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PERFORM 60 – Prediction of the effects of radiation for reactor pressure vessel and in-core materials using multi-scale modelling – 60 years foreseen plant lifetime

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ABSTRACT

In nuclear power plants, materials may undergo degradation due to severe irradiation conditions that may limit their operational life. Utilities that operate these reactors need to quantify the ageing and the potential degradations of some essential structures of the power plant to ensure safe and reliable plant operation. So far, the material databases needed to take account of these degradations in the design and safe operation of installations mainly rely on long-term irradiation programs in test reactors as well as on mechanical or corrosion testing in specialized hot cells. Continuous progress in the physical understanding of the phenomena involved in irradiation damage and continuous progress in computer sciences have now made possible the development of multi-scale numerical tools able to simulate the effects of irradiation on materials microstructure. A first step towards this goal has been successfully reached through the development of the RPV-2 and Toughness Module numerical tools by the scientific community created around the FP6 PERFECT project. These tools allow to simulate irradiation effects on the constitutive behaviour of the reactor pressure vessel low alloy steel, and also on its failure properties. Relying on the existing PERFECT Roadmap, the 4 years Collaborative Project PERFORM 60 has mainly for objective to develop multi-scale tools aimed at predicting the combined effects of irradiation and corrosion on internals (austenitic stainless steels) and also to improve existing ones on RPV (bainitic steels).

PERFORM 60 is based on two technical sub-projects: (i) RPV and (ii) internals. In addition to these technical sub-projects, the Users' Group and Training sub-project shall allow representatives of constructors, utilities, research organizations... from Europe, USA and Japan to receive the information and training to get their own appraisal on limits and potentialities of the developed tools. An important effort will also be made to teach young researchers in the field of materials' degradation.

PERFORM 60 has officially started on March 1st, 2009 with 20 European organizations and Universities involved in the nuclear field.

1. Introduction

In nuclear power plants, reactor materials may undergo degradation in physical and mechanical properties due to severe in-service irradiation. So far, the material databases needed to allow for this degradation in the design and safe operation of installations have mainly relied on long-term irradiation programs in test reactors as well as on mechanical or corrosion testing in specialized hot cells.

This predominantly-empirical approach can now be complemented and improved. Indeed, continuous progress in physical understanding of radiation damage and in computer technology has made it possible to develop multi-scale numerical tools capable of simulating the effects of neutron irradiation on mechanical and corrosion properties of reactor materials [1].

A first step towards this goal has been successfully reached through the development of the RPV-2 and Toughness Module numerical tools by the European and wider international scientific community created around the FP6 PERFECT project [2]. These simulation tools are now able to predict irradiation effects on the mechanical properties of the ferritic light water reactor pressure vessel, and with further development have the potential of providing the constructors and utilities with alternative sources of data related to the residual lifetime prediction of such components.

A similar exercise dedicated to predicting the irradiation effects on austenitic stainless steels (internal structures) has also been performed in the FP6 PERFECT project.

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Relying on the existing PERFECT Roadmap, the 4 years Large Scale Integrating Project PERFORM 60 has the overall objective of developing multi-scale modelling tools aimed at predicting the combined effects of irradiation and corrosion on internals (austenitic stainless steels) and also of improving existing ones on RPV components (low-alloy bainitic steels). Where possible, these new and improved tools will be experimentally validated at each characteristic time or length-scale.

This large-scale collaborative project over 48-months has been produced in response to Fission-2008-2.2.1.3: "*Prediction of irradiation effects on reactor pressure vessel, internals and/or claddings using multi-scale simulation tools*". The research activities will build on previous actions in project PERFECT, which focused on initial multi-scale modelling of irradiation effects on reactor pressure vessels and internals using a qualified software integration platform. The work in progress, and the sustainable scientific and technical community in the EU member states that is expected to result from it, will contribute to the creation of a European Pole of excellence in numerical simulation for residual lifetime prediction in nuclear power plants. PERFORM 60 includes:

(i) the production of more advanced versions of RPV-2 (→RPV-n), together with an improved Fracture Toughness Module to produce an Advanced Fracture Toughness Module to model the irradiation degradation on reactor pressure vessels of PWRs and BWRs for durations of up to 60 years;
(ii) a platform of simulation tools (based on the same concept as the one developed for RPV components) to couple corrosion and irradiation effects on reactor internals in PWRs and BWRs;
(iii) experimental validation and model qualification using industrial plant data and results of existing or new experiments (including non-EU sources) as necessary. In addition, other means of validation such as benchmarking with existing qualified calculation codes will be considered. A Users' Group has been established to test the newly developed modelling tools in a number of benchmark exercises with a view to their qualification. Close links will be established where possible with the NEA and/or IAEA databanks and activities.

2. PERFORM 60 goals and objectives

In order to achieve the above objectives, PERFORM 60 is based on three technical sub-projects: (i) reactor pressure vessel (SP-1), (ii) internals (SP-2) and (iii) Users' Group (SP-3). The organisation of these technical sub-projects is described below.

2.1. Sub-project 1 "reactor pressure vessel"

Light water moderated and cooled fission reactors provide a significant contribution to Europe's electrical energy production needs. With the increasing age of these plants, there is a growing need for predictive capabilities to assess the performance of materials subject to ageing-related degradation phenomena.

Ferritic pressure vessel materials (generally low-alloy bainitic steels) are subject to neutron irradiation during their operational lives and, if damage doses reach only ~0.2 dpa at the end of life (40 years), the irradiation-induced shift in the brittle to ductile transition temperature for current RPV steels would typically be no more than 100 °C. For this level of damage, the damage mechanisms are understood reasonably well, but, in the case of an end of life of more than 40 years, different questions arise:

- Does accumulation of more than 0.2 dpa induce other damage mechanisms (for example: segregation of phosphorus to the grains boundaries or development of new phases after a certain incubation time)?
- What is the effect of temperature (~320 °C) for a duration of more than 40 years?

A first attempt to simulate the evolution of irradiation-induced degradation of mechanical properties has been included in RPV-2 and the Toughness Module of FP6 project PERFECT for Fe–Cu model alloys. However, gaining physical insight into the behaviour of more realistic RPV materials is necessary in order to develop practical applications. The research activities described under SP-1 "reactor pressure vessel" build on previous actions in project PERFECT, with the following objectives:

- Produce an Advanced Fracture Toughness Module (AFTM) based on development and integration of the multi-scale simulation tools RPV-2 (→RPV-n) and Fracture Toughness Module created in FP6 project PERFECT to simulate the irradiation degradation on reactor pressure vessels of PWRs and BWRs for durations up to 60 years.
- Benchmark the numerical results from the AFTM and compare these, where appropriate, with existing analytical methods and data (e.g. via the NEA and (or) IAEA databanks).
- Provide additional experimental validation and model qualification for the AFTM using industrial plant data and results of existing or new experiments (including non-EU sources) as necessary.
- Build the AFTM based on a strong interaction with the End Users' Group (SP-3) of PERFORM 60.

