

# Code Assessment Program for MELCOR1.8.6

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## ABSTRACT

The MELCOR code developed at Sandia National Laboratories for the USNRC is established in Switzerland as the preferred code for analysis of severe accident transients in light water reactors, from initiating event through to potential release of fission products to the environment. One area of international concern is that of air ingress, either into the reactor core during the late stages of an accident initiated at power, into the vessel during shutdown operation with the upper head removed, or to spent fuel in a storage pool or transport cask. This can lead to accelerated core degradation and enhanced release of fission products, especially the highly radiotoxic ruthenium. Assessment of the code models for oxidation of Zircaloy cladding has shown that the present treatments do not fully represent all the relevant physical processes, and cannot be guaranteed to be conservative under all circumstances. By the end of the second year of the project, progress with relevant separate-effects and integral experiments has been assessed, alongside review of new, detailed calculations on the boundary conditions governing air ingress into the reactor vessel. Following a survey of progress with air ingress models in other codes, the key physical mechanisms that need to be considered in a new MELCOR model have been identified, and an outline for such a model formulated in such a way that would allow, in a further project, treatment of advanced cladding materials (M5, Duplex, Zirlo, E110) as well as of Zircaloy-4, which is the target material for the current work. The next stage will be detailed coding of the model and testing against integral data.

Das MELCOR-Programm, entwickelt von den Sandia National Laboratories für die USNRC, ist in der Schweiz als das bevorzugte Programm für die Analyse von schweren Unfällen vom einleitenden Ereignis bis zur

Freisetzung von Spaltprodukten in die Umgebung anerkannt. Ein Gebiet von internationalem Interesse ist das Gebiet des Lufteinbruchs entweder in den Reaktorkern während der Spätphase eines schweren Unfalles im Normalbetrieb, in den Reaktordruckbehälter während der Wartungsphase bei geöffnetem Druckbehälterdeckel, oder bei den abgebrannten Brennelementen im Speicherbecken oder im Transportbehälter. Dieser Lufteinbruch kann zu einer beschleunigten Kernzerstörung und einer erhöhten Freisetzung von Spaltprodukten führen, speziell von stark radiotoxischem Ruthenium. Verifizierungen von Programm-Modellen zur Oxidation von Zirkaloy haben gezeigt, dass der momentane Stand der Programme nicht alle relevanten physikalischen Prozesse zur Zufriedenheit beschreibt und deshalb die Konservativität der Ergebnisse nicht unter allen Umständen garantiert werden kann. Zum Ende des zweiten Projektjahres können Fortschritte bei der Beschreibung von wichtigen Einzeleffekt-Tests und auch bei integralen Tests beschrieben werden mit einem Überblick von neuen detaillierten Rechnungen unter den Bedingungen eines Lufteinbruchs in den Reaktordruckbehälter. Unter der Berücksichtigung von Fortschrittsberichten der Lufteinbruch-Modelle von anderen Computer-Programmen konnten die wichtigsten physikalischen Mechanismen identifiziert werden, welche in dem neuen MELCOR-Modell berücksichtigt werden müssen. Ein Modell wurde formuliert, welches nicht nur das Verhalten von Zirkaloy-4 beschreibt, dem zu betrachteten Material für dieses Projekt, sondern welches in einem zukünftigen Projekt auch erlaubt, das Verhalten von fortschrittlichem Hüllrohrmaterial (M5, Duplex, Zirlo, E110) zu implementieren. Der nächste Abschnitt des Projektes beinhaltet die detaillierte Programmierung des Modells und das Testen des Programms mit integralen experimentellen Daten.

## Project Goals

The safety impacts of air ingress on nuclear fuel elements at high temperature have been studied for many years, in situations such as those in-vessel following hot-leg failure in a PWR severe accident with subsequent failure of the reactor pressure vessel (RPV) lower head [1], in-vessel in shutdown conditions with the lower head removed [1] and with loss of residual heat removal, and in spent fuel ponds after accidental loss of coolant water [2], [3]. The presence of air can lead to accelerated oxidation of the Zircaloy cladding compared with that in steam, owing to the faster kinetics, while the 85% higher heat of reaction drives this process further. Air ingress is typically associated with poor heat transfer; the combined effect of these factors can give rise to an increased rate of core degradation. Furthermore, the exposure of uranium dioxide to air at elevated temperatures can lead to increased release of some fission products, notably the highly-radiotoxic ruthenium [4], [5]. The situation is kept under continual review, with experimental and modelling studies still ongoing, notably within the European Union 6<sup>th</sup> Framework SARNET project [6], [7], and the International Source Term Programme (ISTP) [8], [9], in both of which PSI participates.

