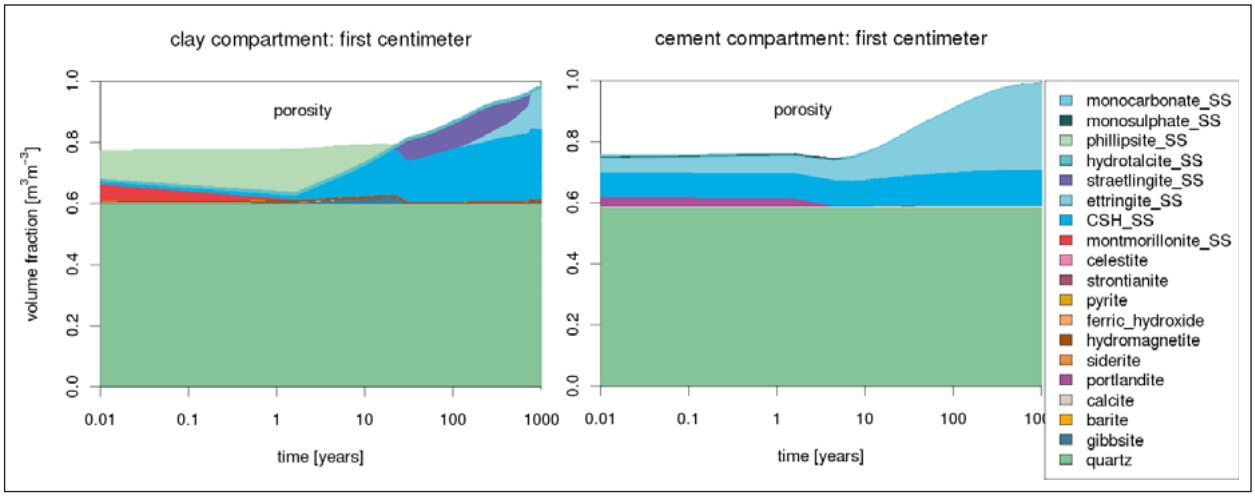

Figure. 2: **Evolution of the volume of mineral phases on both sides of the bentonite/sand-concrete interface.**

The bentonite model, representing MX-80 bentonite, was calibrated using data from [5]. The definition of montmorillonite, the main constituent of bentonite, includes cation exchange processes as well as amphotheric ≡SOH edge sites, and is based on a newly developed, multi-end-member, solid-solution model.

Strong chemical gradients are established between concrete and bentonite/sand if the connecting pore space becomes saturated with water. These gradients are the driving force for the diffusion of solutes across the interface boundary, in both directions. In this scenario, it is assumed that only dissolved species diffuse, and that water movement induced by pressure differences is negligible.

Figure 2 shows the evolution of the volume fraction of the mineral phases in the first centimeter of material, on both sides of the interface. On the concrete side, portlandite is seen to dissolve within a few years, and ettringite to precipitate, filling the free-pore space. On the clay side, montmorillonite dissolves, while the zeolites precipitate. At later stages, several precipitating cement minerals fill up the pore space. This gradual blocking of the pore space slows the diffusion in this region until the interface is effectively clogged.

The existence of these mineral alteration zones has been confirmed experimentally, but the anticipated ‘full stop’ to the transport and chemical reactions in real systems remains an open issue.

Linking the model time-scale to the real time-scale is still hindered by conceptual shortcomings. Porosity changes depend on the selected reference volumes for the chemical calculations, and are therefore dependent on the spatial discretisation, whereas transport is independent of the discretisation. Consequently, the non-linear empirical relationship between porosity and transport parameters also makes clogging time discretisation dependent.

In summary, current models only allow different scenarios with similar spatial discretisations to be compared. Transformation to real time-scales calls for calibration experiments.

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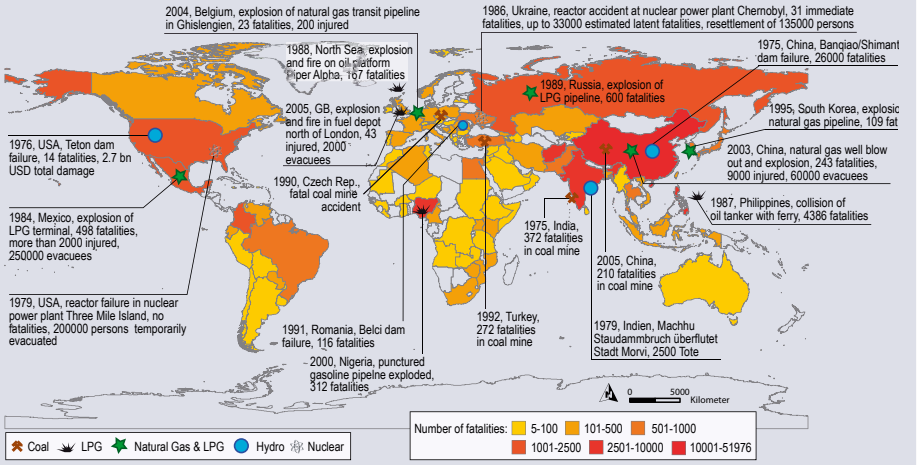
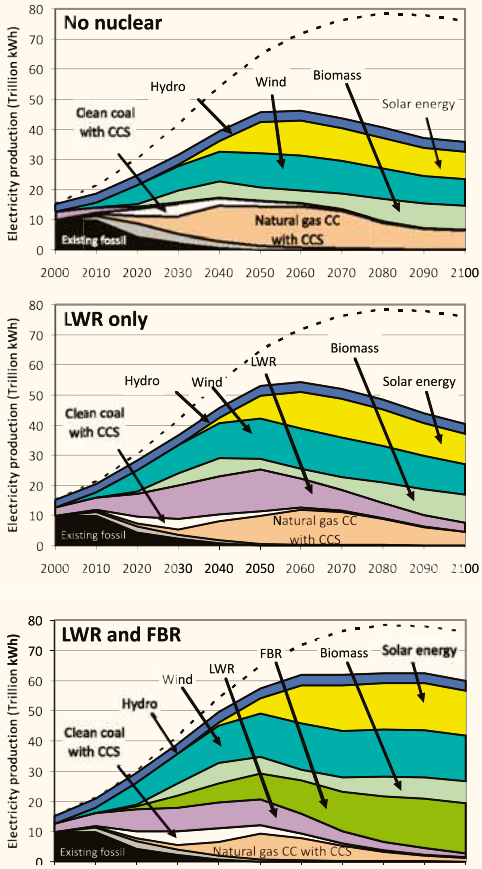
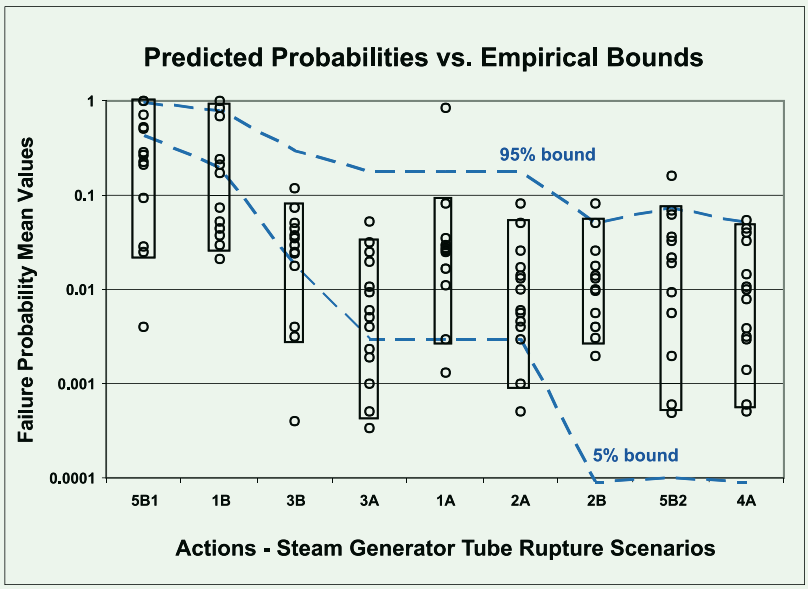
Technology Assessment



Energy Economics



Risk and Human Reliability



Laboratory for Energy Systems Analysis (LEA) 37

LEA is an interdisciplinary Laboratory supporting both NES and the General Energy Department (ENE). The Laboratory aims to contribute to effective decision-making on long-term technology strategies in energy supply and demand, ensuring full integration of all environmental, economic and social factors. LEA also develops methodologies, and carries out the associated risk analyses, within the framework of Human Reliability Assessment (HRA).

The activities within LEA, in cooperation with its various external partners, cover the following three project areas.

Technology Assessment (GaBE)
The project involves analyses of fossil, nuclear and renewable energy technologies. It is based on an interdisciplinary framework, thus enabling comparisons to be made between current and future options for the electricity, heating and transport sectors.

Energy Economics
Analyses are undertaken of energy systems, and associated technological changes, at the Swiss, European and global levels, all aimed at improving understanding of available options for the realisation of more sustainable energy mixes for the future.

Risk and Human Reliability
Main contributions here are to the solution of current and future issues relating to the handling of human factors in the context of Probabilistic Safety Assessment (PSA).

◀ **Safety, environmental impacts and economics of energy technologies are in focus in the work of the Laboratory for Energy Systems Analysis (LEA): accidents and their impacts in a geo-referenced visualization, strategies and scenarios for a sustainable global energy system, and a comparison of human reliability predictions for safety assessment (clockwise from upper left).**

Climate change mitigation options for the global energy system

Hal Turton, *Laboratory for Energy Systems Analysis, PSI;*
Bertrand Magne, *International Energy Agency, France;*
Socrates Kypreos, *Dysenos AG, Switzerland*

Current patterns of energy supply and use across the world are contributing to global climate change. The Energy Economics Group at PSI has analysed scenarios of possible pathways for the future development of the global energy system that respond to the challenge of reducing greenhouse gas (GHG) emissions. This is made possible by deploying new methods for identifying important technology options for achieving very low stabilisation targets for atmospheric GHG concentrations, such as carbon capture and storage, renewable energy (particularly biomass), nuclear energy, and increased efficiency. This effort is supporting the development of energy policy in Europe.

The world today is confronted by a number of challenges arising from the supply and use of energy. Among these, climate change represents a major threat to long-term, sustainable, economic, social and environmental development. To forestall the potentially most severe consequences of climate change, policy-makers in Europe and elsewhere have set the goal of avoiding a greater than 2°C increase in average global temperature above pre-industrial levels. The realisation of such a target is likely to entail technological change and the application of new technology options in the energy sector to substantially reduce GHG emissions. However, questions remain as to whether existing and prospective energy technologies are sufficient to achieve such a stringent target, and which technology options are the most suitable.

Approach and methodology

Analyses undertaken at PSI have sought to address these questions by exploring scenarios that achieve stringent atmospheric GHG concentration targets (specifically 550, 450 and 400 parts per million (ppm) carbon-dioxide-equivalent) over the 21st Century. These scenarios present 'what-if' descriptions of the future, and help to identify trends, robust technology strategies, interactions across the energy system, and unforeseen challenges. Such scenarios are not predictions, but rather possible and relevant future outcomes, based on a set of clearly understood assumptions.
To quantify and analyse these scenarios, a global, energy-economic integrated assessment model has been applied.

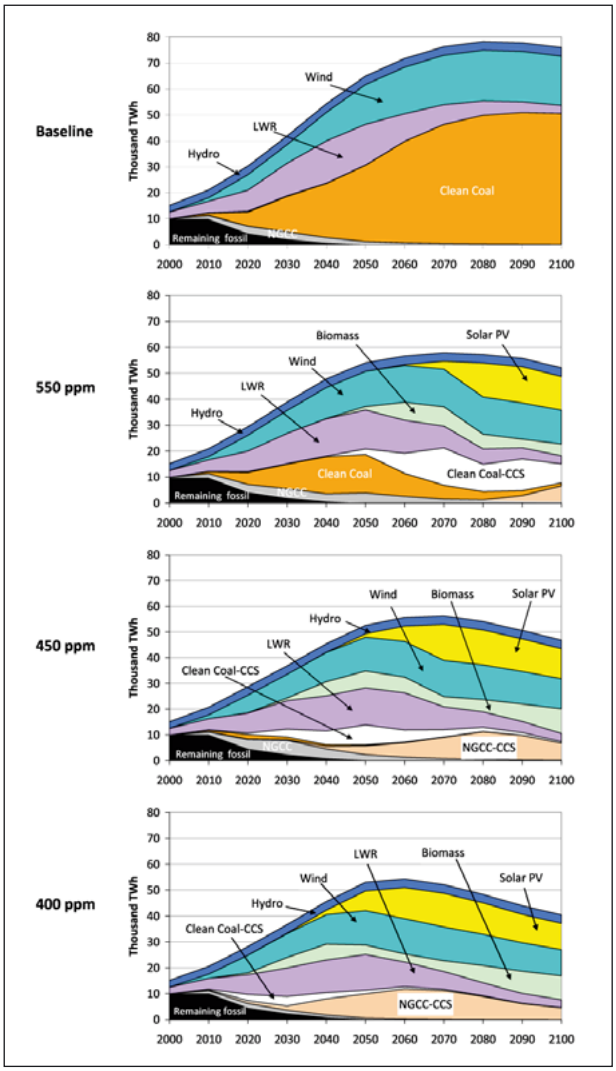


Figure 1: **Electricity output in mitigation scenarios.**

This model – MERGE-ETL – represents the energy sector and economy of nine regions, covering all the countries of the world. MERGE-ETL estimates energy demand, and selects technologies that are cost-effective in the long-term, to maximise global economic utilisation. The model includes a range of technology options for energy supply and conversion, covering fossil-fuel power plants (both conventional and more advanced technologies), renewables and nuclear energy. PSI has implemented into this model technology research and development (R&D) and/or experience. Further, a more detailed representation of the nuclear fuel cycle has also been included, to account for the constraints inherent to the management of fissile material stocks, and the recycling of nuclear materials.

Selected results and conclusions

Four global scenarios for the mitigation of climate change are presented in Fig. 1. Each scenario considers a different target for atmospheric concentration of GHGs, ranging from 'baseline', in which there is no target, to the very stringent 400 ppm, and shows the utility-maximising set of technologies for global energy generation for each. It can be seen that responding to increasingly stringent climate change targets brings a number of technological advancements. These include the adoption of carbon-free power plants, as well as reductions in energy demand, mainly from improvements in efficiency. Under a 550 ppm target, clean coal (Integrated Gasification Combined Cycle, IGCC), nuclear power (Light Water Reactors, LWRs), wind farms and biomass play important roles in the mid-term, while clean coal (with Carbon Capture and Storage, CCS) and renewables represent long-term options. Nuclear (LWRs), biomass and CCS face geological resource and land availability constraints.

Under the 450 ppm and 400 ppm targets, clean coal technologies become significantly less competitive, due to the stringency of the target. This is true even for CCS, since not all emissions can be captured. In contrast, natural gas (NGCC) is more attractive early in the century, and maintains this position later with the adoption of CCS.