In order to do this SP-1 is organised into four technical work packages as follows:

- WP1-1 "fracture behaviour".
- WP1-2 "flow behaviour".
- WP1-3 "microstructural evolution".
- WP1-4 "integration".

2.1.1. WP1-1 fracture behaviour (AREVA GmbH)

The main objective of WP1-1 is to evolve existing methods for describing cleavage fracture toughness behaviour in bainitic RPV steels. Improved engineering models as well as at least one common local approach (LA) to fracture type model are under development, and physical understanding of the calibration parameters used in these models are sought. Because of the link between flow and fracture properties, a strong link with WP1-2 is essential.

Parallel to the development of the cleavage fracture toughness models, transferability issues such as crack-tip constraint, biaxiality, load history (WPS) and crack front length are being addressed.

To validate the models/methods, the available experimental database set up in PERFECT and, if necessary, additional experimental data are being used to define reference cases. These reference cases allow a comparison of the newly-developed methods with existing ones, and also demonstrate their application to components or structures.

As part of the process of integration onto the platform of PERFORM 60, the engineering models and the LA model(s) must be well documented, to include their theoretical basis and calibration procedures.

In addition to these developments, significant contributions in kind are foreseen from Oak Ridge National Laboratory (ORNL) and Phoenix Engineering Associates Inc. (PEAI), and the CRISM Prometey Institute.

In the case of ORNL and PEAI these contributions are mainly on the further development of the DISFRAC Code and its integration into the FTM. These contributions in kind are expected to build on existing successful collaborations established during the course of FP6 PERFECT.

2.1.2. WP1-2 flow behaviour (CEA)

Flow behaviour is the basic information which allows the computation of stresses and strains acting in a material under an applied load. Knowledge of this behaviour is essential to predict damage evolution and the fracture of materials which is the objective of WP1-1. Constitutive laws describe the flow behaviour in a mathematical form. To be accurate and reliable, these laws need to be physically founded. This means incorporating explicitly the mathematical description of the main mechanisms which are at the origin of the flow of the material.

The constitutive laws developed in WP1-2 are able to take into account the major features of the plasticity of RPV steels: thermally activated slip, hardening mechanisms and dislocation interaction with irradiation-induced defects. We also consider the effect of Carbon on dislocations and irradiation-induced defects. This is the most critical yet least fully addressed solute element effect. In comparison, the effect of atoms such as Cu and Ni are negligible when they are in solid solution and can be treated reasonably well in dislocation dynamics when they are present in the form of precipitates.

We must consider the different scales corresponding to the different mechanisms we want to account for. Different modelling tools of the different scales will be used; mainly ab initio density functional theory (DFT), molecular dynamics (MD), dislocation dynamics (DD), crystal plasticity (CP) and homogenization.

The main objective of WP1-2 is to produce tools which are able to predict the macroscopic mechanical behaviour of the irradiated RPV steel using the results of WP1-3 tools as an input. The "macroscopic tensile curve" is the major result of this prediction for which two different approaches are being used: the fast track based on crystal plasticity (CP) and homogenization, and the more refined track based on CP computations of representative grain aggregates.

2.1.3. WP1-3 microstructural evolution (SCK.CEN)

In a multi-scale modelling framework, the starting point for the prediction of the macroscopic changes induced by neutron irradiation in structural materials is a proper description of the microstructure evolution in terms of defect and precipitate populations, versus time/dose and temperature. These models must, as much as possible, include mechanisms and parameters obtained from fundamental atomic level studies, while treating phenomena occurring at a length-scale that may be already defined as "mesoscopic" (hundreds of nanometers to micrometers), over time-scales of macroscopic significance (seconds to years). Models of this type can be defined as coarse-grained microstructure evolution models and are generally based on approaches such as rate theory (RT) or kinetic Monte Carlo (KMC).

The former (RT) corresponds to using equations very similar to those used to describe the kinetics of chemical reactions, substituting chemical species with radiation-induced defects, and can only provide concentrations of defects versus time/dose, in a mean-field approximation, i.e. supposing that all species are uniformly distributed in the piece of material studied. The latter (KMC) exists in multiple versions and there is no widespread consensus on the terminology to be used. Within this project, consistently with the nomenclature used in the PERFECT IP, two KMC classes are distinguished: those in which atoms are explicitly treated (atomistic KMC, AKMC), whereby the microchemistry evolution can be described (at the price of a still limited encompassed length-scale and time-scale); and those in which atoms are not explicitly treated (object KMC, OKMC), which use similar input and provide similar output as RT models, but include space correlations that, as mentioned above, RT models cannot include (although at the price of a much higher computational cost). The higher computational speed of RT and the higher accuracy of OKMC are the reason why these types of tools are developed in parallel.

In this framework, the main objective of WP1-3 is to develop coarse-grained models (RT, object KMC (OKMC)) describing the microstructure evolution undergone by body-centred-cubic Fe (α-Fe) model alloys under irradiation. The output of these models is the input for flow behaviour models developed in WP1-2. The models developed in WP1-3 and WP1-2 are at the core of the RPV-2 and Toughness Module suite of codes, advanced versions of which will be produced within the proposed project. In addition, the improvement of other parts of the RPV-2 suite is being pursued, as well as the development of long-term atomic-level models not yet implemented in RPV-2, which may at some point become mature enough to be included in it.

Since models need to be validated, a number of experimental microstructural studies must be selected as reference cases, by extending the database available from PERFECT with either new data offered by partners or (in a few cases) further microstructural characterisation of materials already studied in the previous project. A literature review can also be considered.

The codes are delivered with all the specifications required for their inclusion in the advanced versions of RPV-2($\rightarrow$RPV-n).

2.1.4. WP1-4 integration (EDF)

The primary objective of the Integration work-package is to collect in a multi-scale modelling numerical platform the scientific and technical advances performed within SP-1 "RPV". For this purpose, the PERFORM 60 numerical platform architecture, structure and development language is developed based on continuity with the PERFECT project numerical platform. The existing set of codes and knowledge already available for the scientific community in the existing platform are continuously optimised and enriched with new physical schemes and computational tools.

The other main objective of WP1-4 is to ensure and maintain a high level quality process for the integration of the scientific and technical products developed by the research teams involved in PERFORM 60. In this aim, the documentation and validation of the computational tools integrated in the numerical platform is seen as an essential element which will allow the European scientific community to exchange information on the state of the art and on their recent advances and developments still classified as "work in progress".

2.2. Sub-project 2 "internals"

The internal components of light water reactors are fabricated from austenitic stainless steel and surround the fuel elements and ensure their positioning and cooling by supporting them and guiding the coolant flow. The internals are exposed to intense neutron irradiation (over 1 dpa per year, depending on the reactor design), mechanical and thermal stresses and the corrosive action of the high temperature water coolant. This exposure may lead to several degradation mechanisms, limiting the useful life time of the internal components. The three main degradation mechanisms under consideration are: irradiation assisted stress corrosion cracking (IASCC), irradiation creep and irradiation induced swelling.