The MELCOR code [10] is the major tool in use in Switzerland for analysis of severe accidents in light water reactors, from initiating events through to potential release of radionuclide fission products to the environment. This is supported by SCDAP-based codes (SCDAP/RELAP5/MOD3.2 [11] and SCDAPSIM/MOD3.4 [12]), for more detailed analysis of thermal hydraulics in the vessel and primary circuit, and treatment of core degradation phenomena. The modelling of air ingress in MELCOR is not sufficient to capture all aspects of the associated phenomena; in particular the accelerated oxidation of the Zircaloy cladding that can occur under air conditions. Therefore, the current three-year project aims finally to develop and validate an improved Zircaloy/air oxidation model for the code. In the first year, relevant data were collected and reviewed, while in the second year the review was updated, the status of modelling in other codes was assessed, and an outline of the proposed model has been formulated. In the third year, detailed model development, consistent with the engineering-level approach adopted in the code, is planned based on separate-effects data, with assessment using the results of independent integral data.

The end result will lead to improved predictability of core degradation and fission product release under air ingress conditions, for Zircaloy-clad fuel in light water reactors.

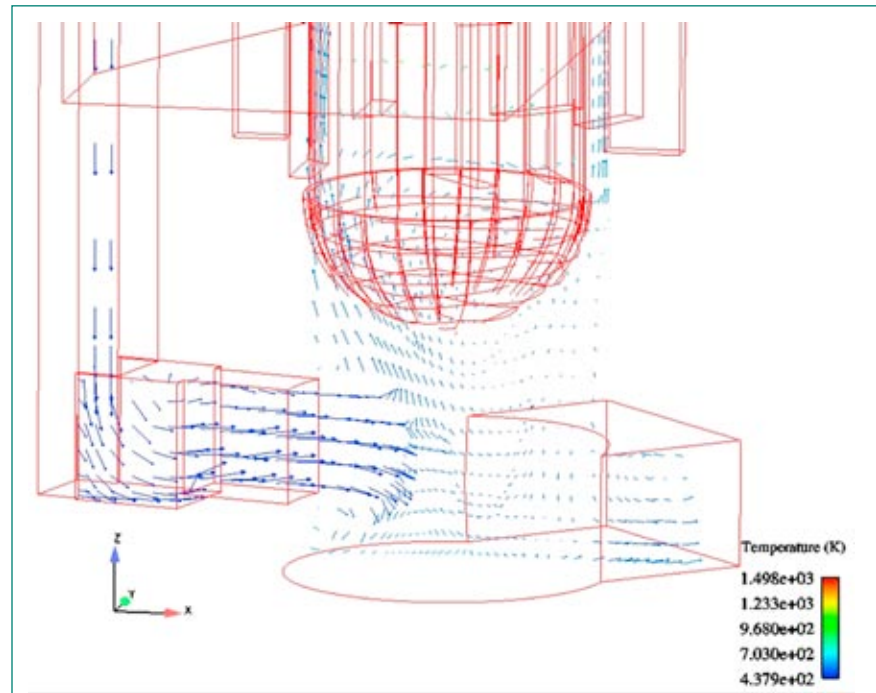
## Work Carried Out and Results Obtained

The state of knowledge concerning boundary conditions, experimental results, air oxidation models in other codes, and current understanding, is now summarised. The status of knowledge within SARNET [6] experimental work was summarised in a review paper [13] to the ERMSAR2007 meeting, to which PSI contributed, while information on the boundary conditions was given in a further paper [14] that included a summary of new reactor calculations for air ingress conditions. The analytic work showed that traditional models for Zircaloy/air reaction kinetics, based on parabolic reaction rates, do not fully represent all relevant physical processes, and cannot be guaranteed to be conservative under all circumstances. One reason is that the observed transition from parabolic (protective) to linear (breakaway) kinetics, which leads to an acceleration of the reaction rate, is not treated. These sections below draw on the material presented at the ERMSAR2007 meeting. Finally, the basis for the proposed new MELCOR models is described.

### Boundary Conditions

This section summarises current knowledge on air ingress rates that might occur into the reactor vessel, following rupture of the hot leg, then later failure of the lower head, allowing air to be drawn in from the reactor cavity. The initial studies at Sandia [1] concluded that the air flow would likely be in the range 10 to 200 mol/s, while later studies [15] favoured 2 to 20 mol/s. Since then, IRSN have published work [16] with ICARE/CA-THAREV2 [17], looking to predict the regions of oxygen starvation in the core where nitriding might take place, using 2-dimensional modelling of the flows in the vessel. A comprehensive evaluation of the likely flows using state-of-the art methods has been conducted [14] within the SARNET project, using the lumped-parameter system code ASTEC [18], the computational fluid dynamics (CFD) code SATURNE [19] (both for a 900 MWe French PWR containment), and again with ICARE/CA-THAREV2 (using a representation of TMI-2).

Fig. 1: Velocity field in the reactor pit calculated by SATURNE, French 900MWe PWR (Auvinen et al., ERMSAR2007, calculations by EdF).