Overall, the results in Fig. 1 show that major technological change is needed to realise very stringent mitigation targets, and that new technologies are likely to play a significant role. Many such technologies are still rather immature, but are expected to become more competitive with increasing experience and further R&D. In all scenarios, technology-learning plays an important role in bringing down the cost of new technologies (especially renewables and CCS), substantially reducing the economic costs of achieving the climate change targets.

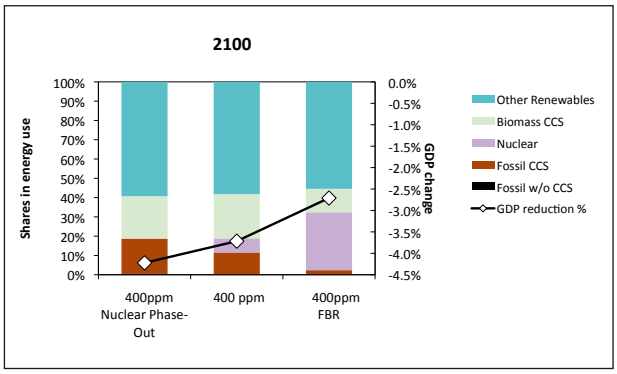


Figure 2: **Electricity generation shares for alternative nuclear scenarios and associated losses in GDP.**

Further analysis of future options has also been carried out, focusing on the technologies identified above to assess some of the uncertainties, such as the availability of CCS, nuclear power or biomass, or the rate of development of renewable technologies, such as solar.

Figure 2 shows the electricity generation mix in the year 2100 under the stringent climate target of 400 ppm across three scenarios of nuclear availability. These are: total nuclear phase-out; continuing use of LWR technology; and the introduction of advanced reactors, including Fast Breeder Reactors (FBRs). The Figure also indicates the economic result in achieving this level of climate mitigation in terms of loss of Gross Domestic Product (GDP). The results suggest that targets can be achieved with a phase-out of nuclear power, but at high economic cost. On the other hand, the availability of advanced FBRs lowers the economic cost, reduces the use of fossil fuel, and avoids the need to use expensive CCS options.

In summary, it appears that stringent mitigation targets can be met under a variety of technology scenarios, but major technological change is needed. Important technology options include carbon capture, renewables (particularly biomass), nuclear energy and improved efficiency.

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Advancements in the Sustainability Assessment of Energy Systems

Stefan Hirschberg, Warren Schenler, Peter Burgherr, Christian Bauer, *Laboratory for Energy Systems Analysis, PSI;* Marek Makowski, *International Institute for Applied Systems Analysis (IIASA), Austria*

The present article summarises progress made in indicator-based sustainability assessment of energy technologies. Achievements include: establishing a comprehensive set of technology-specific indicators of a high level of acceptability to the engaged stakeholders; quantification of all indicators for four countries; development and web-based implementation of new Multi-Criteria Decision Analysis (MCDA) methods; and application of MCDA by a variety of stakeholders to demonstrate the merits of the process, the strengths and weaknesses of the technologies, and the unavoidable impact of stakeholder preferences.

The recently finalised EU Project NEEDS (New Energy Externality Developments for Sustainability) generated a wide range of results within such areas as Life Cycle Assessment (LCA), assessment of external costs and scenario modelling. The research stream *Technology Roadmap and Stakeholder Perspectives* was aimed at broadening the basis for decision support by examining the robustness of the results under various stakeholder perspectives. This objective was realised by combining knowledge expressed in terms of technology attributes with stakeholder preferences. The use of Multi-Criteria Decision Analysis (MCDA) has enabled explicit and integrative consideration to be given to a wide spectrum of technology-specific, environmental, economic and social characteristics.

Analytical approach

The development and implementation of the MCDA approach included: (a) developing a structured set of sustainability criteria, and surveying stakeholders on their appropriateness and acceptance; (b) integrating environmental, economic and social indicator results from this and other research streams into a technology database for use in the MCDA process; (c) developing a range of new MCDA tools for ranking the NEEDS technologies and selecting the most suitable; (e) implementing an interactive, web-based interface for collecting stakeholder criteria preferences; and (f) collecting the individual user inputs, ranking the technologies, identifying patterns by means of sensitivity mapping, and comparing MCDA results with total (internal plus external) costs. It is worth noting that the social aspects associated with energy systems are to a limited extent reflected in the external cost estimates.

Sustainability criteria and indicators

PSI, with support from its partners within the project, has established a full set of technology-specific evaluation criteria and indicators covering the environmental, economic and social dimensions of sustainability [1], building partially on the results of a literature survey and quantitative sustainability assessments from earlier projects. Social criteria and indicators were established in a pioneering work by University of Stuttgart within this project.

The overall set enables the essential characteristics of the different technologies to be identified, and differentiates between them. In general, the proposed criteria and indicators have found wide acceptance among stakeholders, both in terms of content and in its hierarchical structure. In total, there are 36 associated indicators. Of these:

- 11 are *environmental,* covering energy and mineral resources, climate change, ecosystem impacts from normal operation and severe accidents, and special chemical and medium-to-high level radioactive waste;
- 9 are *economic,* including impacts on customers (i.e. the price of electricity), on overall economy (employment and autonomy of electricity supply), and on the utility aspects (financial risk and operational issues);
- 16 are *social,* addressing security/reliability of energy provision, political stability and legitimacy, social and individual risk, both expert-based (normal operation and accidents) and perceived, terrorist threat, and quality of residential environment (landscape, noise).

These indicators were first quantified and then combined to form a unique database for each of the 26 future technologies analysed (for the year 2050) for the four countries: France,

Germany, Italy and Switzerland. Comparisons between the various indicators illustrate the differences in the profiles, and thus the strengths and weaknesses of the various technological options and associated fuel cycles. While improvements are envisaged for all the technologies considered, the most notable is the future economic performance of renewables, in particular solar.

Results of the assessment and conclusions

Using MCDA, the technology-specific set of sustainability indicators is combined with stakeholder preferences. This approach enables a ranking of technologies based on distinct stakeholder profiles to be established, and to explore the associated sensitivities. IIASA has developed a number of new MCDA methods satisfying the requirements of the NEEDS project, while IIASA and PSI together have implemented a web-based tool for the method deemed to be most suitable. This has enabled stakeholders to specify their preference profiles, iterate between them, and obtain a ranking for future technologies. An overview of the results, based on all stakeholder responses, is shown in Fig. 1 along with the total costs [2].

Within the external cost estimation framework applied in NEEDS, nuclear energy exhibits the lowest total cost (i.e. is ranked first), but its ranking in the MCDA framework tends to be lower, mainly as a result of considerations given to a variety of social aspects not reflected directly in the external costs. Thus, in MCDA, nuclear energy ranks lower than renewables, which themselves benefit from their much improved economic performance. Generally, coal technologies have lower total costs than natural gas. However, in the MCDA framework, coal performs worse than the centralised natural gas options, which, being in the midfield, are ranked similar to nuclear. The performance of Carbon Capture and Storage (CCS) is mixed.

The individual preference profiles have a decisive influence on the MCDA ranking of technologies. Given equal weighting of the environmental, economic and social dimensions, the emphasis on protection of the climate and ecosystems, minimisation of objective risks and affordability for customers, the nuclear options are top ranked. In contrast, focusing on radioactive waste, land contamination due to (hypothetical) accidents, risk aversion and perception issues, terrorist threat and conflict potential, the ranking changes to the disadvantage of nuclear. This aspect endorses the need for further technological development aimed at mitigating the negative impact of these areas.

The ranking of fossil technologies strongly depends on the emphasis placed on environmental performance, which in relative terms remains weak, and more pronounced for coal than for gas. Overall, the renewables perform very well in terms of stability and relatively low sensitivity to changes in preference profiles, due to their much improved economics.

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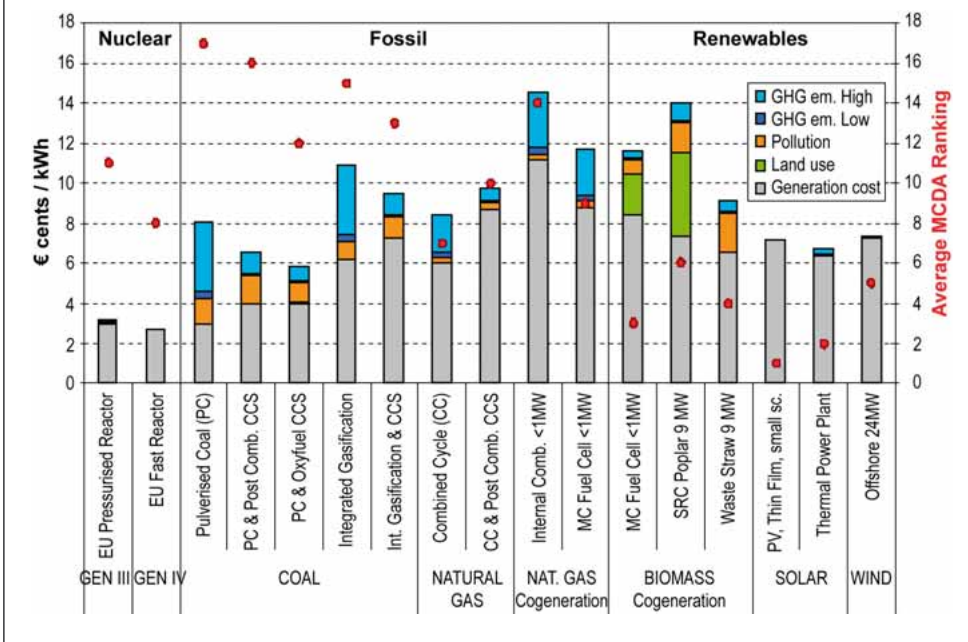

Figure 1: **Average MCDA ranking of future (for the year 2050) technologies compared to total costs [2].**
GHG em.: Greenhouse Gas emissions;
CCS: Carbon Capture & Storage;
MC: Molten Carbonate;
PV: Photovoltaic.

International benchmark of HRA methods based on data from a simulator study

Vinh N. Dang, Luca Podofillini,
Laboratory for Energy Systems Analysis, PSI

In Probabilistic Safefy Assessment (PSA), the safety of nuclear power plants is analysed by modelling the ways in which accidents may occur. Estimating accident scenario probabilities provides insights into many important weaknesses, and their potential fixes. In a PSA, potential human failure events and their probabilities are estimated by means of Human Reliability Analysis (HRA). A major international effort is underway to assess HRA methods by comparing their predictions against actual crew performance data from simulated emergency scenarios. Such data-driven evaluations yield valuable evidence in regard to the qualitative and quantitative accuracy of the methods.

Assessing the safety of nuclear power plants, or other complex systems, involves developing an understanding not only of what accidents could occur but also of how likely these accidents may be. Probabilities allow decision-makers responsible for safety to understand the relative importance of the various accident scenarios, and to identify the contributing causes and failure events that should be prioritised in efforts to ensure safety or reduce risk. In the PSA framework, HRA deals with the Human-related Failure Events (HFEs) that may contribute to these scenarios.

A number of diverse HRA methods are currently available. These methods reflect traditional concerns in PSA scenarios, such as human/machine interfaces, operational procedures, and the adequacy of the time allotted for operator action. In addition, many of the methods have also been developed to address errors of commission, and errors in decision-making. Given the differences in the scope of the methods, their underlying models and variability of the predictions, and in the light of the importance of human actions towards safety, there is considerable interest in assessing the various HRA methods [1].

PSI performs a leading role in the *International HRA Empirical Study,* a major effort coordinated by the OECD Halden Reactor Project, with additional support from the U.S. Nuclear Regulatory Commission, the Electric Power Research Institute, and the Swiss Federal Nuclear Safety Inspectorate. The Halden Project signatory organisations composed the HRA analysis teams, whose predictions form the basis of HRA method assessment. An essential feature of the Empirical Study is its focus on comparisons of predictions to reference data from a dedicated simulator study as the basis for method assessment.

Predictions versus observed performance

Thirteen HRA teams analysed 13 HFEs, defined for 4 nuclear power plant accident scenarios. The scenarios were a Steam Generator Tube Rupture (SGTR) and Loss of Feedwater (LOFW) in a Pressurised Water Reactor, each including a base case, as well as a more complex variant. Each team used one of the 13 HRA methods to be assessed in the study (without knowledge of the simulator results). In a within-subject experimental design with randomised ordering, 14 licensed operator crews responded to 4 emergency scenarios using Halden's Hammlab simulator facility. The crews' performance in the 48 scenario runs provided 14 observations of the majority of the HFEs, and 7-10 observations of 5 more. (One HFE could not be observed, because it was defined as conditional on the failure of a preceding HFE, which did not occur.)

In spite of the large number of operating crews and scenarios involved, the statistical limitations of the data had already been recognised at the outset of the work. The statistically small sample size precludes the option to concentrate solely on the failure counts and the resulting reference failure probabilities, since these can have very large uncertainties (as seen in Fig. 1). In many ways, the limitations are to be expected in HRA, because human performance is known to be situation-specific, making it difficult to aggregate data across different scenarios and situations [2].

Separate from the statistical limitations, it is important to PSA that the HFE failure probabilities predicted in the HRA are underpinned by the identification of the key performance factors and issues contributing to HFEs. As a result, the

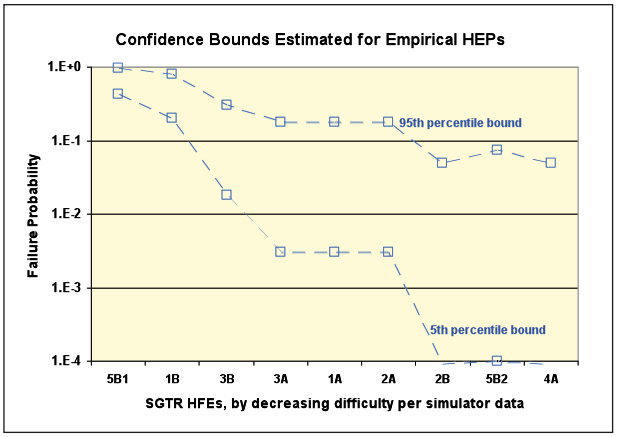

Figure 1: **Bounds for the reference HFE probabilities (HEPs) obtained from the SGTR scenario data.**

methodology for data analysis, and the criteria for method assessment, prioritised the qualitative predictions, giving quantitative performance a significant, but secondary, role among the method assessment criteria. A core component of the simulator study data analysis performed to obtain the reference data is the detailed analysis of the response of the crew in determining the factors that influenced their response and performance. The HRA predictions of the factors driving performance, and of how the scenario or human failure event would unfold, have been compared against these qualitative data. However, the quantitative data are also relevant: (1) because the predictions for the more difficult HFEs, where the evidence is stronger, are considered more important; and (2) in identifying the predictions that could be considered outliers (i.e. those outside the boxes, or confidence bounds, in Fig. 2) for the detailed examinations of the contributors not captured by the HRA analyses [2].