For the light water reactors, currently in operation, no systematic data are available on the long-term behaviour of the materials used for the internal components. This is due to a number of reasons:

- the lack of planned surveillance programmes for internals (as opposed to the reactor pressure vessel);
- insufficient experimental development and optimisation (as is the case for fuel cladding materials);
- insufficient information obtained from extracted components.

The available knowledge on degradation of the internal components of LWRs originates mainly from the analysis of materials from extracted components or from tests on materials, irradiated in test reactors (mostly under somewhat different conditions than occur in LWRs). Due to the difficulty and cost of these tests on irradiated materials, the scope of research programmes has been limited so far, bringing mainly only qualitative understanding of the degradation phenomena and only partial parameterisation of the observed degradation behaviour against the large number of variables to be considered.

Irradiation affects the three degradation mechanisms under consideration for LWR austenitic stainless steel internals, namely irradiation assisted stress corrosion cracking, swelling and irradiation creep.

Stress corrosion cracking (IASCC) is induced or accelerated by irradiation of the environment and by irradiation induced modifications of the material. These modifications consist of changes in the mechanical behaviour of the material due to irradiation damage accumulation in the matrix and of the redistribution of alloying elements in the material, noticeably on the grain boundaries. However, no clear correlation has been found empirically between a single irradiation induced effect and IASCC.

Swelling is caused by precipitation of helium gas bubbles in the material. Correlations exist between the swelling rate of materials and the irradiation conditions (dose, dose rate and temperature). These correlations suggest a fast swelling rate after reaching a threshold dose. This phenomenon has been well illustrated for fast breeder reactor applications, but so far, no significant swelling has been observed in LWRs. The influence of spectrum, dose rate, temperature and material condition on the onset of swelling is so far not well understood for LWR conditions.

Creep is known to be accelerated by neutron irradiation and has been investigated mainly for the fast reactor applications, with some data being obtained in LWR relevant conditions. The fast reactor data show a strong synergy between creep and swelling. At this point however, there is no clear understanding how creep may interfere with swelling and/or IASCC under LWR conditions.

From this short discussion, a clear need emerges to understand and parameterise the irradiation-induced degradation mechanisms, relevant to internals in LWRs. Therefore, the sub-project on austenitic stainless steel internals focusses on producing models that are able to describe the occurrence of swelling, creep and IASCC under light water reactor conditions. The objective of the sub-project is to develop and qualify this set of simulation modules for application in light water relevant conditions. This approach will provide mechanistic and physical insight in the phenomena described, in order to allow a reliable parameterisation and prediction over dose and time ranges and environmental conditions relevant to the full lifetime of light water reactor internals. The development of theoretical models and computer simulation tools for internals has been started in Europe by launching the SIRENA project under the FP5 and the PERFECT project under FP6. These projects pioneered the use of multi-scale and multi-physics modelling whereby the understanding of the underlying mechanisms could be used to develop robust physical basis for the prediction of irradiation damage in internal components in a LWR environment.

The sub-project on internals develops the above approach to provide predictive tools for describing the degradation mechanisms, listed above. These tools are being assembled from a chain of modules, each describing a single physical phenomenon. The validation of the models is done to a maximum extent for every module within the final products, in order to estimate the contribution of each module to the general uncertainty on the prediction. Although some of the verification experiments need to be done on model materials or calculations, reference to industrially relevant materials and conditions are to be made to a maximum extent.

2.2.1. Conceptual approach

The presence of irradiation defects strongly modifies the behaviour of dislocations and in particular induces strain localization at the grain scale. At the macroscopic scale, this results in a strong hardening and a loss of ductility which are both dose dependent. To establish a link based on the best physics models available, a multi-scale approach starting from ab initio to macroscopic scales is applied. A top-down multi-scale approach has been adopted, focussing on the contribution of the smaller scale module developments to the end products, to describe the macroscopic behaviour. The refinement of the end products is performed by iteratively adding more detailed modules. The individual modules are parameterised in a combined theoretical and experimental effort at the task level, while each of the end products is to be validated by dedicated experiments at the level of the work package.

Following the top down approach, the sub-project is divided into four technical work packages (WP), each contributing to a higher work package in terms of scale or complexity in the multi-physics model chaining. Leading the four work packages is work package (*WP2-0*) concerned with the scientific *coordination* of the technical work package activities *and* the numerical *integration* of the codes and modules, developed in the work packages. The objective of the WP2-0 is to deliver the following end products:

- the INTERN module dedicated to the development of the microstructure of austenitic stainless steels under irradiation;
- the IASCC module dedicated to the susceptibility of austenitic stainless steel internals to IASCC initiation.

WP2-1: irradiation assisted stress corrosion cracking (SERCO) involves the highest degree of complexity in the multi-physics chain, as it integrates aspects of radiation induced microstructure modifications, environmental interactions and mechanical behaviour. Within the limits of the project resources and in accordance with the expression of interest of the potential end-users, the option has been taken to focus the efforts on predicting crack initiation. For parameterisation and validation, the initiation of IASCC in irradiated AISI type 316 stainless steel is taken as the reference case. In order to address different physical aspects and to integrate inputs from the underlying WPs, WP2-1 produces models at different scales:

- *Component-specimen scale:* a statistical model is being developed, predicting the distribution of cracks initiated as a function of time, load and material properties. This scale relies on the lower scale models for parameterisation beyond purely empirical data fitting.
- *Continuum scale* (“*representative* volume element”): at this scale, deterministic models are formulated, integrating the mechanical and chemical contributions to crack nucleation and growth, as described in the statistical model at the component scale.
- *Aggregate scale:* at this scale, physics based models are chained in order to predict the occurrence of elementary cracking events by integrating the description of the mechanical behaviour of the irradiated material with the corrosion and oxidation behaviour of the grain boundaries.

WP2-2: flow and creep under irradiation (*CEA*) considers the plastic behaviour of irradiated material and also creep behaviour under irradiation. The former is an essential input to the IASCC modelling in WP2-1. The latter output is part of the final objective of the sub-project and needs input from the microstructure evolution prediction from WP2-4. The prediction of the flow behaviour is addressed at different scales. The first step of the multi-scale approach is the simulation of the dislocation motion and of their interactions with the irradiation-induced defects. Then dislocations dynamics is used to derive, from the collective behaviour of dislocations, information concerning the hardening and the strain localization in clear bands. From the microstructure evolution (in particular Helium production and the consequences on loops and voids formation and on point defects cluster formation kinetics) obtained from WP2-4, cluster dynamic models are used to identify the irradiation creep mechanisms from which a phenomenological constitutive law can be derived. Based on the qualitative and quantitative information obtained from lower scales, a generalized constitutive law able to describe the main plasticity and damage mechanisms (strain localization, irradiation hardening, irradiation creep and swelling) can be derived at crystal scale.