The ASTEC calculations by IRSN [14] were based on a large break LOCA in the hot leg, with no safety injection available. After hot leg breach and lower head failure, gases from molten core concrete interactions (MCCI) exit the reactor cavity, and all the oxygen in the cavity is blown away, with no air ingress into the vessel. This period was calculated to last about after 11 min; after this air flow into the vessel is established, in the base case at about 7 mol/s, and typically 10 mol/s in a range of sensitivity cases. It was found that the flow rate was more sensitive to temperatures in the cavity and adjacent zones than of the remaining fuel in the vessel.

The CFD work by EdF [14] to confirm air ingress was based on a detailed mesh of 41000 cells for the French reactor building, with special detail in the vessel supporting ring in the annular space. The boundary conditions were taken from simulations with MAAP4\_EdF, and confirmed by TOLBIAC [20] for core-concrete interactions. The calculations clearly showed a convection loop, see Figure 1, with humid air flowing down the ventilation duct, heated by the corium pool in the reactor pit, and then up through the annular gap or inside the vessel. Decay heat inside the reactor pressure vessel heats the gas passing through the vessel. Sensitivity studies addressed meshing detail, position of vessel breach, MCCI gas flow, and hot leg breach size (29" down to 7"). The biggest influence was the hot leg breach size; the air flow in-vessel was 24 mol/s for the 29" large breach down to 1 mol/s for the 7" medium breach. The MCCI gas flow had only a weak influence.

The ICARE/CATHAREV2 work performed by an INR Pitești attached at IRSN Cadarache [14] addressed conditions in the RPV after lower head failure; boundary conditions were provided by previous containment calculations by IRSN for a 12" break and by EdF for a 29" guillotine rupture of the hot leg. The calculation followed the circulation of oxygen inside the core and the degradation status of the fuel rods. Depending on the blockages and oxygen availability in each scenario, the possibility exists for degraded fuel and mixtures composed largely of  $UO_2$  to come into contact with oxygen and therefore be prone to oxidation itself, with enhance release of ruthenium.

The main conclusions from the above studies are:

- 1) under conditions of hot leg breach and lower head failure, air will flow through the core from the cavity, at a rate of a few moles/s;
- 2) gases resulting from MCCI may delay the air ingress initially by a few minutes, but will not prevent it occurring;
- 3) it is possible for oxygen to come into contact with bare fuel pellets and  $UO_2$ -bearing mixtures, favouring oxidation/volatilisation of the fuel and hence enhanced ruthenium release.

The results of these calculations were used to define and confirm boundary conditions for the Zircaloy/ air cladding oxidation experiments, and ruthenium release and transport studies performed elsewhere under the source term topic in SARNET.

## Separate-effects tests

### Forschungszentrum Karlsruhe tests, Germany

The comprehensive experimental work on Zircaloy-4 reactions in different atmospheres summarised last year has now been formally reported [21]. Three basic series of experiments were performed: oxidation of Zircaloy on mixed air-steam and nitrogen-steam atmospheres, using the resistance furnace BOX (2 cm long specimens) [22] with temperatures in the range, offgas is measured by mass spectrometry, with mass gain determination and final specimen composition performed post-test; oxidation in air and nitrogen of Zircaloy pre-oxidised in steam or oxygen; in the inductive QUENCH-SR facility (15 cm long fuel rod simulator specimens and 1 cm long cladding tube segments) [23], using a thermal balance to measure mass gain continuously; and specialised thermogravimetric tests on nitrogen attack, aimed at elucidating the mechanism.

The main results, covering the temperature range 800–1600 °C, are summarised in the ERM-SAR2007 review paper [13]. The weight gains of Zircaloy-4 and alpha-Zr(O) measured as a function of time in different atmospheres at 1200 °C are illustrated in Figure 2 [23], showing the complex time dependencies of the reactions, for example pre-oxidation seems to lead to higher oxidation in air in short times, but affords protection at longer times through suppressing the breakaway effect. Also, it is observed that nitriding takes place more readily on samples containing oxygen (either dissolved or in an oxide layer) than with as-received metal itself. Microstructures corresponding to some of these reactions are shown in Figure 3 [13]; their very different nature is clearly seen.

A new test programme has started, measuring oxidation of different Zr-bearing alloys, including those of advanced type marketed for new reload fuel, in different atmospheres [24], initially in oxygen, for Zircaloy-4, Duplex-D4, M5 and E110 (Zr1%Nb). Although the alloys have only slightly different composition, there are quite strong differences up to 1000 °C, less at higher temperatures. The kinetics are mainly determined by the oxide scale (breakaway, crystallographic phase and degree of sub-stoichiometry). New experiments are planned also with Zirlo, and under different atmospheres including air. It is also noted that the next 3 bundle reflood tests will use M5, Zirlo and Duplex respectively, in addition to one test (QUENCH-12) already performed with E110; apart from this the tests up to now have used Zircaloy-4. Although the tests to date were performed in an oxygen atmosphere, they are part of the overall programme

on oxidation of different cladding materials, and the results are relevant to understanding the breakaway behaviour.