The thorough, detailed, qualitative analysis of the simulator data in the Empirical Study produced data supporting the robust findings of what was good and what was poor in regard to the HRA predictions of these HFEs, and provided a firm basis for the broad insights gained into the HRA methods considered in the study so far. For instance, the empirical evaluations show that the cognitive aspects of following procedures and executing tasks (as opposed to situation-assessment or decision-making) have not been addressed, or not adequately addressed, in some of the methods in common use [3]. In this way, the Empirical Study provides valuable information for HRA method selection, and highlights specific shortcomings in the methods, thus enabling them to be improved. In addition, the study has contributed valuable evidence to the specific impacts of situational factors on performance in concrete scenarios, and the associated mechanisms through which they influence performance. These outcomes have led to follow-up work to improve HRA methods, and have motivated further efforts to collect HRA data in simulator studies.

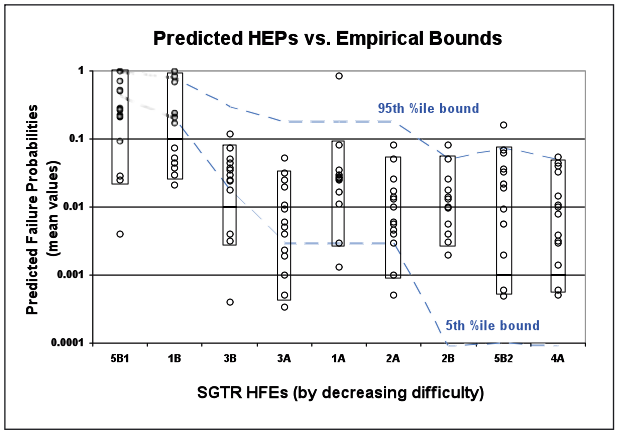

Figure 2: **Overall predictions for SGTR scenarios.**

Acknowledgements

PSI participation in this study is supported by The Swiss Federal Nuclear Safety Inspectorate. The authors also gratefully acknowledge the essential contributions of the nuclear power plant, whose operating crews participated in the simulator study, and those of our colleagues at OECD Halden and the assessment team.

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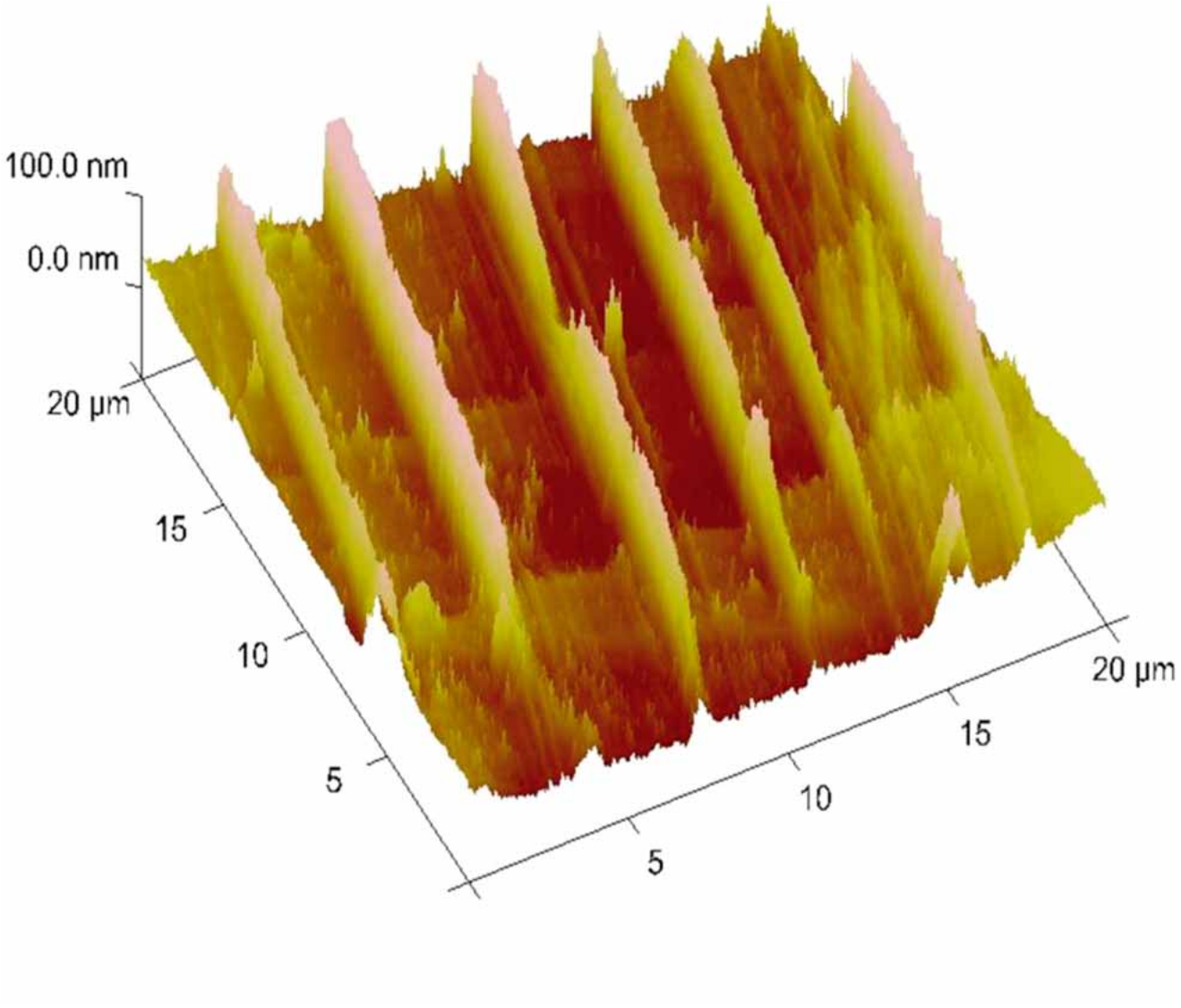
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Laboratory for Nuclear Materials (LNM)

LNM addresses material-related, scientific issues with regard to safety, life-time (extension), performance and sustainability of current and future nuclear reactors.

Currently, LNM focuses on three main project areas.

High Temperature Materials

This activity involves characterisation of materials to be used in the future Generation IV reactors (particularly Gas Cooled Reactors), which will operate at significantly higher temperatures, and will be subject to a more intense radiation environment than current Gen II reactors. Mechanistic models are being developed for the prediction of material behaviour, from the atomic level up to the scale of the continuum. Experimental validation of the models is also undertaken using advanced spectroscopic methods, and, in particular, synchrotron radiation.

Nuclear Fuels

This project focuses on micro-structural/micro-mechanical examination of the ageing of core internals (fuel rods, structural materials), and the development of associated theoretical models. In particular, investigations of fuel damage, and identification of possible causes of failure, are being carried out, and methods for the production of Gen IV fuels, and their associated fuel cycles, are also under consideration.

Component Safety (INTEGER)

This activity involves the experimental characterisation of important ageing mechanisms (stress-corrosion-cracking, thermal fatigue and irradiation embrittlement) in primary pressure boundary components, the development and validation of advanced, mechanistic material-ageing models, and the application of probabilistic methods for improved integrity assessments and life-time predictions. The work also encompasses evaluation of advanced, non-destructive techniques for the early detection of fatigue and initiation of stress-corrosion-cracking, and characterisation of the actual degree of embrittlement in the reactor components.

◀ **Evolution of intrusions and extrusions at the surface of stainless steel at a very early stage in fatigue life during a thermo-mechanical fatigue experiment under light water reactor operating conditions, as revealed by atomic force microscopy. These regions act as micro-crack initiation site later on in the fatigue life.**

From Fe-Cr to steel: atomistic calculations of binary Fe-Cr alloys

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Laboratory for Nuclear Materials, PSI

The suitability of Fe-Cr steels in the 2 to 20 at%Cr concentration range as structural materials for the next generation of nuclear power plants is currently under discussion worldwide. In the context of materials design through modelling, first-principles atomistic calculations are being performed on the pure Fe-Cr alloy to determine the preferred configuration of Fe and Cr atoms as a function of the Cr concentration. A tendency for the Cr atoms to cluster above 12.5 at%Cr has been observed, and is characterised by a short-range-order parameter. The inclusion of carbon is expected to shed some light on precipitations in realistic steels.

As well as being cheap and abundant, iron (Fe) is also incredibly versatile. For example, its interdependent magnetic, structural and mechanical properties can be drastically altered by alloying with other elements. Hard steels can be formed by the inclusion of small amounts of carbon (C), and corrosion-resistant steels by the further addition of chromium (Cr). Recent years have seen a renewed interest in the understanding and developing of new Fe-Cr-based steels, in view of the challenges posed by the requirements for structural materials for future nuclear power plants (of both the fission and fusion type). In the future, computer modelling is expected to play a crucial role in materials design [1], and in the prediction of the long-term effects of irradiation and harsh environments on material properties. Computations using Density Functional Theory (DFT) form the basis of a multi-scale modelling approach to gain insight at a fundamental level into the mechanisms affecting the behaviour of Fe-based alloys.

Cr in Fe: the reluctant solute

While the main features of the phase diagram of pure, non-irradiated Fe-Cr alloy are widely accepted, many of its details require further evaluation [2]. This is particularly true at the onset of the Cr-rich phase known to form at low Cr concentrations at the temperatures relevant to nuclear power plant operation. Magnetic interactions play a major role in the ability of Cr atoms to form a solid solution with Fe, and exhibit a tendency to cluster, depending on the Cr content [3]. The ground state of pure Fe is ferromagnetic, while that of pure Cr is described by an anti-ferromagnetic, spin-density wave. The substitution of Fe atoms by Cr atoms therefore creates situations of magnetic 'frustration', and it is to be expected that the preferred configurations for the Fe and Cr atoms will be heavily constrained by magnetism at any given Cr concentration. Configurations of lowest energy can be identified and studied by means of the super-cell approach within spin-polarised, total-energy DFT calculations.

Density Functional Theory calculations

Possible ways of treating random alloys have traditionally included the virtual-crystal and coherent-potential approximations. These are effective approaches, but ones that are not suitable if the details of the local environments are expected to play key roles. An appropriate method in these circumstances is to construct super-cells: i.e. repeated *body-centred-cubic* (BCC) unit cells in all spatial directions. The total energy of a range of different Cr arrangements is first calculated, and then used as the discriminating criterion.

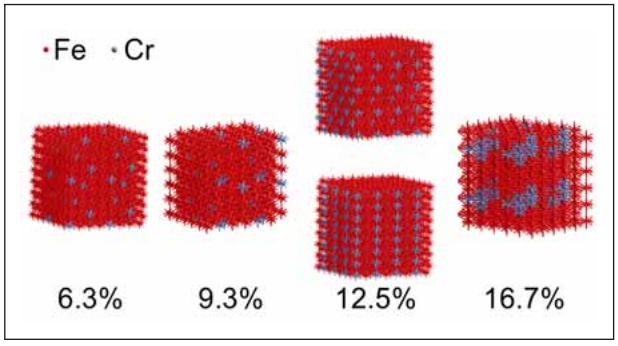

Figure 1: **Representation of the lowest energy structures found for 6.3, 9.3, 12.5 and 16.7 at%Cr alloys.**

Figure 1 shows the lowest energy structures found using the projector-augmented wave implementation employed in the code VASP [4]. A clear tendency of the Cr atoms to cluster is evident at 16.7 at%Cr. In contrast, at 6.3 at%Cr and 9.3 at%Cr, the Cr atoms tend to be more widely spaced. At 12.5 at%Cr, there are clear indications of transitional behaviour, with two different structures having near-degenerate energies after relaxation of the ionic positions. While no guarantee exists that these structures correspond to an absolute energy minimum, results are consistent for the range of super-cell sizes tested (up to 4×4×4).

Short-range ordering versus clustering

A quantitative means of qualifying the configurations of Cr and Fe atoms at any given concentration is by calculating the so-called *short-range-order parameter* for each configuration. For the binary alloy $Fe_{1-x}Cr_x$, the parameter can be defined per shell '*l*' around a Cr atom as $\alpha^l = 1 - n_{Fe}^l / [(1-x)n\_pos^l]$, in which n_{Fe}^l is the number of Fe atoms in the l^{th} shell, and n_pos^l is the total number of sites in the shell. This purely structural parameter is particularly important for Fe-Cr alloys, and can be measured experimentally by diffuse neutron-scattering measurements [5]: typical results are reproduced in Fig. 2 (full circles).
In this Figure, a negative short-range-order parameter indicates short-range ordering, while a positive value indicates a tendency to cluster. Superimposed on the experimental measurements are the calculated values from the lowest energy structures found using DFT. There is reasonable agreement between model predictions and experimental measurement at the lower end of the atomistic scale. The picture correlates with the calculation of formation energies at low Cr concentrations [2], for which negative mixing enthalpies for Cr concentrations below 6% are predicted.

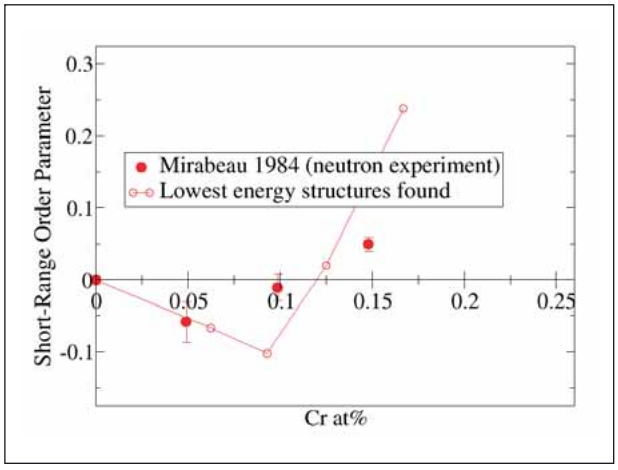

Figure 2: **Weighted (1st and 2nd shell) short-range-order parameter: full circles are as measured by Mirabeau [5], and empty circles are calculated for the lowest energy structures. The line is simply a guide for the eye.**

Modelling steel

The ab *initio,* first-principles calculations outlined above illustrate the dependency of the formation of Cr-rich regions in the pure Fe-Cr system on concentration. A further step to be taken is the study of the effect of interstitial carbon impurities in the system. While complete understanding of the role of carbon on the mechanical properties of steel, both in normal environments and under irradiation, necessarily includes phenomena beyond the scope of DFT, static *ab initio* calculations can provide insights into the formation of carbon precipitates. After analysing the large local deformation caused by the introduction of a single carbon atom in pure Fe, the affinity of the carbon for Fe or Cr was investigated for small supercells of the 12 at%Cr Fe-Cr system (Fig. 3). A first round of calculations indicates a preference of carbon for Fe rather than Cr, while nitrogen, another impurity commonly found in Fe, prefers proximity with the Cr atoms. The results are preliminary, and are part of the ongoing work.