WP2-3: corrosion behaviour (*VTT*) of irradiated stainless steels in LWR environment: preferential corrosion along the grain boundaries in irradiated material is considered as a primary precursor for nucleation of stress corrosion cracks. In this WP the processes underlying grain boundary attack are being assessed on a multi-scale approach, coupling electrochemistry, diffusion in the bulk, and oxide film growth modelling. On the continuum scale, the relative oxide film production rates at the surface versus the grain boundaries is coupled to electrochemistry, taking into account the local radiation-induced composition changes (radiation induced segregation, modelled in WP2-4). On the aggregate level the model describes the element fluxes through the oxide film, taking into account the diffusion properties in the oxide and metal (input from WP2-4). Coupling of plasticity and corrosion is also done at this level, in a second stage of model refinement, and then can be extended to the case of irradiated conditions and IASCC. On the atomistic level, a KMC code for simulation of the oxidation of Fe-NiCr alloys is developed, and parameterised using DFT calculations of ionic transport in the oxide film and oxide/metal interface.

WP2-4: microstructure and segregation (*CNRS/EDF*) in stainless steels under irradiation is also described in a multi-scale model framework. The goal of the WP is to produce the components of the INTERN end product for the prediction of the microstructure evolution of austenitic steels under irradiation. This includes:

- the prediction of the production of invisible primary damage, its evolution into the experimentally observable microstructural features (e.g. Frank loops), in terms of density, size and spatial distribution;
- the onset of swelling when He is present in significant concentration due to transmutation;
- the production of fundamental data and tools necessary to describe microchemical processes occurring under irradiation, such as precipitation and radiation induced segregation (RIS) at grain boundaries (GB) and surfaces, in model alloys for austenitic steels.

3. State of the art and progress to be accomplished by the end of the project

3.1. Sub-project 1 "reactor pressure vessel"

3.1.1. WP1-1 fracture behaviour

In the PERFECT project a basis to understand the fracture toughness behaviour of irradiated RPV materials was built. Micromechanical models have been further developed; however, it is desirable to have improved understanding of the physical principles behind these models, especially those relating to the calibration parameters. Therefore one of the main objectives in WP1-1 is to develop at least one consensus micromechanical model of cleavage fracture behaviour.

The results attained within PERFECT serve as an input for the specification of the new multi-scale cleavage fracture model. Sub-modelling at the level of single grains serve as input for the LA model to account for local stress and strain fields (i.e. stress and strain heterogeneity).

In addition, existing engineering fracture models will be further developed to address fracture toughness transferability issues from test specimen to RPV component such as crack-tip constraint, biaxiality, load history (WPS) and effects of crack front length.

In order to develop new reference cases (aside from the experimental data resulting from previous projects) new experimental data for constraint-modified fracture toughness specimens (small cruciform specimens) must be obtained from testing irradiated materials. This allows a better understanding of the effect of irradiation on fracture toughness transferability.

3.1.2. WP1-2 flow behaviour

During the course of FP6 PERFECT project, new crystal plasticity constitutive equations have been proposed and validated to describe the flow behaviour of un-irradiated RPV steel. This model is able to account for different phenomena such as the thermal activation of plasticity, hardening due to the dislocation–dislocation interactions and its temperature dependence. Aggregate and homogenization computations have shown the capability of this model to predict the macroscopic tensile stress versus strain curve taking into account the actual crystallographic microstructure of the RPV steel.

Applications to the irradiated material have been attempted assuming that only the "friction stress" parameter is affected by irradiation-induced defects through the increase of the critical resolved shear stress (CRSS) of a pure Fe single crystal. This approach is clearly not sufficient and the constitutive law needs to be improved to introduce directly the distribution of irradiation-defects through the internal variables of the crystal plasticity model.

The foreseen evolution of the crystal plasticity constitutive equations implies the use of different modelling techniques in order to identify which characteristics of the irradiation defects are pertinent parameters. Dislocation Dynamics, which is used for this objective, needs the inputs of ab initio computations and molecular dynamics for dislocation mobility laws, and local rules for interaction of dislocations with irradiation-induced defects. This work has been already started in the frame of the FP6 PERFECT project, but only considering pure Fe. In PERFORM 60, we also take into account the effect of Carbon on dislocation slip and its interaction with irradiation-induced defects.

3.1.3. Carbon effect on dislocation slip

The energy map of carbon–dislocation interactions in iron is calculated from ab initio calculations for a straight $\langle 1\,1\,1 \rangle$ screw dislocation. These calculations are performed using the SIESTA code and optimised simulation cells in the recently developed dipole approach. Molecular static simulations are used to compute the dislocation interaction with C atom in α-Fe and we compare these results with elasticity theory. Molecular dynamics simulations at constant strain rate are performed, using established techniques to determine critical resolved shear stress (CRSS) for edge and screw dislocations on (1 1 0) and (1 1 2) slip planes in Fe and Fe–C systems, with emphasis on the effect of the different possible locations of C with respect to the dislocation. The non-Schmid behaviour is also investigated through the introduction of a tensile stress component in the stress tensor applied to the simulation "box".

3.1.4. Dislocation interaction with irradiation-induced defects

Established molecular dynamics techniques are used to study, as a function of temperature and strain rate, the interaction of screw and edge dislocations with the classes of defects observed in irradiated RPV steels and their model alloys, with special emphasis on self-interstitial loops and the effect of the presence of C. Both static and dynamic simulations are performed. From static simulations, it is possible to calculate the interaction energy and to determine the mechanism of interaction and the work to be applied to make the dislocation move through a regular (or irregular) array of obstacles. Dynamic simulations are used to verify the mechanism of interaction at finite temperature and the effect of temperature on the CRSS. Different strain rates can be used to study the sensitivity of the CRSS and the interaction mechanism (which now may be different compared with the one obtained from static simulations) to this parameter.

3.1.5. Crystal plasticity law

DD simulations are essential for the integration of results of simulations at the atomic level in the continuum models of crystal plasticity. This technique is the only one possible with which to incorporate, without adjustable parameters, the whole physical knowledge about microstructure and deformation mechanisms into a larger scale simulation of the macroscopic mechanical properties. The work initiated several years ago provided some dispersed results on the interactions with irradiation defects. The role of thermal activation is expected to be fully and explicitly considered in the DD simulations.

The results of these simulations is used to identify a new crystal plasticity constitutive law taking into account the effect of Carbon and the irradiation-induced defects.

3.1.6. Macroscopic behaviour through crystal plasticity modelling

The objective of the crystal plasticity modelling is to predict, using the finite elements (FE) technique, the macroscopic behaviour (and the tensile stress versus strain curve) of the irradiated RPV steel. In fact, the RPV steel is modelled as an Fe–C alloy with the same crystallographic microstructure. As described above, the constitutive law is developed from the DD simulations results, although the microstructure modelling needs to be improved. Two tracks to model the microstructure are being followed: the fast track using the homogenization technique as the input needs only the underlying sets of crystallographic orientation; the refined track uses 3-D aggregates taking into account the true shape of the bainitic lath packets (or blocks). These representative aggregates and their associated FE meshes must be built according to the crystallographic information of the actual RPV steel being modelled. A method is developed for this objective. Large computations are performed on these meshes and the resulting stress and strain fields are analysed and modelled for further use as input to the LA model(s) in WP1-1.