### IRSN MOZART tests, France

Separate-effects tests have continued in the MOZART facility [13], under the auspices of ISTP. The results to the middle of the year were summarised at ERMSAR2007; thermogravimetric tests were performed for air oxidation of as-received and pre-oxidised specimens in the temperature range 800–1600 °C. The pre-oxidation was carried out in steam at 500 °C, to simulate in-reactor corrosion. The pre-transition regime, the transition to accelerated kinetics, and the post-transition regime were investigated, including the effect of a pre-existing scale; the effect of the latter is illustrated in Figure 4 [25]. In contrast to the delayed transition that would occur at elevated temperatures during a reactor transient, pre-oxidation simulating waterside corrosion tends to accelerate the transitions. As with the FZK experiments, there has been a move to characterize the behaviour of advanced cladding materials, the first results to become available are those for M5 [26]. An example is given in Figure 5 [25] showing the dependence of the thickness to breakaway on temperatures; in the initial bare state, M5 is more resistant to breakaway than Zircaloy-4, while there is no more breakaway from 1100 °C for Zircaloy-4. As a further example, Figure 6 [25] shows the effect of alloy type on pre-transition parabolic kinetics.

Currently the work is being extended to Zirlo. Further possibilities are extending the work further to include thick-walled samples, pre-hydrated samples, more com-

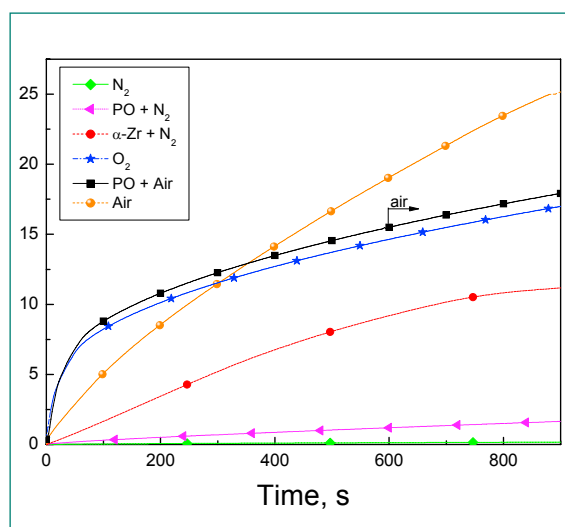
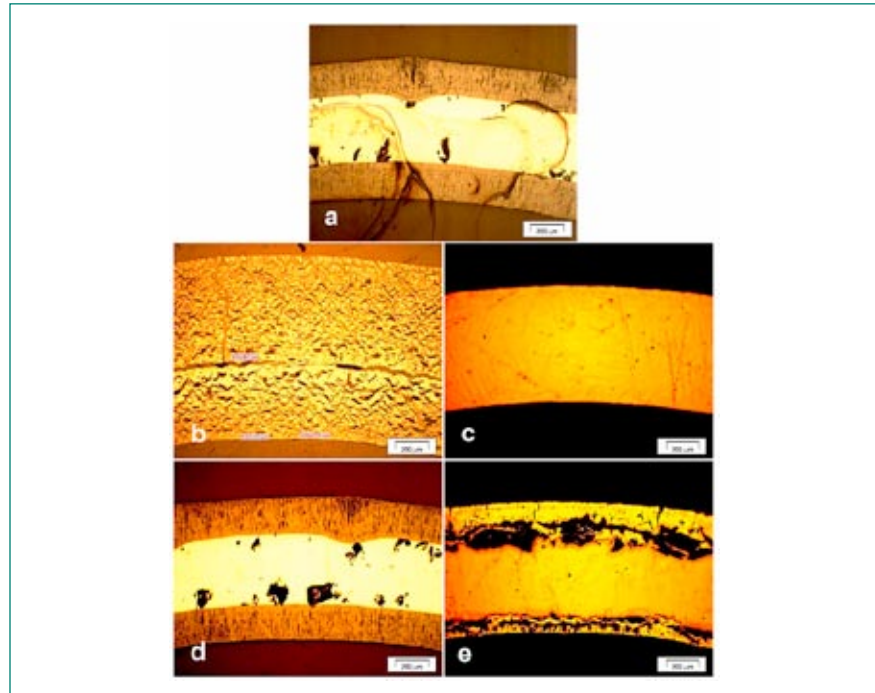


Fig. 2: Oxidation of Zircaloy-4 in different atmospheres at 1200 °C. (Steinbrück, 13<sup>th</sup> QUENCH Workshop 2007, FZK data).