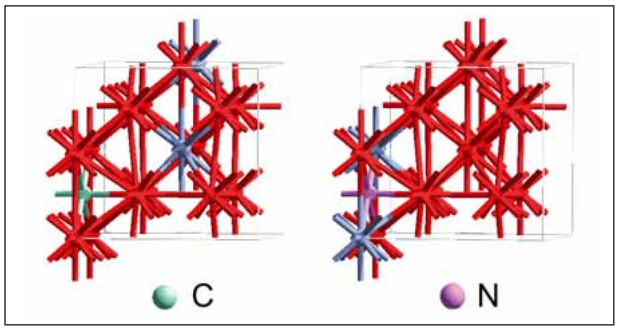

Figure 3: **2×2×2 supercells with 14 Fe, 2 Cr and either 1 C or 1 N.**

Conclusions

First-principles calculations have been utilised to obtain a quantitative description of Fe impurities, of both the substitutional (Cr) and interstitial (C,N) type, and their impact on, and preferred configurations in the Fe matrix. These investigations highlight the power of DFT calculations in predicting material properties, and, in the future, on designing new materials.

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XAFS analyses of Cu precipitates leading to reactor pressure vessel steel embrittlement

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Laboratory for Nuclear Materials, PSI

The irradiation of a reactor pressure vessel with a high dose of neutrons leads to embrittlement of the Reactor Pressure Vessel (RPV) steel, with the potential to limit the lifetime of the reactor. This embrittlement is closely related to the creation of ultra-fine precipitates of low-concentration elements produced as a result of radiation-induced diffusion processes. Copper (Cu) is the most important element in cluster formation, due to its high initial diffusivity. In this study, we report the use of X-ray Absorption Fine-Structure (XAFS) spectroscopy to investigate radiation damage and 'next-neighbour atomic environment' around Cu in neutron-irradiated RPV steels.

Irradiation-induced embrittlement of a Reactor Pressure Vessel (RPV) steel is a vital issue for ensuring the continued safe operation of Nuclear Power Plants (NPPs) around the world, especially since many are close to their (initially-designated) operational lifetimes. Earlier studies [1] have revealed that nano-precipitates of constituent trace elements (e.g. Cu and Ni), enhanced by long-term neutron irradiation, are the principal causes of embrittlement. Hence, it is of considerable importance to examine the nano-structural changes of Cu-rich precipitates during long-term operation of commercial NPPs, and to provide an atomic-scale description of the irradiation effects on RPV steels.

The basic mechanism of radiation embrittlement of RPV steels is due to matrix damage. Embrittlement manifests itself as an increase in the ductile-to-brittle transition temperature, a parameter normally used as an indicator of the degradation status of the material. In addition to mechanical testing, methods based on non-destructive measurement techniques, such as positron annihilation spectroscopy and atom-probe topography, can also be used to follow embrittlement [2].

In the present study, using synchrotron light, XAFS spectroscopy has been applied for the first time at the Cu 'K-edge' to systematically investigate neutron-induced radiation damage to the metal-site, body-centred cubic (*bcc*) structure of RPV steels. The technique is sensitive to the average atomic environment just a few atoms away from the probe (specific element), this providing a measure of the 'short-range-order' of the system (ca. 1 nm). Selected RPV surveillance specimens from a Swiss NPP and the IAEA reference steel JRQ [3], bombarded with neutrons in a test reactor with a fluence range of 0.85 – 5.0×10^{19} cm^{-2}, have been used in this study. Thermal annealing has also been carried out for a few selected JRQ specimens to study the thermal stability of defects developed by neutron irradiation. These specimens are from two heatings of A533B Class 1 plates containing a very low concentration (0.14 wt%) of Cu in the Fe matrix.

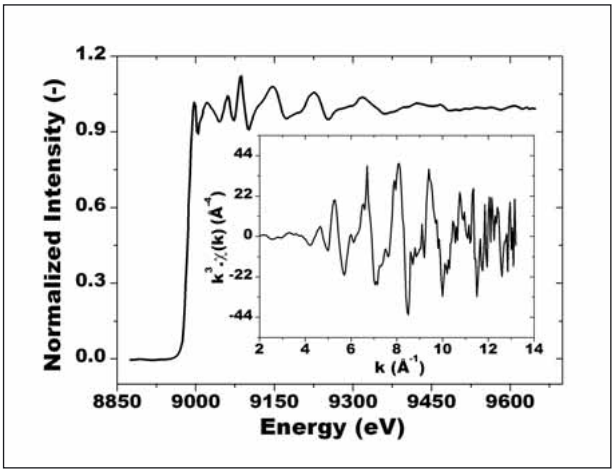

Figure 1: **Normalised and background-removed K-edge absorption spectra of the IAEA reference RPV steel JRQ in the 'as-prepared' state before neutron irradiation. The inset shows the XAFS signal versus photo-electron wave number *k*.**

Atomic environment around Cu in an RPV

Figure 1 shows an example of the measured XAFS spectrum from a non-irradiated JRQ sample. The data clearly demonstrate the excellent quality of XAFS for the Cu signals, even though the concentration is very low.

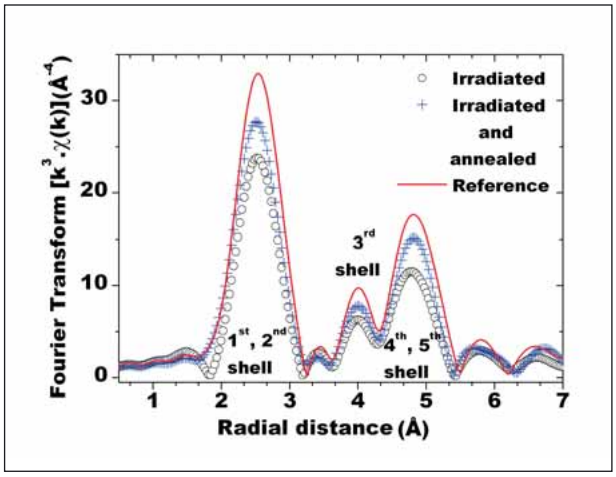

Figure 2: ***k*³-weighted Fourier-Transformed XAFS data at the Cu K-edge measured from three JRQ samples: non-irradiated, and irradiated before and after annealing.**

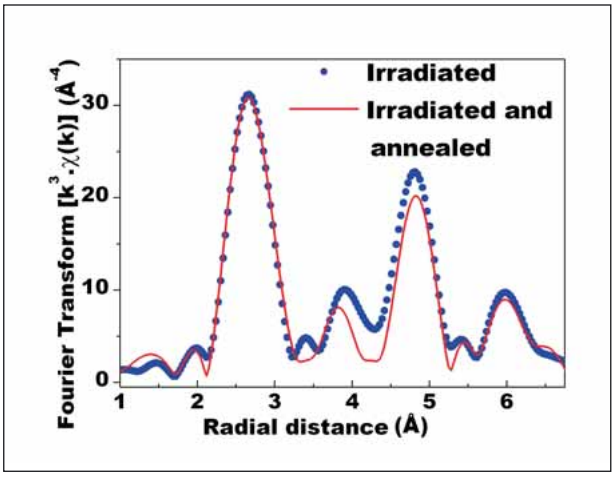

Figure 3: **Fourier Transforms of the XAFS data at the Fe K-edge measured from the irradiated specimen in the as-irradiated state and after thermal annealing at 735 K for 168 hours.**

For a quantitative analysis of these data, a fitting procedure has been applied [4]. The optimised structural parameters of the next-neighbour coordination numbers and interatomic distances are derived from the data analysis.

Figure 2 depicts Fourier-Transformed (FT) experimental data from a JRQ sample, irradiated at a neutron fluence of 5.0×10^{19} cm^{-2}, measured in the as-irradiated state, and after thermal annealing (at 735 K over 168 hours). The data from the non-irradiated JRQ reference sample is also included for comparison. The results illustrate Fourier features which are characteristic of a bcc Cu-site environment, each peak corresponding to the distance to the neighbouring Cu atoms.

From the pristine data, long-range order (i.e. beyond the first and second shells) is apparent in the spectrum, which features several nearest-neighbour peaks. In the irradiated specimen, all these peaks are greatly reduced in magnitude, typical of damaged materials. The reduction in the number of interfering atoms is due to the formation of structural vacancies resulting from the irradiation. Prolonged annealing leads to a reduced damage fraction in the sample, indicating the recombination of vacancy- and interstitial-like defects, and giving rise to an increase in the coordination numbers of near-neighbour atomic shells, approaching values close to those of the non-irradiated material, but not suppressing the formation of nano-sized, Cu-rich precipitates.

Atomic environment around Fe

In the following, the XAFS results at the Fe K-edge obtained for the irradiated JRQ samples before and after thermal annealing are compared. The experimental FT data are shown in Fig. 3. Prolonged annealing after neutron irradiation appears to have no influence on the Fe first-nearest and second-nearest neighbour shells, although a small change can be observed in the higher-order shells (third to fifth, see Fig. 2) of the Fe. The Fe environment, reflected in the XAFS data for the REF sample (not shown here), is very similar to the results presented in Fig. 3.

The main structural difference between the two samples is the Debye-Waller factor of the higher-order shells [4]. In fact, from the data measured at the Fe K-edge, and from the subsequent analyses, no essential structural changes in the first two neighbour shells are observed between the REF and irradiated JRQ samples. However, this is not the case for the Cu neighbours, which are indicative of more specific vacancy-type defect environments, in close proximity to the solute Cu atoms. Computer simulations of the cascade and defect micro-structure evolution have also predicted similar results: that is, the size and fraction of self-interstitial atoms clusters are larger in Cu than in Fe. On the other hand, the vacancies in Cu are mostly in the form of clusters, though they do not cluster in Fe [5].

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Effect of the LWR coolant environment on fatigue, crack initiation and growth in stainless steels

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Material fatigue is one of the major concerns associated with ageing in nuclear power plants, and is becoming increasingly important with extended plant life. Isolated fatigue cracking and leakage incidents in pressurised components have been reported. Traditionally, fatigue design does not consider the potentially corrosive effects of the reactor coolant environment, and is based solely on fatigue behaviour in air. However, laboratory tests have revealed that there are significant environmental effects on fatigue initiation and crack growth, which have thus raised concerns regarding the adequacy of safety margins in accepted fatigue design and evaluation procedures. These aspects are currently being addressed at PSI within the ENSI-sponsored KORA project.

In Boiling and Pressurised Water Reactors (BWRs & PWRs), corrosion-resistant, austenitic stainless steels are widely used as construction materials for the piping circuits enclosing the primary reactor coolant. This boundary is an engineered barrier for radiation protection, and is critical for plant safety during its operational lifetime.

Evidence of cracking of such components has been discovered during BWR & PWR service inspections over the past decades which could be attributed to stress-corrosion-cracking (SCC) or low/high-cycle fatigue (LCF/HCF). Fatigue-cracking incidents are rare, and have mainly been related to either HCF, through flow-induced vibrations from power up-ratings in BWRs, or to thermal fatigue (HCF/LCF) caused by temperature stratification, striping and/or turbulent mixing in both BWRs & PWRs. At least the LCF (or combined LCF/HCF) damage, as a result of thermal loadings, may have been aggravated by corrosion effects resulting from coolant attack [1,2].

The original fatigue design was based purely on the fatigue behaviour of the materials in air, and ignored potential environmental effects. However, laboratory tests have now revealed that there could be significant environmental effects on fatigue initiation and crack growth, and have thus raised concern regarding the adequacy of the safety margins associated with current fatigue design and evaluation procedures.

Clarification of these issues has become important to the Swiss Nuclear Safety Inspectorate (ENSI), who have sponsored a research effort at PSI to address them [1,2]. Within this activity, the corrosion fatigue behaviour of different stainless steels has been characterised by means of cyclic-fatigue tests carried out using pre-cracked/notched-only fracture mechanics samples in the temperature range 70°C to 320°C under normal-water-chemistry (NWC) and hydrogen-water-chemistry (HWC) conditions in BWRs, and under primary-circuit conditions in PWRs.

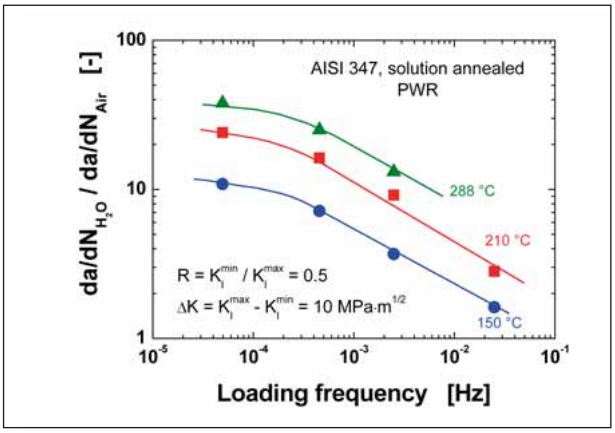

Figure 1: **Effect of temperature and loading frequency on the environmental acceleration of fatigue crack growth in a solution-annealed, Nb-stabilised stainless steel in a PWR primary environment.**

Results and discussion

Relevant environmental acceleration of fatigue crack growth (and reduction of fatigue initiation life) has been observed in all steels at loading frequencies ≤ 0.1 Hz (strain rates ≤ 0.1 %/s), and could be sustained down to the lowest investigated loading frequencies (or strain rates) in all three environments (Figs. 1,2). Subsequent to initiation, the stationary, short-crack growth rates, after crack advances of 50 to 300 µm from the notch-root, were in the typical range of corresponding results from tests with long cracks (pre-cracked specimens), and showed the same system parameter re-

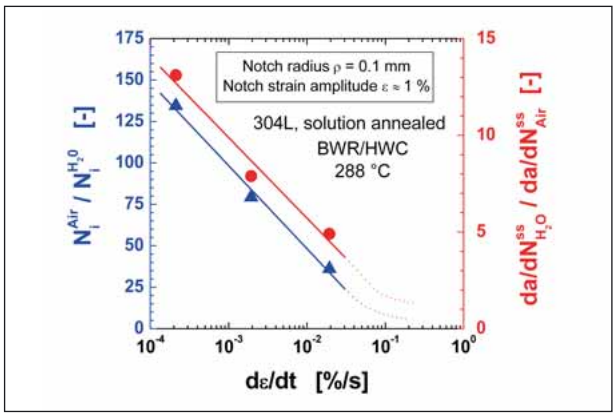

Figure 2: **Effect of strain rate on environmental reduction of fatigue initiation life, and acceleration of subsequent, stationary, short-crack growth in a low-carbon stainless steel in a BWR/HWC environment.**

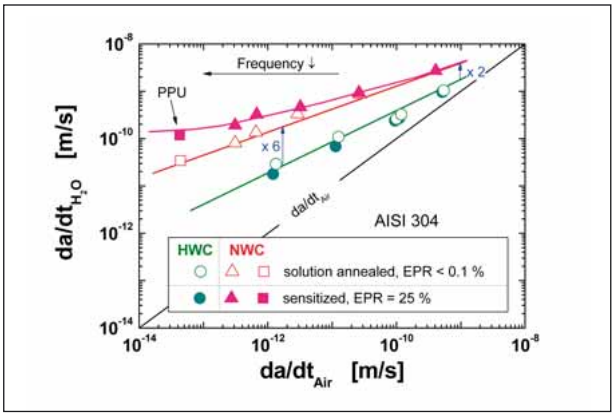

Figure 3: **Effect of sensitisation and corrosion potential (NWC vs. HWC) on corrosion fatigue-crack growth in a high-carbon stainless steel in BWR/HWC and NWC environments.**

sponse. The effect of environment on the genuine initiation process (Δa≈10 µm) was stronger than on the subsequent stationary, short-crack growth (Fig. 2).