In summary, WP1-2 contributes to SP-1 through the development of three tools:

(i) a tool to simulate the irradiation-induced microstructure of the RPV steel;
(ii) a tool to compute the macroscopic flow behaviour through aggregate computations;
(iii) a tool to compute the macroscopic flow behaviour through homogenization computations.

3.1.7. WP1-3 Microstructural evolution

In the current version of the RPV-2 suite of codes developed in PERFECT, a number of drastic approximations are made.

The damage source term in RPV-2 comes from a database providing the defect distribution at the end of displacement cascades of different energies, as simulated by molecular dynamics, after short-term annealing by means of KMC techniques. This scheme may be improved in terms of flexibility, correctness and statistical relevance, by devising a different scheme, allowing "equivalent cascades" to be produced for any recoil energy, e.g. with the aid of binary collision approximation (BCA) techniques.

In the microstructure evolution models implemented in RPV-2, many of the atomic-level mechanisms of defect mobility and reaction in α-Fe, identified in the last few years, are not taken into account. The effect of impurities, such as C and Cu, is allowed for only in a very tentative way. The effects of other elements, such as Ni and Mn, or P, are totally disregarded.

Even independently of the specific case of RPV-2, no model currently exists that is capable of correctly describing the microstructure evolution under irradiation in a multi-component alloy as a function of dose and temperature.

In PERFORM 60, a physically more correct description of the mechanisms of defect mobility and reaction in α-Fe is introduced in both rate theory and Kinetic Monte Carlo models. This is based on results obtained in PERFECT and worldwide in recent years, as well as on specific studies performed in PERFORM 60, including a systematic validation against experimental reference cases. The important problem of properly treating the effect of C on the microstructure evolution is specifically addressed. This is done by using ab initio data (available from PERFECT and complemented within PERFORM 60) and also by exploiting inter-atomic potentials, developed within PERFECT, to perform dynamic studies, aimed at providing information concerning mechanisms of defect-C interaction and corresponding characteristic energies. Similarly, inter-atomic potentials and atomistic KMC (AKMC) approaches developed in PERFECT are further developed and exploited to provide a better description of the processes leading to Cu precipitation under irradiation, to be implemented in the coarse-grained microstructure evolution models.

In addition, inter-atomic potentials for ternary alloys are fitted to ab initio data, so as to be able to study, at the atomic level, e.g. by means of molecular dynamics (MD) techniques, the combined effect of other elements to Cu or C, such as Ni and Mn, or P (Currently, no ternary inter-atomic potentials exist in the literature). Correspondingly, AKMC studies of the first stages of precipitation under irradiation in multi-component systems, using technically varied approaches (based on ab initio and inter-atomic potentials, employing methods developed in PERFECT), are performed. The ultimate aim is that, at the end of the project, at least some of the effects of the presence of multiple alloying elements, e.g. Ni and Mn, or P, can be reflected in the RT and object KMC coarse-grained models. This provides a description of the microstructure evolution closer to the one expected in a multi-component system, such as a RPV steel. The selection of the most suitable ternary model alloy to be targeted is based on the indications from the available experimental data, as well as from the advice of the end-users (via SP-3 Users' Group), based on an assessment of feasibility within the timeframe of the project.

3.1.8. WP1-4 integration

The PERFORM 60 integration numerical platform is based on the existing numerical platform. It keeps the same structure (chaining of modules and integration of codes from diverse origins) and language of development (strictly speaking Python language for the integration and Python Qt for the development of the graphical interface).

The existing modules and approaches integrated at the end of the PERFECT project are improved in the PERFORM 60 integration numerical platform:

- the CPU intensive nature of the computations is reduced;
- a library of meshes is proposed and the user also has the possibility of configuring his own specimen mesh;
- the cascade database and convolution spectrum is improved and the size of solute number in rate theory is increased.

The innovative approaches which are developed in the others WPs must be integrated. Thus, the new local approach model(s) of cleavage fracture and the newly-developed rate theory and Kinetic Monte–Carlo code will be integrated on the platform.

The creation of a "link" in the graphical user interface of the numerical platform allows the user to launch a browser directly to the URL of the PERFORM 60 database, thus providing a useful new functionality.

Particular attention is given to the validation of the integrated approaches. From a numerical point of view, verification Code to Code is realised for finite element computations. A new function which allows experimental results to be imported from the PERFORM 60 database (tensile curves for example) supports the validation of the modules via reference cases, defined by WP1-1, WP1-2 and WP1-3.

3.2. Sub-project 2 "internals"

The first steps towards multi-scale modelling of irradiation damage effects in austenitic alloys were made in the sixth framework integrated project PERFECT. In this project, a first set of tools was constructed, describing the accumulation of irradiation damage in austenitic alloys and its effect on the hardness or yield stress. A prediction tool called INTERN-1 is able to predict from a known neutron spectrum the increase of the critical resolved shear stress (CRSS) on each slip system for a given dose. The mechanical sub-module which performs this operation is a Dislocation Dynamics code which uses as input the computed distributions of irradiation defects. At the end of the PERFECT project, the tools that make up the INTERN-1 module describe only binary Fe–Ni alloys and hence yield only qualitative information on the evolution of stainless steels. Regarding the microstructure, an Object Kinetic Monte–Carlo code developed to simulate the point defect cluster evolution under irradiation in ferritic alloys has been modified to treat austenitic alloys (accounting for interstitial helium atoms, substitutional helium atoms as well as helium-vacancy clusters) also in the framework of PERFECT. At the moment, the code employs a very simple parameterisation which predicts correctly the saturation of the evolution of the Frank loops and of the vacancy clusters in pure Ni. A Mean Field Rate Theory code, originally devoted to the co-clustering of point defects and substitutional atoms has been modified in order to treat in an improved way the possible co-clustering of helium atoms and point defects. In a same manner, the fusion community has undertaken a similar effort to describe the evolution of the irradiation damage in ferritic martensitic steels, based on the simulation of Fe–Cr alloys.

The PERFECT project also resulted in prototype numerical tools for prediction of stress corrosion crack propagation and initiation. The stress corrosion crack propagation model, is based on the mechanistic slip dissolution model as applied by Ford & Andresen or Shoji to describe crack propagation in sensitised stainless steels exposed to oxygenated pure water (representative of boiling water reactors). The electrochemical interaction between the stainless steel and the primary environment in PWRs has been characterised and modelled, including effects of irradiation on the environment. The resulting model allows the prediction of the stress corrosion crack propagation rate as a function of the environmental conditions and the material properties (which are affected by irradiation). However, at the end of PERFECT, insufficient tools were available to fully describe the effect of irradiation on the parameters, required by the IASCC propagation model. These material parameters include yield stress (the evolution of which is qualitatively described by the INTERN-1 module), strain hardening coefficient (for which no quantitative information is provided by the numerical tools in PERFECT) and repassivation kinetics of the material in primary environment. The latter material property is dependent on the (local) chemical composition at the crack propagation path (i.e. the grain boundary), for which no quantitative model is available. Also, no model or experimental database was produced to link the local composition at the grain boundary to repassivation kinetics.