Fig. 3: Post-test images of Zircaloy-4 cladding walls after reaction at 1100 °C in different atmospheres  
a) oxygen;  
b) air;  
c) nitrogen;  
d) air following pre-oxidation in oxygen;  
e) nitrogen following pre-oxidation in oxygen  
(Duriez et al., ERMSAR2007, FZK data).



plex atmospheres (air plus steam, oxygen plus nitrogen), and oxidation of zirconium nitride; these will be discussed within the ISTP framework.

#### INR Pitesti tests, Romania

The experiments at INR Pitesti, Romania on 21 mm long Zircaloy-4 cladding samples of CANDU geometry, under the auspices of SARNET, have now been reported openly [27]. The experimental apparatus and technique, thermobalance, is very similar to that used in the MOZART programme. The test series concentrated on bare Zircaloy-4 oxidation in argon plus steam atmospheres,

and oxidation of steam pre-oxidised samples in air, mixed air plus steam, and argon plus steam atmospheres. For the bare samples, the isothermal oxidation tests were performed at 100 K intervals in the temperature range is 600–1400 °C, in an 18.6 vol%/81.4 vol% steam/argon mixture. The pre-oxidised samples were oxidised in a mixture of the same composition for 24 h at 600 °C, then isothermal tests were made under 3 sets of conditions; 18.6 vol% steam plus argon, 37.2 vol% steam plus air, and 50 vol% air plus argon. Evaluation of the results presented in the ERMSAR2007 review paper [13] concluded that mass transfer limitations might have in-

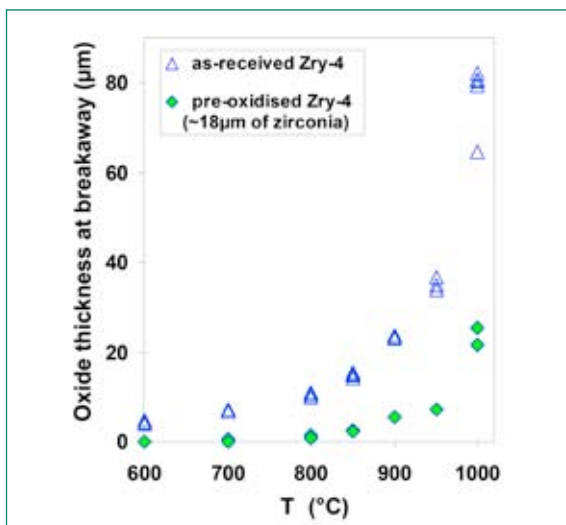


Fig. 4: Effect of pre-oxidation in steam on oxidation in air (Duriez et al., 15<sup>th</sup> Int. Symp. on Zirconium in the Nucl. Industry, IRSN data).

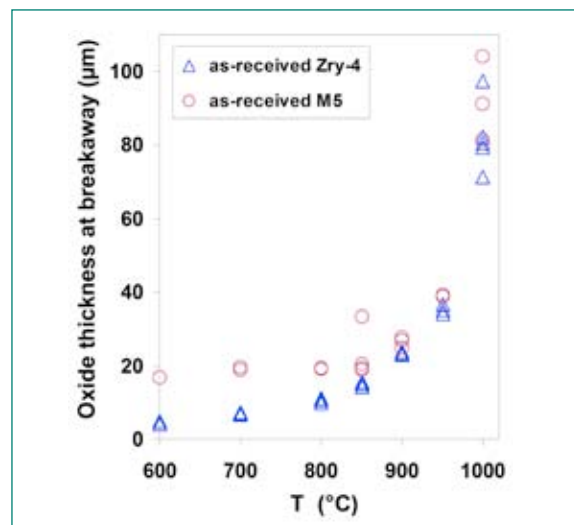


Fig. 5: Effect of material composition on breakaway oxidation in air (Duriez et al., 15<sup>th</sup> Int. Symp. on Zirconium in the Nucl. Industry, IRSN data).