At low corrosion potentials, under BWR/HWC and PWR conditions, relevant environmental acceleration of fatigue-crack growth (and environmental reduction of fatigue initiation life) occurred in all the low-carbon and stabilised stainless steels investigated for the combination of loading frequencies ≤ 0.1 Hz (strain rates ≤ 0.1%/s), temperatures ≥150°C (≥100°C), and ΔK values ≥ 3 MPa · $m^{1/2}$ (notch strain amplitudes ≥ 0.3 %), respectively. If these conjoint threshold conditions were simultaneously satisfied, the environmental enhancement increased with decreasing loading frequency (or strain rate) and increasing temperature. Generally, material and water chemistry parameters had only a minor effect, and sensitisation only affected the corrosion fatigue behaviour under highly oxidising BWR/NWC conditions (Fig. 3).

The current ASME Boiler & Pressure Vessel Code Section XI [3] on fatigue-crack growth curves do not include environmental effects, and are not conservative in LWR environments if the above-mentioned conjoint threshold conditions are satisfied. A modification of Section XI should therefore be pursued to include environmental effects in the appropriate manner.

Similarly, the fatigue design curves in Section III of the Code [3] do not represent excess conservatism to cover environmental effects, and are also not conservative for some critical parameter combinations. The initial studies conducted at PSI have qualitatively confirmed the NUREG/CR-6909 approach [4] of the new US NRC Regulatory Guide 1.207 [5], which defines a procedure to include environmental effects in Section III for new plants. Nevertheless, this approach should be critically evaluated by additional tests under more realistic and plant-relevant conditions before it is applied to existing plants.

Summary and conclusions

The possibility of coolant effects on fatigue under BWR and PWR conditions is undisputed, but there is no general consensus on the practical consequences. The valuable field experience accumulated for fatigue-designed stainless steel components does not indicate any generic deficiencies in current procedures resulting from lack of knowledge of such effects. This is due to the large overall conservatism embodied in current fatigue-design and evaluation procedures, and to the fact that for many plant transients one or several of the above-mentioned conjoint threshold conditions are not satisfied, resulting in moderate coolant effects only. Furthermore, in the case of fatigue, the very high ductility of austenitic stainless steels results in a rather large critical crack size, and a noticeable flaw tolerance. Consequently, there is no incentive to take immediate action. Higher priority should be given to a modification of Section XI of the ASME Code, including SCC. In flaw-tolerance evaluations, the contribution of SCC usually overwhelms that of fatigue under many conditions (e.g. for BWR/NWC or cold-worked stainless steels).

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EXIT

Hot Laboratory Division (AHL) 53

The Hot Laboratory (Hot Lab) is the largest nuclear research facility under the supervision of the Swiss Federal Nuclear Safety Inspectorate (ENSI), and the only Swiss research facility capable of examining large quantities of radioactive materials. The Hot Lab incorporates a complex infrastructure to ensure that all radioactive materials inside the building are contained, and that a safe workplace for its staff is guaranteed. AHL is the operator of the Hot Lab, as well as being its main user. The two main tasks of the division are to ensure a safe and efficient utilisation of its infrastructure, and to conduct state-of-the-art service work for the Swiss nuclear industry.

Highlights of current activities are listed below.

- AHL offers Hot Lab users modern analytical tools for the manipulation and investigation of radioactive materials. In particular, the laboratory is very well equipped for structural and chemical analyses of the materials used in Nuclear Power Plants and accelerator facilities.
- The Hot Lab is one of the nominated 'PSI User-Lab Facilities', and is responsible for the preparation and handling of radioactive specimens prior to their deployment in the large facilities at PSI: namely, SINQ, SLS and PROTEUS.
- AHL has strong links to the Swiss NPPs, and undertakes the necessary detailed material investigations for ensuring their continuing safe and economic operation. AHL also collaborates with several research projects concerned with the fuel and structural materials used in nuclear installations. Through this involvement, AHL has established recognition of its competence within the nuclear material research community worldwide.
- AHL benefits directly from its very competent staff, in that it is also successfully developing new analysis methods and infrastructure for tackling the challenging and ever-changing needs of the nuclear community, and is also able to undertake its own safety evaluation to ensure its continuing safe operation.

◀ **Hotcell line for research on nuclear fuel rods, for material testing and mechanical material processing.**

New measurement of the half-life of ^{60}Fe

Ines Günther-Leopold, Niko Kivel, *Division Hot Laboratory, PSI;* Dorothea Schumann, Regin Weinreich, *Laboratory for Radiochemistry and Environmental Chemistry, PSI;* Michael Wohlmuther, *Laboratory for Accelerator Operation and Development, PSI;* Georg Rugel, Thomas Faestermann, Klaus Knie, Gunther Korschinek, Mikhail Poutivtsev, *Technische Universität München, Germany*

A sample containing ^{60}Fe has been extracted from a copper beam dump irradiated for more than ten years with high-energy protons from the PSI ring cyclotron. In a joint collaborative project between the Technische Universität München (TUM) and PSI, the sample has been used to produce a new estimate of the half-life of ^{60}Fe using gamma spectrometry and multicollector inductively coupled plasma mass spectrometry. The new value for the ^{60}Fe half-life is 2.62 (± 0.04) x 10^6 yr, significantly higher than the previously reported value of 1.49 ± 0.27 x 106 yr. This result has a significant impact on the interpretation of time-scales of the formation of the early Solar System.

Radioactive nuclei produced by astrophysical processes are a key to understanding the evolution of the Universe, and the half-life of ^{60}Fe plays an important role in different astrophysical investigations. Most prominent examples are nucleosynthesis in the Galaxy, as observed through gamma rays; the history of the early Solar System, as observed through meteoritic inclusions; and supernova deposits on Earth, as indicated in ocean crust material.

Only two measurements of the half-life of ^{60}Fe have been reported to date: 3×10^5 yr (with an uncertainty of a factor 3) [1], and $1.49 \pm 0.27 \times 10^6$ yr [2], which was the currently accepted value before our investigations. Obviously, a more accurate determination of the half-life is warranted, since its value may have a significant impact on the interpretation of astrophysical data.

In general, half-lives can be determined by measuring the two factors *N*, A of the following equation:

$$T_{1/2} = \frac{N}{A} \cdot \ln 2 \qquad (1)$$

where A represents the ^{60}Fe activity, and *N* the number of ^{60}Fe atoms.

Sample preparation *N*

The ^{60}Fe sample to be examined was extracted from a copper beam dump of the ring cyclotron at PSI in use between 1980 and 1992. In 2004, after the short-lived radionuclides had decayed, chemical separation of iron from the bulk material, as well as from the main contaminant, ^{60}Co, was performed by the Rad Waste Analytics Group at PSI using liquid-liquid extraction and precipitation techniques [3]. About one order of magnitude more ^{60}Fe material was available for the investigation compared to that reported in [2].

Activity measurement

Our colleagues at TUM determined the activity A of the ^{60}Fe sample in a shallow underground laboratory, with a shielding of 15 metres water-equivalent to reduce cosmic-ray-induced background radiation. The activity of the sample was monitored by the 'growth' of the daughter isotope ^{60}Co, via the two prominent gamma-ray lines of 1.17 and 1.33 MeV, over a period of almost 1000 days (Fig. 1).

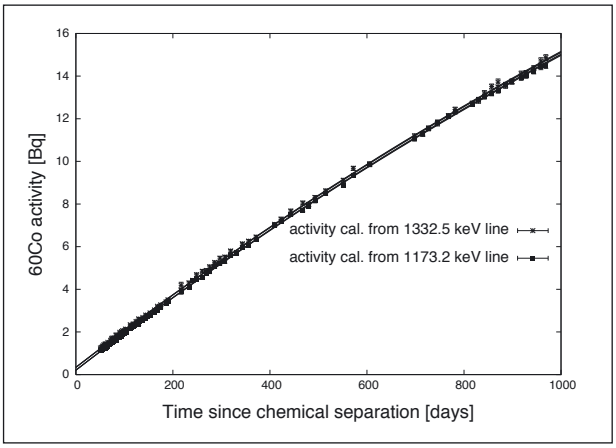

Figure 1: **Activity of the two ^{60}Co lines as a function of time.**

Figure 2: **MC-ICP-MS in the PSI Hot Laboratory.**

The measurement of the two ^{60}Co lines yielded a value of $A^{60}Fe = 49.19$ (± 0.11) Bq, from an initial ^{60}Co activity of 0.2 Bq (background in the sample).

Measurement of the number of atoms

The Isotope and Elemental Analysis Group at the PSI Hot Laboratory determined the number of ^{60}Fe atoms using a multicollector inductively coupled plasma mass spectrometer (MC-ICP-MS, Neptune, Thermo Fisher Scientific, Bremen, Germany; Fig. 2) with a desolvating sample introduction system for higher sensitivity [4,5].

For the determination of the number of atoms of ^{60}Fe, a master sample aliquot of 100 mg was taken and diluted with 3% nitric acid to approximately 4 µg/g. For calibration purposes, a certified reference material (IRMM-014) was prepared in the same manner to match the matrix, and to achieve similar signal intensities. The method of isotope dilution (ID) was used for the quantification, and the analyte solutions were prepared as five replicates with different spiking ratios from $^{57}Fe/^{56}Fe = 0.75$ to 1.5 to eliminate any systematic errors. The analysis procedure employed was the standard sample-bracketing method, by which potential drifts of the mass spectrometer can be detected, and the data corrected for these drifts. All data were corrected for background, mass bias and isobaric interferences (including ^{60}Ni).

The iron concentration in the ID sample was determined to be 585.6 ± 1.6 µg/g, corresponding to 2.662 ± 0.009 mg of iron in the master sample. The ratio N_{60Fe}/N_{Fe} was found to be 2.0483 (± 0.0035) $\times 10^{-4}$, and so the number of ^{60}Fe ions in the master sample was estimated to be $N = 5.873 \pm 0.020 \times 10^{15}$.

Results and conclusions

From Eq. (1), a half-life for ^{60}Fe of $2.62 \pm 0.04 \times 10^6$ yr was calculated, based on the measured quantities. This new value is much more precise (1.5% relative uncertainty), and significantly higher, than the previously accepted estimate given in [2].

Understanding the early evolution of the Sun requires precise data for the half-life of ^{60}Fe. There is no conclusive model at present which can explain the presence of ^{60}Fe in the early Solar System in a satisfactory manner. Since this new determination of the half-life yields a value more than 75% higher than previously thought, any models based on these earlier data now need to be critically reviewed.

Perspectives

In the near future, it is planned to extract an even larger quantity of ^{60}Fe from the copper beam dump, and to send subsamples of the material to interested laboratories worldwide. This will enable a cross-check of the half-life estimation undertaken at PSI to be made by the wider scientific community.

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The use of scanning electron microscopy and electron probe micro-analysis in the study of nuclear materials

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Investigations of cladding and fuel behaviour at different service times in nuclear power plants are important for the improved development of fuel rods. The commissioning in 2009 of the fully-shielded, field-emission Electron Probe Micro-Analyser (EPMA) JEOL 8500F, powered by remX, has provided a capability to investigate the local distribution and concentration of elements in highly radioactive samples, including fuel rod segments. Acquisition of this new instrument has broadened the scope of the investigations, from polished specimens to fractography samples, and has enhanced the electron optical imaging capability and X-ray resolution analysis. Selected results of scanning electron microscopy and electron probe microanalysis on a highly irradiated fuel rod are presented here.

Scanning electron microscopy (SEM) and electron probe micro-analysis (EPMA), performed on a Boiling Water Reactor (BWR) fuel rod specimen, with an average burn-up of 57.5 MWd/kgU, illustrate the capability of the newly acquired, fully-shielded, field-emission EPMA JEOL 8500F, powered by remX. Both electron-optical and micro-analytical methods have been used to characterise CRUD, oxide-layer and fuel at high burn-up, all of which are crucial factors in overall reactor fuel performance. The results yield important information with respect to cladding corrosion, morphology, and the distribution of fissile and fission products in the fuel, all which are important parameters in regard to fuel behaviour, its efficiency and integrity.

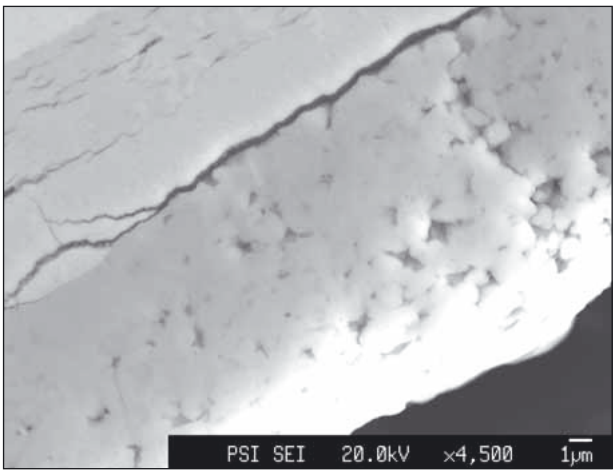

Figure 1: **SEM image of the outer oxide (zirconium) and CRUD layers of an irradiated BWR fuel rod.**

CRUD structure and composition

CRUD is a deposit of oxidation products on the external surface of fuel rods that can modify locally important parameters concerning fuel rod behaviour, such as thermal conductivity, or the corrosion condition of the cladding. In the current programme, the CRUD thickness and the water-side oxide-layer thickness have been measured at different azimuthal locations around the cladding circumference of an irradiated BWR fuel rod. The variability of the CRUD layer thickness indicates that much loose, fine-grained CRUD had fallen off during handling and transportation.

The texture of the deposit is quite homogeneous, with a dense layer near the CRUD/oxide interface, and a granular, less dense CRUD layer at the outer rim, close to the interface. The CRUD sometimes appears more porous, and gives the impression of being a less compact material, as seen on the SEM image in Fig. 1.

At the same location, Fig. 2 shows a typical example of the back-scattered electron (BSE) image, in which the CRUD layer is contrasted against different material compositions. Complementary to this, the Ni, Fe, Zn and Mn X-ray mappings are shown in Fig. 3. The element Fe is rather homogeneously distributed, whereas Zn, Ni and Mn are scattered, with a stronger presence near the CRUD/oxide interface, indicating a spinel-type oxide formation. The element ratios are also complex, with strong, non-systematic variations observed locally, but which can be analysed quantitatively taking into account the EPMA resolution below 0.5 µm.