The IASCC crack initiation module, consists of a statistical calculation framework, chaining stochastic defect nucleation to microcrack coalescence and growth in a 2.5 D microstructure. The nucleation parameters are distributed according to a Weibull type of distribution (with two data fitting parameters) and deterministic interaction and growth rules (taken from empirical data). No "hard" coupling between the initiation and growth module was performed in PERFECT and no mechanistic or physics based defect nucleation model were formulated.

Concerning the description of the mechanical behaviour of irradiated stainless steels, the PERFECT project produced a basic approximation for the evaluation of the effect of the dislocation channelling, which is observed in irradiated stainless steels, on the stress–strain concentration on the grain boundaries and free surfaces. This approach relies on experimental observations and does at this point not contain a physics based prediction of the nucleation of dislocation channels nor their development with dose or strain.

From the experimental parameterisation point of view, the PERFECT project generated some data on crack propagation in neutron irradiated stainless steels and showed that model alloys (cold worked stainless steels and alloy 286, exhibiting "channelling" type of plastic deformation) are not fully representative for generating crack growth data. For crack initiation, tests on model alloys with compositions close to those measured on grain boundaries of irradiated materials, have produced a database, suitable for a first parameterisation of the model produced.

Moreover, a number of relevant activities have been developed over the past years:

- Atomistic modelling of development of irradiation damage in Fe–Cr alloys: this activity has been developed in the fusion community and tackles for the first time the development of irradiation damage in concentrated alloys, based on Fe–Cr. The description of the Fe–Cr interaction is of relevance to the development of the ternary Fe–Ni–Cr model alloy for austenitic stainless steel.
- Experimental programmes have provided mechanistic insight into the governing parameters of IASCC:
  - o Crack growth tests have shown the detrimental effects of silicon
  - o Slow Strain Rate Tests (SSRT) and crack growth tests have shown the limitations of using cold worked stainless steels as model for irradiated materials.
  - o The threshold stress for IASCC crack initiation has been observed to decrease with increasing dose beyond the range where radiation induced segregation and radiation induced hardening are saturating with dose. This observation may be due to the increasing tendency for flow localization and-or the increasing level of silicon segregation.

Taking into account the above state of the art, each SP-2 work package provides progress as follows.

3.2.1. WP2-0: coordination and integration

The linking of the atomistic modelling of radiation damage to its effect on the mechanical behaviour and stress corrosion cracking behaviour for austenitic materials is a significant improvement with respect to the state of the art, following from the PERFECT project.

3.2.2. WP2-1: IASCC

The multi-scale approach is innovative with respect to the previous IASCC modelling efforts. It allows both mechanisitic issues as well as user relevant ones to be addressed. Also, it allows the incorporation of different mechanisms in a single calculation chain, yielding a more flexible model with a larger validity range. At the different scales, the following progress is expected:

- *Component-specimen scale:* the statistical prediction framework, as developed in PERFECT is to be parameterised for irradiated stainless steel in primary environment, as opposed to the parameterisation with model materials. The multi-scale approach feeds physics based parameters into the framework and replaces the empirical fitting parameters: the defect nucleation rate is predicted using corrosion-oxidation models, linked to the mechanical behaviour of the material. The coalescence and growth description is refined using the output of PERFECT (crack growth laws) and the aggregate calculations of WP2-2.
- *Continuum scale:* the coupling of environmental interaction at the grain and grain boundary surface is an evolution of the PERFECT ECHEM model, based on the local material compositions after irradiation and allows for a first approximation of the nucleation time of a defect.
- On the aggregate level, coupling of the point defect model for oxide films to the grain boundary segregation model in the metal is a new development. The current state of the art comprises two unlinked models, the point defect model (which assumes a homogeneous substrate) and the radiation induced segregation models (making abstraction from surfaces). In a second stage, this coupling will be extended to the plastic behaviour.

3.2.3. WP2-2: flow and creep under irradiation

The multi-scale description of the flow and creep behaviour in irradiated stainless steels represents a major advance in the modelling of the mechanical behaviour of these materials with respect to the PERFECT project. The improvements at the different scales are:

- Improved accuracy of the dislocation mobility laws by considering more realistic inter-atomic potentials (for austenitic alloys) and enriched description of the interaction between dislocation and irradiation defects by considering more types of irradiation defects. Using this new knowledge, the DD simulations are used to evaluate more accurately the increase of the CRSS but also the plastic behaviour and the kinetic of the strain localization (clear bands formation) in individual grains.
- From these DD simulations and from the identification of the creep mechanisms under irradiation and description of the swelling effect on mechanical behaviour, a generalized crystal plasticity law for irradiated material can be derived and used to quantify the effect of clear bands on the loading of the grain boundaries.
- These stress concentration factors are provided to the models developed in the WP2-1 (IASCC). The computation on representative grain aggregates with the same crystal plasticity law provides the macroscopic mechanical behaviour which is needed to compute the stress and strain states in the modelling of IASCC. The information obtained at different scales also contribute to the development of the modelling in the other work packages, e.g. the DD simulations describing the stress and strain in front of a crack tip within a grain are input data to the oxygen diffusion modelling (WP2-3), the vacancy and void densities provided by the cluster dynamic model (WP2-2 and WP2-4) are used to quantify the corrosion–plasticity interaction described in WP2-3.

3.2.4. WP2-3: corrosion behaviour

Addressing the oxidation and dissolution behaviour of materials in primary water from a multi-scale multi-physics point of view is highly innovative.

- On the continuum level, the allowance for a heterogeneous substrate yields to a first estimate of the effect of grain boundary segregation in promoting a faster local corrosion rate, which in turn can promote intergranular cracking.
- At the aggregate and atomistic levels, parameterising the models to the primary environment, and coupling them to a heterogeneous substrate represents an evolution in the level of complexity handled by the approaches.
- Finally, the incorporation of plasticity–corrosion interaction effects makes significant progress towards modelling the synergistic relationship between two areas which have previously been handled separately, thus bringing the model closer to the real conditions expected.