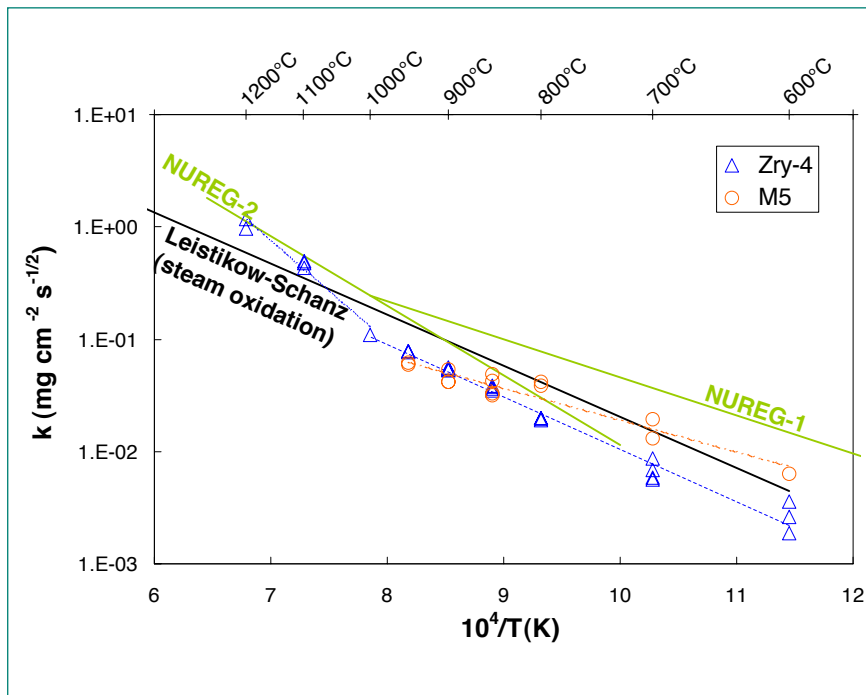


Fig. 6: Comparison of pre-transition parabolic rate constants for Zircaloy-4 and M5 in air (Duriez et al., 15<sup>th</sup> Int. Symp. on Zirconium in the Nucl. Industry, IRSN data).

fluenced the results and more experiments would be needed with higher oxidising gas flow rates to interpret the results properly.

## Integral Tests

No further integral air ingress tests were performed in the last year. The three performed to date, namely the 9-rod electrically-heated AIT1 [28] and AIT2 [29] tests in the CODEX facility at AEKI, Budapest, Hungary, and one, the 21-rod electrically-heated QUENCH-10 [30], [31], Figure 7, in the QUENCH facility in the Forschungszentrum Karlsruhe, Germany, were summarised in last year's report.

The PARAMETER facility [32] operated at Luch, Podolsk, Russia under the auspices of the International Science and Technology Centre (ISTC) incorporates a 19-rod electrically-heated bundle of VVER-1000 dimensions, materials (cladding E110, Zr1%Nb) and geometry. The overall capability is similar to that of QUENCH, but with top as well as bottom flooding, and the rods have a heated length of 1.275 m compared with 1 m in QUENCH. Two tests have been carried out with two more planned; the fourth, SF4, scheduled probably for 2009, is planned as an air ingress experiment similar to QUENCH-10, with pre-oxidation in steam at 1200–1300 °C to an extent to be decided, followed by cooling to 900 °C, then an air ingress phase with maximum temperatures envisaged of 1800 °C, likely top reflooding. The detailed test conditions will be determi-

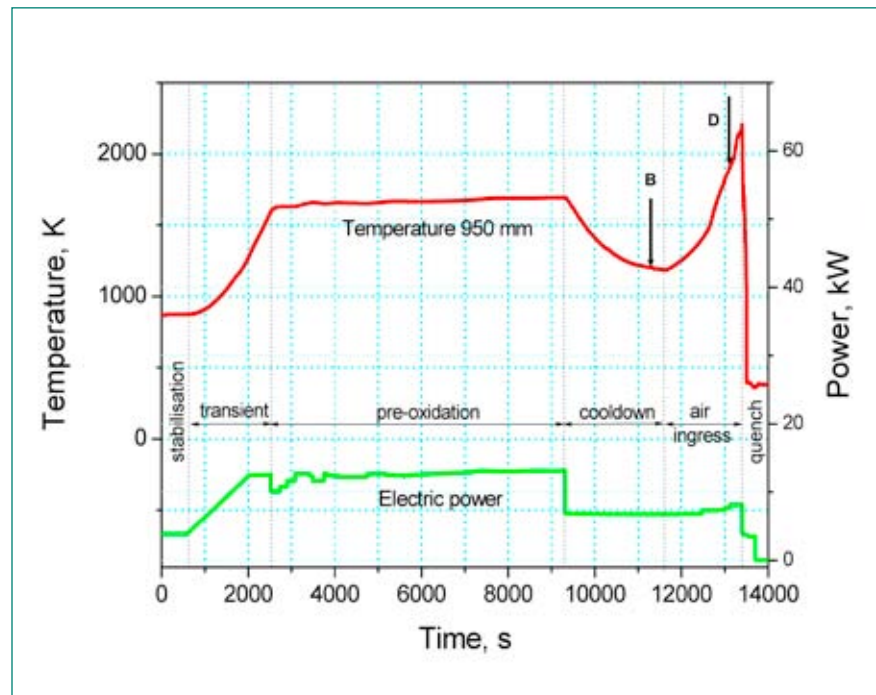
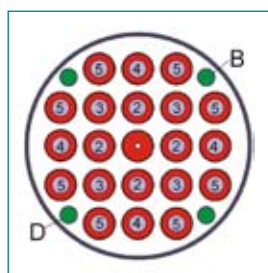
ned following a cooperative series of pre-test calculations, in which PSI may be involved. This experiment will enable models for air oxidation for the E110 cladding to be assessed under integral conditions