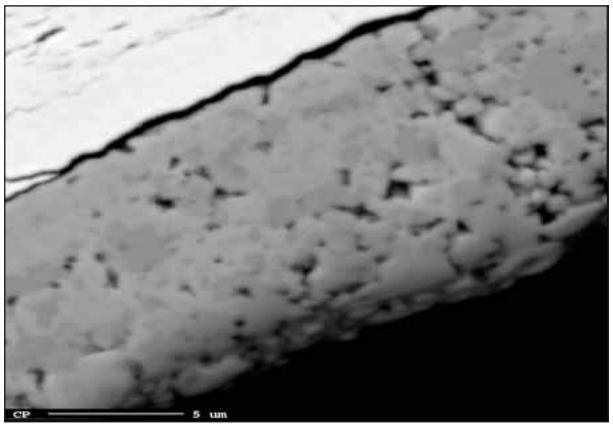

Figure 2: **BSE image of the CRUD layer.**

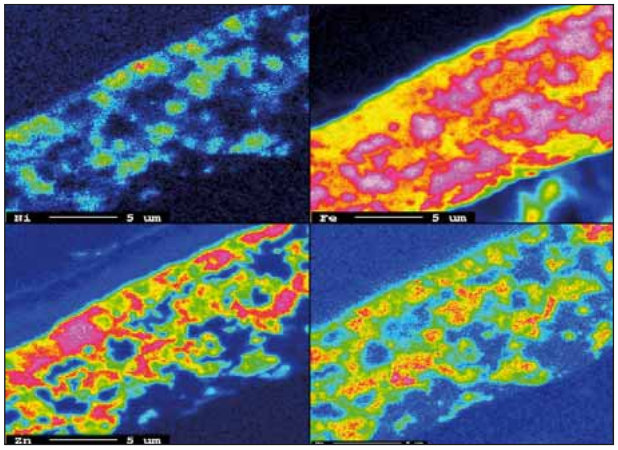

Figure 3: **X-ray mappings of Ni, Fe, Zn and Mn in CRUD material.**

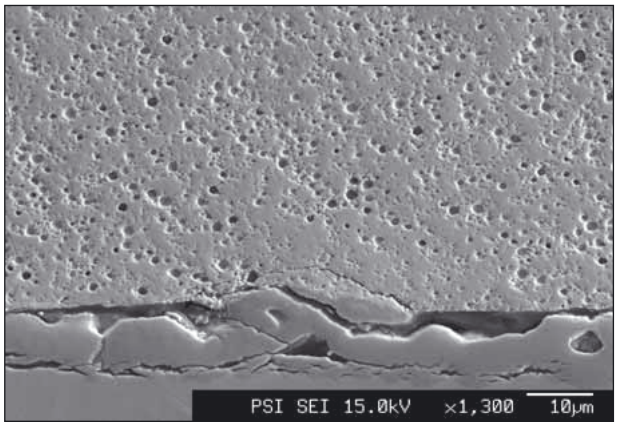

Figure 4: **SEM image showing the porosity at the rim adjacent to the inner oxide layer of the fuel rod.**

Fuel structure and composition

The fuel has been analysed using standard PSI procedures. The porosity and element distribution across the fuel pellet yield important information concerning the fuel and fission-gas behaviour during reactor operation. An SEM image of the porosity in the fuel rim zone (where the pore density is at a maximum) following high burn-up is given in Fig. 4.

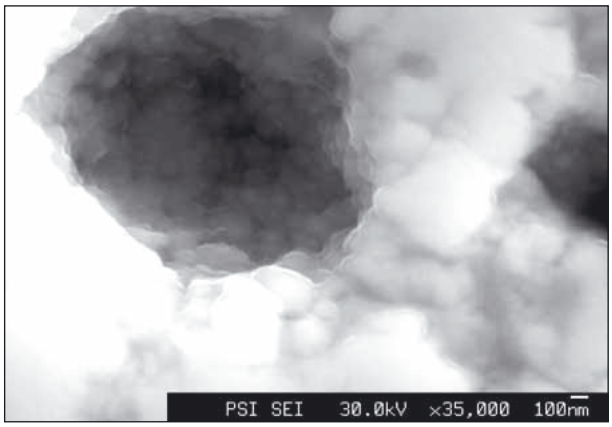

Figure 5: **SEM image of a pore in the rim zone with fission product particles and sub-micron fuel grains.**

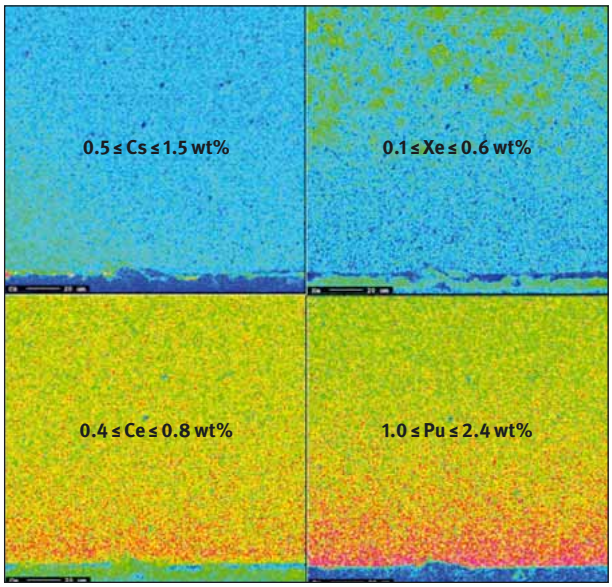

Figure 6: **Cs, Xe, Ce and Pu distribution in the high burn-up structure of the fuel rim.**

An example of the high-resolution imaging possible with the new instrument is given in Fig. 5, which shows the details of the internal surface of an open pore in the high burn-up zone. Finally, element mappings acquired at the periphery of the pellet are presented in Fig. 6. At the periphery, dissolved Xe in the matrix is present only up to 70 µm from the fuel edge. The Ce, Cs and Pu concentrations increase towards the pellet periphery, due to the higher fission and breeding rates.

Conclusions

The new instrument, EPMA JEOL 8500F, powered by remX, makes possible a complete and quantitative element-distribution analysis of the surface of highly irradiated materials. The field emission electron gun, combined with elaborate spectrometer shielding, produce high electron-optical and X-ray resolution performance.

FIXBOX: a complex installation for the treatment of liquid radioactive waste

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The conditioning of liquid waste containing radioactive materials, in particular waste containing non-irradiated and/or irradiated nuclear fuel material in solution, is a safety-relevant problem in many Hot Laboratories around the world. At PSI, the FIXBOX facility has been developed, featuring the enclosure of the radioactive elements in cement bricks, by which the actinide and fission products are safely combined within a solid matrix. The resulting 'waste bricks' can then be safely conditioned in a package, to be certified for intermediate and final storage. The third-generation facility, FIXBOX-3, has recently been completed, and will be commissioned as soon as all the administrative steps and controls required by the safety authorities have been finalised.

Handling and conditioning of liquid radioactive waste containing dissolved fuel material is difficult, and necessitates the use of complex, dedicated installations. The third generation of the FIXBOX facility is a further development of the installation successfully used at PSI in the past for the conditioning of liquid waste containing non-irradiated fuel. The newly shielded FIXBOX-3 facility has been specifically developed for the handling, treatment and conditioning of highly-radioactive, liquid waste containing irradiated fuel and fission products.

Waste type

The liquid waste results from the treatment of radioactive materials using wet chemical processes, like etching, for optical microscopy investigations, and surface cleaning or material dissolution, for elemental or isotopic analyses. In the PSI Hot Laboratory, the largest amount of liquid waste results from dissolution processes of non-irradiated and irradiated fuel in connection with the fuel development and fuel behaviour research programmes.

Figure 1: **Installation of the distillation column in its alpha-containment.**

General concept of FIXBOX-3

The FIXBOX-3 facility consists of two lead-shielded boxes, together with internal steel boxes to ensure complete alpha containment. In the first box, called the *Concentration Box*, low-active solutions are safely concentrated using a well-controlled distillation process, carried out under vacuum conditions to decrease the waste volume to be treated in the second box (Fig. 1). The concentration rate is carefully determined as a function of the composition of the liquid to exclude exothermic reactions.

In the second box, called the *Solidification Box,* a well-defined volume of liquid, resulting from the concentration process and/or waste to be directly conditioned, is mixed and carefully analysed. Then, the liquid is mixed with a pre-determined volume of cement powder to produce solid bricks, which are then placed in steel casings (Fig. 2).

Figure 2: **Steel casing containing a cement brick (test).**

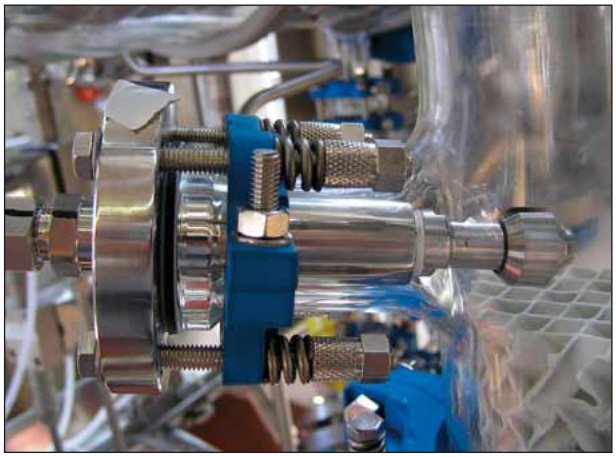


Figure 3: **Complex connector for a water cleaning sprayer nozzle.**

Safety considerations

All the processes carried out in the FIXBOX-3 facility have been developed and optimised to maximise the safety of the operators, and generally to control the contamination of the installation. Complex instrumentation and auxiliary equipment have been specially developed to ensure that operation of the installation can be achieved by remote means (Fig. 3). Additionally, tests have been performed to determine the maximum salt and acid concentrations consistent with the production of dense and solid bricks, with conservative limits imposed on all operational procedures. These measures, together with the experience gained during operation of the previous FIXBOX installation, ensure that the FIXBOX-3 facility will be operated safely when it comes into operation.

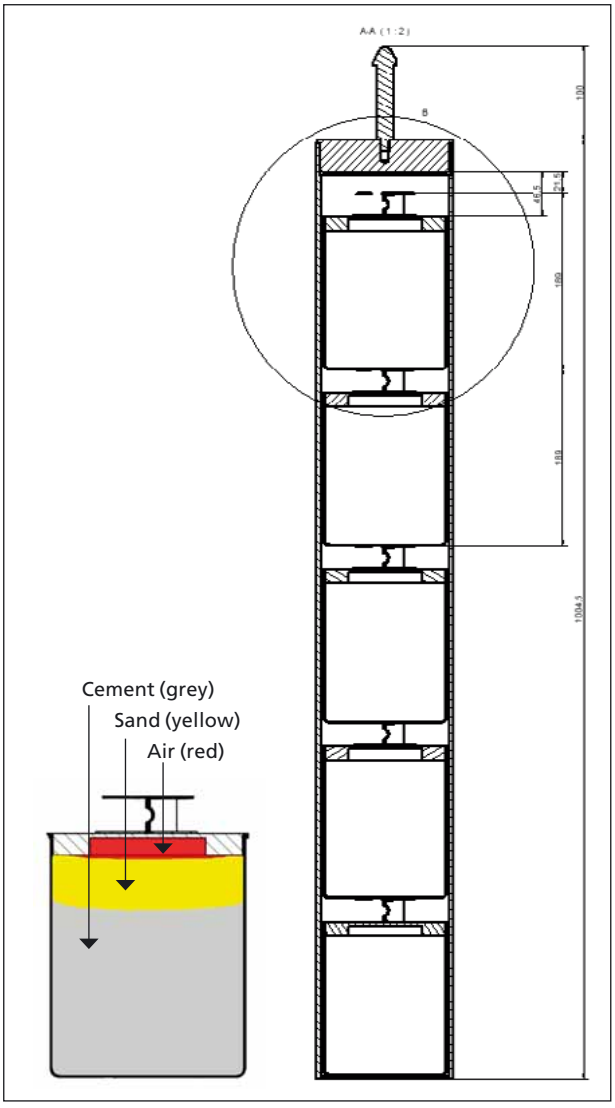


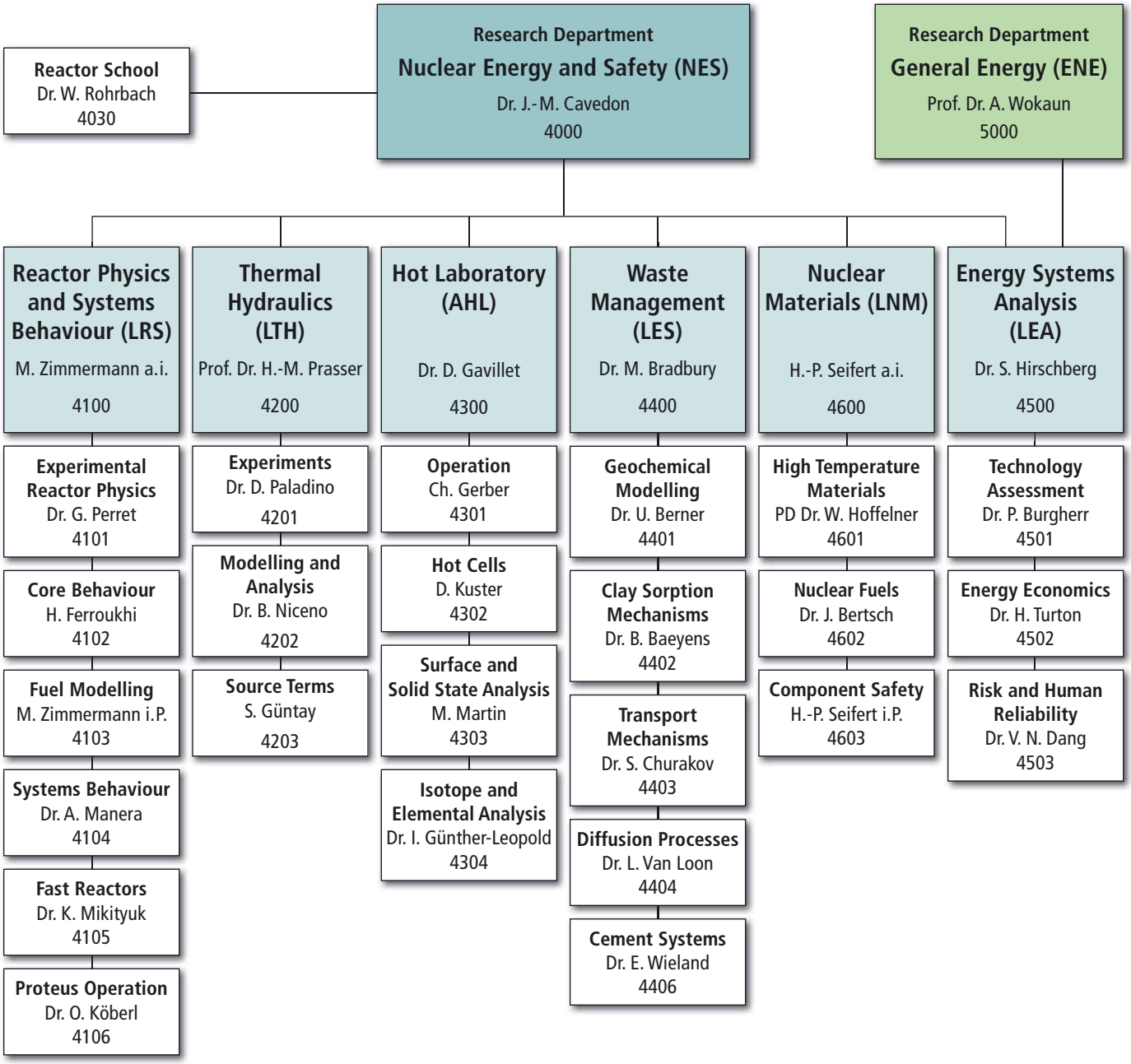
Figure 4: **Sketch of a cement brick in its steel casing and subsequent stacking in the final container.**

Final conditioning

After complete drying/solidification of the bricks in their steel casings, the upper part of the inner casing volume is filled with quartz sand and finally closed with a covering lid. Five such casings are then installed in a sealed, steel cylinder ready for final disposal (Fig. 4). All processes will be realised remotely in the FIXBOX facility itself, and the Hot Laboratory's concrete cells.