3.2.5. WP2-4: microstructure and segregation

In this WP the multi-scale modelling approach from the PERFECT project is extended:

- At the scale of the description of the inter-atomic interactions, developments in the modelling of ternary and concentrated alloys is made in order to describe the Fe–Ni–Cr system, taken as a model for the austenitic stainless steels of relevance. To date, multi-component atomic systems can be reliably studied only by means of density functional theory (DFT) methods, which are limited to only few hundreds of atoms and can hardly be used for dynamic studies. In order to study diffusion processes in multi-component systems, simpler model Hamiltonians (e.g. inter-atomic potentials or pair-energy cohesive models) consistent with both DFT data and experimentally known thermodynamic properties of the system of interest must be first developed and for this a massive quantity of DFT data is needed, which is currently not available from the literature and has to be produced within the project. Inter-atomic potentials have been developed at the most for binary systems and one of the objectives of the sub-project is to produce a FeNiCr potential. Therefore, the development of ternary inter-atomic potentials represents a significant progress in the multi-scale modelling of concentrated alloys.
- The description of the diffusion behaviour at atomistic scale are integrated in an aggregate scale model for grain boundary segregation, yielding a physics based model for radiation induced segregation. This approach (which uses pair-energy cohesive models) has been developed within the PERFECT project for the RPV steels. It will now be applied to transfer the information provided by DFT and inter-atomic potentials into an atomistic kinetic Monte–Carlo code, capable of simulating diffusion processes. This code, at its different levels of approximation and refinement, can then be used to deduce the phenomenological diffusion coefficients (for the improvement of the parameterisation of continuum models) as well as to study the segregation processes. As segregation is inherently an atomic level process, only atomic-level models can eventually provide a detailed and quantitatively correct description of the diffusion mechanisms. These are strongly dependent on the local atomic environment, so the model Hamiltonians used in these models are to be trustworthy. Parameters obtained from these atomic-level models can then be implemented in continuum models to increase the level of reliability of the latter.
- For modelling of the intragranular microstructure (dislocation loops and void swelling), the development of the ternary potential mentioned above allow a more accurate description of the

formation of the hardening defects in the matrix. During the PERFECT project, a Mean Field Rate Theory code, originally devoted to the co-clustering of point defects and substitutional atoms was modified in order to treat in an improved way the possible co-clustering of helium atoms and point defects. The use of a representative potential for FeCrNi ternary alloys improves the accuracy of the microstructure modelled by this method. Alternatively, kinetic Monte–Carlo methods are being considered that allow one going beyond the continuum by explicitly taking into account the spatial correlations of the elements in a physical system with a defined microstructure.

4. PERFORM 60 Users' Group

The scientific approaches developed in the SP-1 and SP-2 subprojects to model the behaviour and degradation mechanisms of reactor pressure vessel (irradiation embrittlement) and internals (IASCC) materials are very innovative both because of the techniques used for numerical simulation and of the challenge to derive the macroscopic component behaviour from the microscopic evolutions of the material.

Although this project deals with fundamental research and modelling, it's still a challenge from an industrial point of view since only such an in-deep physical understanding of the degradation mechanisms is able to provide predictive modelling of these phenomena.

Therefore, to fully reach the goals of the project, a complementary work has to be done through a Users' Group in order to assess the developed modelling with industrial data and share the knowledge and modelling approach improvements among the European Nuclear Community. This work includes a state of the art with a critical evaluation of existing tools and approaches in a 60 years operation context, a collection of experimental reference data and a proposal of industrial applications, and a final evaluation of simulation tools through their applications to collected reference data and applications. A final workshop will be organized at the end of the project, for a final evaluation of all end products with identification of missing gaps.

Within the framework of this Users' Group, it is foreseen to broaden the dissemination of the created knowledge during the PERFORM 60 project among the European nuclear community and outside the European Community. The created knowledge includes both modelling approach improvements and new modelling tools. To improve the assessment of this developed knowledge, the industrial data collection for both reactor pressure vessel and internals aspects (RPV steels, stainless steel for internals) need to be extended and the evaluation and feedback regarding the capability of these tools should be performed by additional organisations. Several major international organizations have a close look at the PERFORM 60 Users' Group: the IGRDM Group, the IASCC Advisory Committee, the NULIFE network of excellence, EPRI, TEPCO, Vattenfall.

The wish to widely associate 'non specific research organizations' (e.g. Utilities, Manufacturers…) to Users Group activity has also been taken into account in the preparation of sub-project SP-3, since the responsibility of two work packages 'RPV applications' and 'internals applications' is undertaken by a Utility and a Manufacturer.

The activity of the Users' Group SP-3 is split into five work packages.

4.1. WP3-0 "coordination, integration, training and dissemination of knowledge" (EDF)

The WP activity includes the constitution of Users Group (involving external partners of the project with a specific contracting to set up), the management and coordination of the WP, the corresponding reporting and feedback towards other members of the project (SP-1 and SP-2), the organisation of specific Training sessions on simulation tools for Users, and the external communication (including a close link with NULIFE network of excellence). Periodic progress meetings will be organised to discuss and validate the work realised or foreseen in the other WP of the UG. High quality publications are encouraged to highlight the achievements of simulation tools and end products. Opportunity of scientific events (Conferences, workshops, seminars, summer schools…) must be used for promotion of technical work and contribution to dissemination of knowledge.

Exchange of research workers for the evaluation of the End Users Tools can be favoured within the Users' Group.

4.2. WP3-1 "reactor pressure vessel applications" (Rolls-Royce)

The main objective of the WP is an evaluation of the simulation tools for reactor pressure vessel applications and their capability to be used in the future for practical industrial applications and assessments (and how to fill the possible remaining gaps). The corresponding work first includes a review of existing methods of predicting the effects of irradiation on RPV materials with their limits in a 60 years operation context. A collection of reference experimental data and a proposal of industrial RPV applications will be prepared, to be used for application and evaluation of simulation tools and end products developed by SP-1. A final synthesis with evaluation of tools for prediction of irradiation degradation on RPV steels will be prepared, including a comparison with existing methods and models. Conclusions and recommendations issued from the WP will be discussed with SP-1 contributors in order to identify how to fill the possible remaining gaps.

4.3. WP3-2 "internals applications" (TRACTEBEL)

With the same goal of scientific and industrial assessment of the project results proposed in the previous WP for reactor pressure vessel, the WP evaluates the simulations tools devoted for internals applications (irradiation creep, swelling and IASCC). The process is the same as in the previous work package.

The corresponding work first includes a review of existing methods of predicting the effects of irradiation on internals materials (for IASCC topic) with their limits in a 60 years operation context. A collection of reference experimental data and a proposal of industrial internals applications will be prepared, to be used for application and evaluation of simulation tools and end products developed by SP-2. A final synthesis with evaluation of tools for prediction of IASCC internals steels will be prepared, including a comparison with existing methods and models. Conclusions and recommendations issued from the WP will be discussed with SP-2 contributors in order to identify how to fill the possible remaining gaps.