## Review of Existing Models

Models for air oxidation are present in many of the major severe accident analysis codes, as well as in MELCOR. A brief review is here given of their status, mainly through open publications on analysis of QUENCH-10. A summary of this experiment, and of PSI analysis using MELCOR and SCDAP-based codes, was given in last year's progress report, with further details in references [33] and [34]. These codes all use parabolic oxidation kinetics for steam and air (local PSI modifications for air oxidation in the case of the SCDAP codes), and no treatment of nitriding was included, except in ICARE/CATHARE.

The detailed ATHLET-CD code from GRS [35] has been modified to include air oxidation effects and assessed against QUENCH-10 [36]. The air oxidation model assumes parabolic kinetics and considers only the oxidation, not the nitriding. An empirical reduction factor on oxidation rate is included to simulate oxygen starvation. The model gives good agreement for temperatures at 850/950 mm elevation and above, but overcalculates between 550 and 750 mm, and while the calculated hydrogen production is nearly identical to the test data, there is less oxygen consumption in the calculation than

Fig. 7: Conduct of the QUENCH-10 experiment (Sepold, ANS2006).



observed. The new model is stated to adequately predict the cladding oxidation under air ingress, however later work simulating CODEX-AIT1 concluded that the effect of nitride formation has an important influence that should not be neglected, and that theoretical knowledge was to date inadequate.

Further work with ATHLET-CD has been reported by Ruhr-University Bochum [37]. The calculations reproduced well the conditions in the steam pre-oxidation phase, a necessary pre-requisite for accurate calculation of the air phase. Compared with the previous calculation, there was better overall calculation of the total oxygen consumption, but its time dependence was not so well reproduced. There was overcalculation of the heatup in the later stages of the air phase, illustrated by data at 750 mm. It was concluded that an improvement of the air ingress model was needed.

Developments in the detailed ICARE/CATHAREv2 code by IRSN regarding air oxidation were tested by application to QUENCH-10 [38]. The new modelling includes several correlations for oxidation kinetics (parabolic or linear) plus standard parabolic kinetics for oxide layer growth. Formation of ZrN in the Zr alpha-layer in the case of oxygen starvation is considered, with nitrogen starvation as well as the usual allowance for oxygen or steam starvation, but oxidation of the nitride is not considered. Good results were obtained for temperature evolution in the pre-oxidation phase, while it was not possible to obtain good agreement at all axial elevations in the air phase. Furthermore, the experimental oxygen mass evolution

during the air phase exhibited trends which were not captured by the parabolic air oxidation model regardless of the correlation used, as with the PSI analysis. It was concluded that the air oxidation model needed improvement, for example by taking into account breakaway kinetics. Such development is under way.

Air oxidation kinetics have been introduced into the code MAAP4\_EDF (EPRI/EdF) and tested against QUENCH-10 data [39]. After calculating the pre-oxidation phase to give appropriate initial conditions for the air phase, the air phase was simulated. The oxidation with air was calculated to take place at a lower level in the bundle than observed. A sensitivity study with an artificial air oxidation law with a 2-regime behaviour (parabolic law followed by a linear one), showed a better trend in the simulation of the test. It was again concluded that the breakaway phenomenon needed to be modelled.

Finally, the very detailed SVECHA/QUENCH code [40] from IBRAE, Moscow, has been applied to QUENCH-10 [41]. Unlike the other codes, it considers a single rod (the centre one), with the temperatures of the surrounding heated rods supplied as a boundary condition. Again, the nitriding reaction is not considered, only the oxygen interaction with Zr with its increased oxidation heat. The temperature history of the centre rod can be adequately reproduced, however this is a less challenging test of the modelling than the other simulations since the imposed experimental temperature boundary condition essentially determines the temperature history of the central rod. The analysis at the time mainly focussed on hydro-

gen evolution, and while the oxide thicknesses were quite well reproduced, the hydrogen production was underestimated; a «mass balance» contradiction noted in the conclusions. Air oxidation model developments continue within SVE-CHA/QUENCH.

The above analyses that consider the whole bundle are consistent in concluding that further model development is required that takes into account the reaction with nitrogen which degrades the integrity of the oxide film, leading to breakaway. A critical quantity to calculate is the time-dependent oxygen flux in the off-gas stream. It is not yet clear whether the take-up of nitrogen itself needs to be modelled, though its effect on oxidation certainly does.

## Summary of Current Understanding

The current knowledge relevant to the current model development is summarised as follows.