Conclusions

The FIXBOX-3 facility is a complex installation in the Hot Laboratory at PSI. It has been specially developed and optimised for the safe handling and conditioning of fuel-containing acidic solutions resulting from the various research activities performed at PSI.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Dr. J.-M. Cavedon
4000
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General Energy (ENE)
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◀ **Organisational chart of the Nuclear Energy and Safety Research Department.**

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Krepel J., Mikityuk K., Sun K., Rimpault G.1
"ESFR – analysis of sustainable fuel cycle" 7th Eur. Commission Conf. on Euratom Research and Training in Reactor Systems (FISA 2009), Prague, Czech Republic, 22-24 June 2009, Prague, Czech Republic
[1] CEA, Cadarache, FR

NES Colloquia

Abolhassani-Dadras S.
"Nuclear materials imaging with electrons: nano-scale", 22 October 2009

Bako B.
"Dislocation dynamics: from micro- to meso-scale description", 19 February 2009

Churakov S.
"Multiscale modelling: clay as repository barrier", 23 April 2009

Dehbi A.
"Particle transport: in nuclear reactors", 28 May 2009

Kosakowski G.
"Particle transport: in geological media", 28 May 2009

Krack M.,
"Multiscale modelling: uranium compounds", 23 April 2009

Martin M.
"Nuclear materials imaging with electrons: micro-scale", 22 October 2009

Samaras M.
"Multiscale modelling: reactor structure material", 23 April 2009

University Level Teaching

Cavedon J.-M.
"From Nuclear Structure to Nuclear Energy", Lecture Course, ETHZ, Zurich, Switzerland, Autumn Semester, 2009

Curti E.
Lectures given in the Course: "Geological Disposal of Radioactive Waste", University of Berne, Switzerland, Summer Semester, 2009

Degueldre C.
"Comportement des radionucleides dans l'environnement", Lecture Course, University of Geneva, Switzerland, Autumn Semester, 2009

Dehbi A.
"Introduction to Lagrangian Methods for Dispersed Flows", "Lagrangian Tracking in Laminar Flows", "Lagrangian Tracking in Turbulent Flows", "Particle-Turbulence Interactions", "Stochastic Methods in Particle Dispersion Modeling", Lectures given in Master Course: Computational Multiphase Thermal Fluid Dynamics, ETHZ, Zurich, Switzerland, Spring Semester, 2009

Gavillet D.
"Advanced Topics in Nuclear Reactor Materials", Lectures given in the Nuclear Engineering Master Program, ETHZ, Zurich, Switzerland, Spring Semester, 2009

Gavillet D.
"Effect of Radiation on Materials – Fission Materials", Lectures given in the Doctoral School Program (MSE-600), EPFL, Lausanne, Switzerland, Summer Semester, 2009

Gimmi T.
"Geochemical Modelling II: Reactive Transport", Master Course in Environmental and Resource Geochemistry, University of Berne, Switzerland, Summer Semester, 2009

Giust F.
Lectures given in Master Course: Special Topics in

Reactor Physics (151-0166-00 G), ETHZ, Zurich, Switzerland, Spring Semester 2009

Günther-Leopold I.
"Fuel Reprocessing", Lectures given in the Course: Nuclear Energy Systems, ETHZ, Zurich, Switzerland, Summer Semester, 2009

Günther-Leopold I.
"Kernbrennstoffe", Strategic Exercise given in the Course: Analytische Chemie V, ETHZ, Zurich, Switzerland, 27 October 2009

Hummel W.
Lectures given in the Course: Nuclear Energy Systems, ETHZ, Zurich, Switzerland, Summer Semester, 2009

Hummel W.
"Landfilling, nuclear repositories and contaminated sites", Lectures given for degree of Master of Biochemistry and Polution, ETHZ, Zurich, Switzerland, Autumn Semester, 2009

Kolbe E.
"Radioisotopes and Radiation Applications", Lectures given in the Nuclear Energy Master Program, ETHZ, Zurich, Switzerland, Spring Semester, 2009

Kosakowski G.
"Geostatistics I & II", Lecture Course: Master in Applied Environmental Geoscience, University of Tubingen, Germany, Autumn Semester 2009

Krack M.
"Introduction to the CP2K DFT module QUICKSTEP", "Accuracy and Efficiency", Lectures given in the Course: 1st CP2K Tutorial: Enabling the Power of Imagination in MD Simulations", CECAM-ETHZ, Zurich, Switzerland, 9-13 February 2009

Kulik D.
"Thermodynamic concepts in modeling sorption at the mineral-water interface", Lecture given at the Short Course in Thermodynamics and Kinetics of Fluid-Rock Interaction, Davos, Switzerland, 19-21 June, 2009

Manera A.
Lectures given in the Course: Multiphase Flow (151-1906-00L), ETHZ, Zurich, Switzerland, Spring Semester 2009

Manera A.
Lectures given in the Course: Nuclear Reactors Laboratory Course (151-0162-00L), ETHZ, Zurich, Switzerland, Spring Semester 2009

Manera A.
"Thermal-Hydraulic System Codes and Hands-On Training", Lecture Course: Training on TRACE – a best estimate thermal-hydraulics code, ENSI, Villigen PSI, Switzerland, 17-21 August 2009

Mikityuk K.
"Coupling for reactor dynamics", Lectures given in the Course: Special topics in reactor physics, part of EPFL/ETHZ Nuclear Engineering Master Program (ETHZ course 151-0166-00L), April-May 2009

Mikityuk K.
"Lead-cooled fast reactor", Lecture given at the 2009 Fréderic Joliot/Otto Hahn Summer School, KIT, Karlsruhe, Germany, 26 August - 4 September 2009

Niceno B.
"Essentials of Multiphase Flows", "Continuum Phase Modeling", "Wall Modeling", "Introduction to Multiphase Flow Modeling", "Two-Fluid Model", "Interface Tracking Techniques", "Mechanistic Modeling of Boiling", Lectures given in Master Course: Computational Multiphase Thermal Fluid Dynamics, ETHZ, Zurich, Switzerland, Spring Semester, 2009

Pelloni S.
"Adjoint flux and perturbation theory", "Fast reactor neutronics methods", Lectures given in the Master Course: Special Topics in Reactor Physics, ETHZ, Zurich, Switzerland, Summer Semester, 2009

Pouchon M..
"Radiation Damage", Lecture given in the Course: Materials for Nuclear Power Plants, ETHZ, Zurich, Switzerland, 11 March 2009

Pouchon M.A.
"Cladding", Lecture given in the Course: Materials for Nuclear Power Plants, EPFL, Lausanne, Switzerland, 27 October 2009

Weidmann N.
"Demand-side measures; supply-side measures: technological learning", Lecture given in the Course: Renewable Energy Technologies I, ETHZ, Zurich, Switzerland, 29 September 2009

Zimmermann M.A.
"Advanced Topics in Nuclear Reactor Materials", Lectures given in the Nuclear Master Program, ETHZ, Zürich, Switzerland, Autumn Semester 2009

Zimmermann M.A.
"Nuclear Fuels & Materials", Lectures given in the Nuclear Master Program, EPFL, Lausanne, Switzerland, Autumn Semester 2009

Habilitation, Doctoral, Master and Bachelor Theses

Girardin G.
Development of the Control Assembly Pattern and Dynamic Analysis of the Generation IV Large Gas-Cooled Fast Reactor (GFR), Doctoral Thesis No. 4437, EPFL, Lausanne, 2009

PSI and Other Reports

Allelein H.J.[1], Auvinen A.[2], Ball J.[3], Guentay S., Herranz L.[4], Hidaka A.[5], Jones A.V.[6], Kissane M.[7], Powers D.[8], Weber G.[2]
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[1] GRS, Köln, DE
[2] VTT Energy, Espoo, FI
[3] AECL, Chalk River, CA
[4] CIEMAT, Madrid, ES
[5] JAEA, Tokai-mura, JP
[6] JRC, Karlsruhe, DE
[7] IRSN, Cadarache, FR
[8] SNL, Albuquerque, US

Bertsch J., Alam A., Zubler R.
"Crack Resistance Curve Determination of Zircaloy-4 Cladding", PSI-Bericht Nr. 09-04

Dreier J., Smith B.L.
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[1] VTT, Helsinki, FI
[2] CEA, Cadarache, FR
[3] SCK-CEN, Brussels, BE
[4] Studsvik Ecosafe, Nykoping, SE
[5] KFKI, Budapest, HU
[6] NRI, Rez, CZ

Seifert H.P., Ritter S.
"Environmentally-Assisted Cracking in Austenitic LWR Structural Materials — Final Report of the KORA-I Project", PSI-Bericht Nr. 09-03

General Communications and Public Relations

Cavedon J.M.
"Une réaction en chaine et son contrôle, ou la vie d'un réacteur nucléaire", Séminaire d'information, Matinée de clarification pour les élus romands, Fédération romande pour l'énergie, Lausanne, Switzerland, 4 May 2009

Cavedon J.M.
"Abfälle, Externalities, Generation III, Risiken", Energieforum Schweiz, Berne, Switzerland, 21 October 2009

Chawla R.
"Les réacteurs d'aujourd'hui, de demain et d'après-demain", Journée d'étude 2009 de l'Association Romande de Radioprotection (ARRAD), Lausanne, Switzerland, 29 October 2009

Hardegger P.
"Les impacts comparés des différentes sources de production d'énergie", Séminaire d'information, matinée de clarification pour les élus romands, Fédération romande pour l'énergie, Lausanne, Switzerland, 4 May 2009

Hardegger P.
"Produktion elektrischer Energie, Vor- und Nachteile, spezieller Einblick in die Kernenergie", Information Schweiz, Reinach, Switzerland, 29 September 2009

Awards

Epiney A.
Best paper: Int. Youth Conf. on Energetics 2009 (3rd ENEN PhD Event 2009), Budapest, Hungary, 5 June 2009

Proff C.
Posterpreis: Microscopy Conference (MC 2009), Graz, Austria, Aug. 30 – Sept. 4, 2009

Wieselquist W.A.
Best student paper: Int. Conf. Computational Methods and Reactor Physics, Saratoga Springs, USA, 3-7 May 2009

Membership of External Committees

Cavedon J.-M.
- Member of the KNS (Swiss Federal Nuclear Safety Commission)
- Member of the Advisory Board of the French Institut de Radioprotection et de Sûreté Nucléaire IRSN
- Swiss representative to the Committee on the Safety of Nuclear Installations (OECD/CSNI)
- Swiss representative to the Policy Group of the Generation IV International Forum

Chawla R.
- Vice Chairman of the OECD/NEA Nuclear Science Committee (NSC)

- Invited Expert on the Scientific Committee of the French CEA's Direction de l'Energie Nucléaire (DEN)
- Member of the Editorial Board of Annals of Nuclear Energy
- Member of the Training and Academic Affairs Committee of the European Nuclear Education Network (ENEN)

Degueldre C.
- Member of the Executive Committee, Symposium N Organiser of the 2010 Meeting of the European Material Research Society (E-MRS), June 7-11, 2010

Froideval A.
- Appointed member as Swiss user representative of the European Synchrotron Users Organisation (ESUO)

Guentay S.
- Vice Chairman of the OECD/NEA Working Group on the Analysis and Management of Acidents (WGAMA)

Janssens K.
- Principal Symposium Organizer (as member of the Computational Materials Science Committee of TMS) of "Fatigue: Mechanisms, Theory, Experiments and Industry Practice" at the TMS Annual Meeting, February 15-19, 2009, San Fransisco, CA

Manera A.
- Member of the Editorial Board: Science and Technology of Nuclear Installations
- Vice-President of the Schweizerische Gesellschaft der Kernfachleute (SGK)

Ritter S.
- Vice Chairman of the Executive Committee of the European Cooperative Group on Corrosion Monitoring of Nuclear Materials (ECG-COMON)

Samaras, M.
- Co-chair of the OECD/NEA Working Party on Multi-Scale Modelling of Fuels and Structural Materials for Nuclear Systems (WPMM) Expert Group on Multiscale Modelling Methods
- Member of the Reviewers' Committee of the Nuclear Engineering and Technology (NET) journal
- Member of the International Advisory Board of CIMTEC 2010: 5th Forum on New Materials

Seifert H.P.
- Member of the Executive Committee of the International Cooperative Group on Environmentally Assisted Cracking of Water Reactor Materials (ICG-EAC)

Smith B.L.
- Chairman of the OECD/NEA Working Group on the Analysis and Management of Acidents (WGAMA) CFD Special Group

Zimmermann M.
- Swiss representative to the Committee for the Safety of Nuclear Installations (OECD/CSNI)
- Chairman of the CSNI Expert Group Safety Margin Assessment and Application (SM2A)
- Swiss representative to the GIF International Expert Group

LEA – Laboratory for Energy Systems Analysis

The Energy Departments (NES and General Energy)

Publications in Books

Burgherr P., Hirschberg S.
"Wiley Handbook of Science and Technology for Homeland Security", in J.G. Voeller (Ed.): Comparative risk assessment for energy systems: a tool for comprehensive assessment of energy security, John Wiley & Sons Inc., Hoboken NJ, USA, 1-19, 2009 (ISBN 978-0-471-76130-3)

Eskeland G.[1], Criqui P.[2], Jochem E.[3], Catenazzi G.[4], Neufeldt H.[5], Eichhammer W.[6], Held A.[6], Jakob M.[4], Mima S.[2], Linnerud K.[7], Schade W.[6], Traber T.[8], Reiter U., Turton H., Rive N.[7], Mideksa T.[7]
"Transforming the European Energy System", in M. Hulme, H. Neufeldt, (Eds.): Making Climate Change Work for Us: European Perspectives on Adaption and Mitigation Strategies, Cambridge University Press, 165-199, 2009 (ISBN 978-0-521-11941-2)

[1] NHH, Bergen, NO
[2] University of Grenoble, FR
[3] ETHZ CEPE, Zurich, CH
[4] ETHZ, Zurich, CH
[5] ICRAF, Nairobi, EAK
[6] FhG-ISI, Karlsruhe, DE
[7] CICERO, Oslo, NO
[8] DIW, Berlin, DE