4.4. WP3-3 "PERFORM 60 database" (FZD)

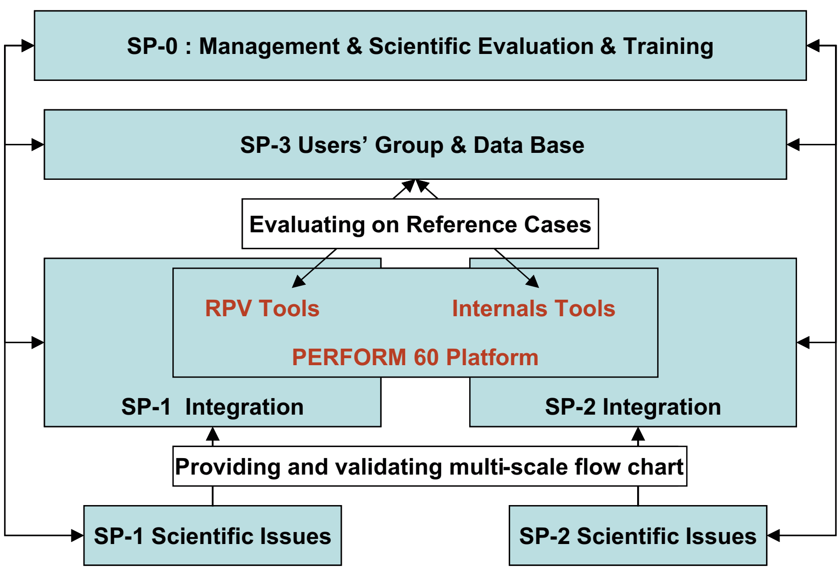
The evaluation of simulation tools requires a collection of reference data (materials properties, conditions of irradiation, metallurgical evolutions…) and industrial applications, to be compared to predictions of simulation tools, both for RPV and internals materials. All these elements are gathered in a specific database (PERFORM 60 Database) developed in a specific WP, using feedback from previous FP6-integrated project PERFECT. This work includes the constitution of the Database, the definition of input and output data, the Quality Assurance of the Database, and its maintenance.

4.5. WP3-4 "*final evaluation of end products*" (NRI)

A final evaluation of simulation tools and end products and their ability to be used in real industrial components assessment will be prepared by industrial Users in a specific report based on SP-1, SP-2 and SP-3 work and progress during the project. Complementary to improvement of tools and approaches, and their validation, possible limitations for practical applications will be emphasized.

A final workshop will be organized at the end of the project to promote and discuss such scientific and industrial approaches with the international community.

5. Overview of the project organisation



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6. PERFORM 60 impacts

Impacts of PERFORM 60 are evidenced on several fields:

The *leading position of the EU's nuclear industry* in the field of numerical simulation for residual lifetime prediction is effective to date, since the FP6 PERFECT produces tools (RPV-2 and Toughness Module) able to predict radiation effects both on RPV steel's (bcc crystalline structure) mechanical behaviour and failure. The objective of the PERFORM 60 project is now to extend the roadmap initiated within PERFECT to austenitic stainless steels (fcc crystalline structure) which were not assessed completely in PERFECT and to improve the RPV tools in order to overcome some scientific issues that have been identified within PERFECT (for instance effectively bridging DDD and local mechanical fields, or accounting for more solute effects in the irradiation damage simulation).

The PERFORM 60 project shall also allow the community settled in FP6 taking a dominant position in the frame of fracture mechanics and stress corrosion cracking simulation (damage mechanics' field indeed), in addition to the actual leading one on irradiation damage simulation.

As a first step, the results obtained in PERFORM 60 will be directly applicable to existing reactors up to possible 60 years of operation, since the numerical tools shall be validated on existing in-reactor data (task of the Users' Group). But of course, these results will be also useful for residual lifetime prediction of the European Pressurized Reactor (the materials involved in this reactor are nearly the same as the ones we can find in existing ones). Moreover, the studies conducted within the PERFORM 60 project shall be of great interest for GenIV reactors. Indeed, even if the materials involved in GenIV are different, the numerical tools developed in the frame of PERFECT and PERFORM 60 shall be able to take into account two types of crystalline structure, i.e. bcc and fcc. No doubt that these kinds of crystalline structure will be present in GenIV reactors.

Acceptability: the building of the proposed tools will demonstrate the will of the European industry to reduce as much as possible production of irradiated materials. Enhancing nuclear energy means also combating global warming. Hence, the project shall enhance the public acceptability of nuclear energy. Moreover, the prediction capability clearly contributes to public acceptability of the safe exploitation of nuclear power.

Capitalization of knowledge: during several years (sixties to eighties), huge experimental and theoretical efforts were carried out to characterize, understand and model irradiation effects in materials. Thanks to the FP6 PERFECT, many of these efforts have been capitalized within numerical tools. But there is still work to do. The PERFORM 60 project will pursue this task, so that the future European Research in these fields can benefit from the amount of work performed 20–50 years ago.

Structuring of the European Research: PERFORM 60 brings together around 20 research centers institutes and academic laboratories working in the field of numerical simulation of materials behaviour. Such a large European team is required to mobilize the necessary competences and skills; no single country could provide all of them. A team involving most of the European Community working in this field has been created within PERFECT, PERFORM 60 still reinforces the strong links between the partners.

Training: Learning about irradiation damage requires a strong involvement of students. Indeed, it is almost impossible for them to carry out experiments aimed at assessing systematically the cross-influence of parameters (temperature, spectrum, ...). They must therefore rely mainly on a theoretical approach in order to fill in gaps of knowledge.

The simulation tools developed in PERFORM 60 do contribute to solve this issue. As it was made possible with RPV-2 and Toughness Module, they allow students to perform virtual irradiations easily and analyse the resulting evolution of mechanical properties and microstructure. Thus these tools shall be an important vector of knowledge that will be disseminated within universities and engineering schools.

The Summer Schools organized within PERFORM 60 also contribute to a better training of doctorate students and engineers from companies involved in the EU's nuclear industry.

Bridging "Eastern" and "Western" countries: The PERFORM 60 project is an important vector of dissemination of recently developed codes and knowledge concerning numerical simulation of materials. This dissemination will be particularly fruitful within Eastern countries. One has also to point out that Institutes from recently integrated Eastern countries are part of PERFORM 60.

Strengthening the links between European and extra-European Research: The fact that EPRI and TEPCO have already accepted to take an active part in PERFORM 60 Users' Group ensures that links between European and extra-European Research in this field will be strengthened.

7. Project partners

Belgium: Studiecentrum voor Kernenergie.Centre d'Etudes de l'Energie Nucléaire (SCK.CEN), Tractebel, Université Libre de Bruxelles.

Bulgaria: BG H2 Society.

Czech Republic: Ustav Jaderneho Vyzkumu Rez.a.s. (NRI).

Finland: Valtion Teknillinen Tutkimuskeskus (VTT).

France: EDF, Commissariat à l'Energie Atomique, Centre National de la Recherche Scientifique, AREVA NP SAS, ARMINES.

Germany: AREAVA NP GmbH, Forschungszentrum Dresden-Rossendorf e.V (FZD).

Spain: Centro de Investigaciones Energeticas, Medioambientales y Tecnologicas, Universitat Politecnica de Catalunya.

United Kingdom: Serco Ltd., Rolls-Royce, The University of Manchester, Loughborough University, The University of Edinburgh.

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