Knopf, B.[1], Edenhofer, O.[1], Barker, T.[2], Baumstark, L.[3], Criqui, P.[4], Held, A.[5], Isaac, M.[6], Jakob, M.[6], Jochem, E.[7], Kitous, A.[7], Kypreos, S., Leimbach, M.[1], Magné, B., Mima, S.[3], Schade, W.[4], Scrieciu, S.[2], Turton, H., van Vuuren, D.[5]
"The Economics of Low Stabilisation: Implications for Technological Change and Policy", in Hulme, M., Neufeldt, H. (eds.): Making Climate Change Work for Us: European Perspectives on Adaption and Mitigation Strategies, Cambridge University Press, Cambridge University Press, 291-318, 2009 (ISBN 978-0-521-11941-2)

[1] PIK, Potsdam, DE
[2] University of Cambridge, UK
[3] University of Grenoble, FR
[4] FhG-ISI, Karlsruhe, DE
[5] PBL, Bilthoven, NL
[6] ETHZ, Zurich, CH
[7] ENERDATA, Grenoble, FR

Publications in Scientific and Technical Journals

Baraldi P.[1], Librizzi M.[1], Zio E.[1], Podofillini L., Dang V.N.
"Two Techniques of Sensitivity and Uncertainty Analysis of Fuzzy Expert Systems", Expert Syst. Appl. (ISSN 0957-4174), **36**(10), 12461-12471 (2009)

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[1] University of Manchester, UK
[2] Queensland University of Technology, Brisbane, AU

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[1] University of Waterloo, CA

Mercurio D., Podofillini L., Zio E.[1], Dang V.N.
"Identification and classification of dynamic event-tree scenarios via possibilistic clustering: application to a steam generator tube rupture event", Accid. Anal. Prev. (ISSN 0001-4575), **41**(6), 1180-1191 (2009)

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Ristovski Z.D.[1], Suni T.[2], Kulmala M.[2], Boy M.[2], Meyer N.K., Duplissy J., Turnipseed A.[3], Morawska L.[1], Baltenpserger, U.
"The role of sulphates and organic vapours in new particle formation in a eucalypt forest" Atmos. Chem. Phys. Discuss. (ISSN: 1680-7367), **9**, 17793-17815 (2009)

[1] Queensland University of Technology, Brisbane, AU
[2] University of Helsinki, FI
[3] BAI Group, Boulder, US

Roth S.[1], Hirschberg S., Bauer C., Burgherr P., Dones R., Heck T., Schenler W.
"Sustainability of electricity supply technology portfolio", Ann. Nucl. Energy (ISSN 0306-4549), **36**, 409-416 (2009)
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"Heuristic Design of Advanced Drives Analysis of Trade-Offs in Powertrain Electrification", World Electric Vehicle Association Journal (ISSN 2032-6653), **3**, 1-7 (2009)

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[1] Polytechnic of Milan, IT

International Conferences with Proceedings

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"A Bayesian Network Model for Dependence Assessment in Human Reliability Analysis", Eur. Safety and Reliability Conference (ESREL 2009), 7-10 September 2009, Prague, Czech Republic, Vol. 1, 223-230, 2009 (ISBN 978-0-415-55509-8)
[1] Polytechnic of Milan, IT

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"Quantifying wood combustion emissions with on-line methods". 13th ETH-Conference on Combustion Generated Nanoparticles, 22-24 June 2009, Zurich, Switzerland, CD-ROM, 2009
[1] University of Applied Sciences, Windisch, CH
[2] Oekozentrum, Langenbruck, CH
[3] Lucerne University of Applied Sciences and Arts, Horw, CH

Miljevic B.[1], Meyer N.K., Keller A.[2], Burtscher H.[2], Good J.[3], Doberer A.[3], Lauber A.[3], Nussbaumer T.[3], Heringa M.F., Richard A., DeCarlo P.F., Prevot A.S.H., Fairfull-Smith K.E.[1], Baltensperger U., Bottle S.E.[1], Ristovski Z.D.[1]
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[2] University of Applied Sciences, Windisch, CH
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[1] Loughborough University, UK

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"Heuristic Design of Advanced Drives Analysis of Trade-Offs in Powertrain Electrification", Electric Vehicle Symposium (EVS 24), 12-17 May 2009, Stavanger, Norway, CD-ROM, 2009

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Bauer C.
"CO_2-Abscheidung & Speicherung: Patentlösung für eine nachhaltige Stromversorgung?", Zürcher Hochschule für Angewandte Wissenschaften (ZHAW), Kompetenzzentrum für Sicherheit und Risikoprävention (KSR), Winterthur, Switzerland, 27 May 2009

Bauer C.
"Life-cycle analysis: a tool supporting rational decision-making", Carbon Management in Power Generation (CARMA) Workshop on LCA, Risk Assessment, External Costs and MCDA, ETHZ, Zurich, Switzerland, 25 September 2009

Bauer C.
"Wie vergleicht man verschiedene Verkehrsmittel? — Methodik und Datengrundlagen der Ökobilanz-Datenbank ecoinvent", Tagung: Umweltvergleich von Verkehrsträgern des SBB Umweltcenters, Zurich, Switzerland, 24 November 2009

Bauer C., Heck T.
"Carbon capture and storage: life cycle assessment and external costs of future fossil power generation", 4th Int. Conf. on Life Cycle Management, Cape Town, South Africa, 6-9 September 2009

Burgherr P.
"Comparative assessment of accidents in the energy sector: risk indicators and monetization issues", IRSN Workshop on Measuring the Cost of Disasters, Zurich, Switzerland, 26 May 2009

Burgherr P., Hirschberg S., Eckle P.
"Comparative assessment of accident risks in the energy sector: results from NEEDS and outlook", Swiss Federal Office of Civil Protection (BABS), Berne, Switzerland, 20 October 2009

Eckle P., Burgherr P., Hirschberg S.
"Risk Analysis Methods", Swiss Federal Office of Civil Protection (BABS), Berne, Switzerland, 20 October 2009

Gül T., Turton H.
"Illustrating perspectives of energy and mobility", Int. Advanced Mobility Forum (IAMF 2009), Geneva, Switzerland, 10-12 March 2009

Heck T.
"Environmental impacts and external costs methods – tutorial overview", Tutorial Workshop, Institut für Atmosphäre und Klima (IAC), ETHZ, Zurich, Switzerland, 12 January 2009

Heck T.
"Assessment of environmental impacts and external costs related to air pollution emissions", Invited Talk, Kolloquium Atmosphäre und Klima, ETHZ, Zurich, Switzerland, 19 October 2009

Heck T.
"Regionalization and parameterization of LCA and LCIA of energy systems", Life Cycle Assessment (LCA) Discussion Forum, ETHZ, Zurich, Switzerland, 13 November 2009

Hirschberg S.
"Technology assessment and stakeholder perspectives", Invited Talk, Policy Session, Conf, on External Costs of Energy Technologies, Eur. Economic and Social Committee, Brussels, Belgium, 16-17 February 2009

Hirschberg S.
"Energy technology roadmap and stakeholder perspectives", Invited Talk, R&D Session, Conf. on External Costs of Energy Technologies, Eur. Economic and Social Committee, Brussels, Belgium, 16-17 February 2009

Hirschberg S.
"Fuels — a competition between resources and global warming", Int. Advanced Mobility Forum (IAMF 2009), Geneva, Switzerland, 10-12 March 2009

Hirschberg S.
"State-of-the-art, technology-specific indicators for sustainability asssessment: methodology, results and options for aggregation", "Multi-criteria decisions analysis", Technical Meeting on Defining and Selecting Integrated Indicators for Nuclear Power Development, IAEA, Vienna, Austria, 24-27 March 2009

Hirschberg S.
"Optionen für die Elektrizitätsversorgung in der Schweiz", Invited Talk, Wissenmanagement ENSI, ENSI, Würenlingen, Switzerland, 5 June 2009

Hirschberg S.
"Multi-criteria decision analysis of power systems", Invited Talk, 38th Life Cycle Analysis (LCA) Discussion Forum, ETHZ, Zurich, Switzerland, 19 June 2009

Hirschberg S.
"Life-cycle assessment activities at the Paul Scherrer Institute", Seminar in connection to the visit by the Federation of Thai Industries, EMPA, Dubendorf, Switzerland, 20 August 2009

Hirschberg S.
"Externalities in the energy system", IAEA Scientific Forum on Energy for Development, Invited Talk, IAEA, Vienna, 15-16 September 2009

Hirschberg S.
"Global energy challenges and Swiss supply system", Carbon Management in Power Generation (CARMA) Workshop, ETHZ, Zurich, Switzerland, 25 September 2009

Hirschberg S.
"Technology-specific indicators for sustainability assessment & MCDA: overview", "Alternative criteria structure and sustainability indicators", Technical Meeting on Experience with the Application of Integrated Indicators for Nuclear Power Development, IAEA, Vienna, Austria, 27-30 October 2009

Hirschberg S.
"Swiss scientific perspective on climate change and related issues", Invited Talk, European Nuclear Council Meeting, ATEL, Zurich Airport, Switzerland, 5 November 2009

Hirschberg S., Burgherr P.
"Risikoanlayse verschiedener Energie-Technologien", Invited Talk, Axpo Executive Meeting, AXPO, Zurich, Switzerland, 18 March 2009

Hirschberg S., Burgherr P.
"Comparative risk assessment", Carbon Management in Power Generation (CARMA) Workshop, ETHZ, Zurich, Switzerland, 25 September 2009

Hirschberg S., Burgherr P.
"Comparative assessment of severe accidents associated with various energy technologies", Invited Talk, Int. Conf. on Nuclear Power: Technology, Investors, Financing, Most Wanted! Conferences & Events, Warsaw, Poland, 19-20 November 2009

Hirschberg S., Heck T.
"External cost assessment", Carbon Management in Power Generation (CARMA) Workshop, ETHZ, Zurich, Switzerland, 25 September 2009

Kypreos S., Cuomo V.[1], Loulou R.[2], Blesl M.[3], Cosmi C.[1], Salvia M.[1], Van Regemorter D.[4]
"European Energy and Climate Change Scenarios Evaluated with the TIMES Model for the EU-NEEDS Project", Invited Talk, ATINER 4th Int. Symp. on Environment, Athens, Greece, 21-24 May 2009
[1] IMAA, Tito Scalo, IT
[2] McGill University, Montreal, CA
[3] University of Stuttgart, DE
[4] University of Leuven, BE

Kypreos S., Turton H.
"Climate Change Scenarios evaluated with MERGE-ETL and Technology Transfer Protocols", Int. Energy Workshop 2009, Venice, Italy, 17 June 2009

Marcucci A.
"NCCR Young Researchers Meeting", NCCR Climate Young Researchers Meeting, National Centres of Competence in Research (NCCR) Climate, Murten, 4 June, 2009

Marcucci A.
"Mitigation and sustainable energy strategies under global uncertainty", National Centres of Competence in Research (NCCR) Climate WP4 and NCCR Trade Joint Workshop, Berne, 27 November, 2009.

Meyer N.K.
"Emissions from Diesel and CNG Buses", HarmonE: Today's Technology, Tomorrow's Drivers, IIASA, Vienna, Austria, 18 May 2009

Meyer N.K., Duplissy J.[1], Gysel M., Metzger A.[1], Weingartner E., Prevot A., Alfarra M., Good N.[1], Dommen J., Fletcher C.[2], McFiggans G.[3], Baltensperger U., Jonsson A.[4], Hallquist M.[4], Ristovski Z.[1]
"Analysis of the hygroscopic and volatile properties of ammonium sulphate seeded and un-seeded SOA particles", Final project meeting: Integration of European Simulation Chambers for Investigating Atmospheric Processes (EUROCHAMP), Rügen, Germany, 13-15 May 2009
[1] Aachen University of Technology, DE
[2] Queensland University of Technology, AU
[3] University of Manchester, UK
[4] University of Gothenburg, SE

Meyer N.K., Heck T.
"Towards assessments of the health and climate impacts of biomass combustion emissions", Energy Use & Emissions in a Co-Benefits World, Workshop I, IIASA, Vienna, Austria, 18 May 2009

Meyer N.K., Heck T.
"Towards assessment of health & environmental impacts of biomass combustion", Impact of Biomass Burning Aerosol on Air Quality and Climate (IMBALANCE) Workshop, ETHZ, Zurich, Switzerland, 27 May 2009

Meyer N.K., Heck T.
"Towards assessments of the health and climate impacts of biomass combustion emissions", Invited Talk, Bundesamt für Umwelt (BAFU) Workshop: emission factors from wood burning, Lucerne, Switzerland, 3 July 2009

Reiter U.
"Climate change mitigation: challenges for the European electricity sector", Invited Talk, Int. Energy Workshop 2009 (IEW), Venice, Italy, 17-19 June 2009

Reiter U., Turton H.
"Climate change adaptation scenario for the European electricity sector", IARU Int. Sci. Congress on Climate Change: Global Risks, Challenges and Decisions, Copenhagen, Denmark, 10-12 March 2009

Wilhelm E., Schenler W.
"Heuristics for the Design of Advanced Powertrains: Strategies for Manufacturers", Int. Advanced Mobility Forum (IAMF 2009), 10-12 March 2009, Geneva, Switzerland, 2009

Wilhelm E., Schenler W.
"Losing Weight to Save Energy: How Advanced Materials could affect Tomorrow's Vehicle Fleet", EMPA PhD Symposium, EMPA, Dübendorf, Switzerland, 19 November 2009

Wokaun A., Turton H.
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Burgherr P.
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Dang V.N.
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Hirschberg S.
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"Nuclear Energy and Sustainability, Lecture 1: Life Cycle Assessment", Lecture given in the Course: Nuclear Energy Systems, ETHZ, Zurich, Switzerland, 7 May 2009

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"Life-Cycle Analysis and other Approaches for Sustainability Assessment", "Life Cycle Analysis and Multi-Criteria Assessment of Energy Systems in View of Sustainability Indicators", Lectures given in the Course: Renewable Energy Technologies I, ETHZ, Zurich, Switzerland, 24 November 2009

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Marcucci A.
"The global energy system: energy demand and supply climate protection goals; potential of renewables", Exercise given in the Course: Renewable Energy Technologies I, ETHZ, Zurich, Switzerland, 22 September 2009

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Habilitation, Doctoral, Master and Bachelor Theses

Conti M.
"A Bayesian Network for Quantifying Human Error Probabilities in Successive Emergency Tasks", Masters Thesis, Politecnico di Milano, Italy, 2009

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"Risiken der Kernenergie im Vergleich zu anderen Energiequellen", Invited Talk, ENSI-Rat, ENSI, Würenlingen, Switzerland, 27 May 2009

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Awards

Karanki D.R.
Outstanding researcher award for research in Uncertainty Management and Dynamic Reliability in PSA of NPPs, 4th Int. Conf. on Quality, Reliability and Infocom Technology (ICQRIT 2009), 18-20 December, 2009, New Delhi, India

Membership of External Committees

Hirschberg S.
- Member of the Review Panel for the Helmholtz Programme "Technology, Innovation and Society"

Turton H.
- Member of the Programme Committee for the Conference on the International Dimensions of Climate Policies, Berne, Switzerland, 21-23 January 2009

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