In the pre-transition regime, the current processes are most significant:

- Adsorption-dissociation of oxygen;
- O<sub>2</sub>- solid state diffusion through the protective dense zirconia scale (the rate-limiting step – displays parabolic kinetics characteristic of oxidation in steam);
- Oxygen dissolution in the metal;
- Formation of oxide at the metal-oxide boundary.

Regarding the *breakaway kinetic transition*, formation of radial and circumferential crack allows access of air to the oxide-metal interface, factors affecting breakaway include:

- Monoclinic to tetragonal phase transition of ZrO<sub>2</sub> at ca. 1100 °C;
- Differing densities: Zry (ca. 6500 kg/m<sup>3</sup>), ZrO<sub>2</sub> (ca. 5800 kg/m<sup>3</sup>), ZrN (ca. 7100 kg/m<sup>3</sup>);
- Dependence on temperature, temperature history, alloy composition etc.

Concerning *post-breakaway oxidation*, the following factors are important:

- Air diffusion through cracks to the metal interface;
- Firstly, consumption of oxygen (local oxygen starvation), then formation of ZrN by reaction between remaining nitrogen and α-Zr(O) or ZrO<sub>2-x</sub>;
- Re-oxidation of ZrN by «fresh» air and release of nitrogen;
- Stress build-up and relief due to different densities of Zr, ZrO<sub>2</sub>, and ZrN cause formation of macro- and micro-cracks.

This gives rise to a self-sustained mechanism that leads to fast, even accelerating formation of porous oxide scale.

These are considered in the outline model summarised in the next section.

## Outline of Proposed Model for MELCOR1.8.6

The findings from the numerous experimental programmes cited above, together with the above observations clearly show two dominant characteristics:

- i) steam oxidation takes place only in the absence of oxygen;
- ii) breakaway of the oxide film has a dominant role during air oxidation.

The kinetics are then no longer limited by the protective effect of a progressively thickening oxide layer; instead the protective effect is itself limited by the flaking or cracking of the oxide scale, once it reaches a certain thickness. The model treats this phenomenon by introducing a maximum effective thickness, δ\*. Then the oxidation rate, in terms of oxide thickness is:

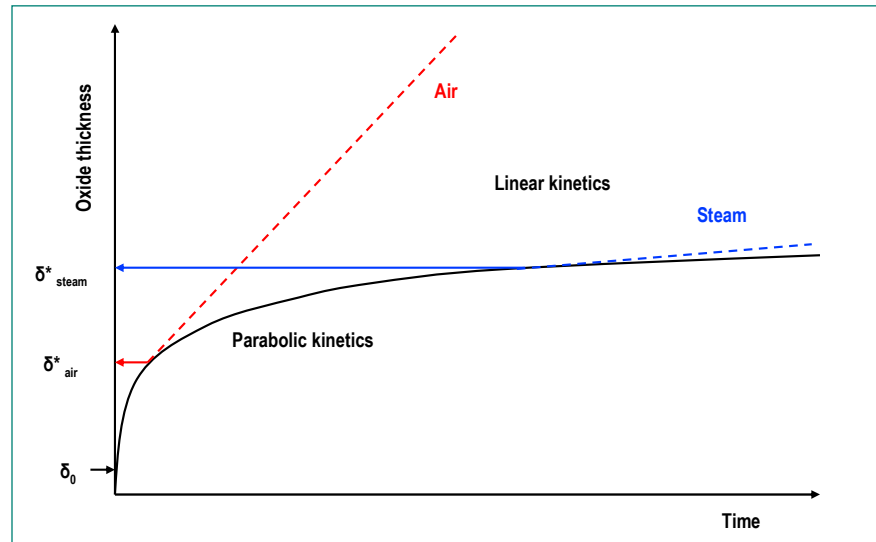
$$d(\delta)/dt = K/\max(\delta_0, \min(\delta, \delta^*)), \quad (1)$$

where the coefficient K is an Arrhenius function of temperature and δ<sub>0</sub> is a prescribed minimum or a starting value. Experimental results show also that δ\* depends on several factors, including temperature, cladding material and previous oxidation history. In the proposed δ\* is considered a function of temperature but which may differ according to cladding material. Eqn. (1) represents the linear nature of post-breakaway kinetics. The effect of oxidation history is approximated by considering the transition from steam to air oxidation kinetics to take place over a finite time period, θ. In this way the accelerating oxidation rate observed in some tests is captured.

To represent breakaway kinetics in both steam and air, separate values (δ\*,air < δ\*,steam) are defined. In fact a more accurate statement is that δ\*,air applies in the presence of nitrogen. Thus the model can represent oxidation in steam, air, steam-air, and steam-nitrogen mixtures that may apply in case of oxygen starvation. Nitride formation is non-exothermic and is not considered in the model. Nitrogen is therefore treated as a catalyst. The values and temperature dependences for δ\* and θ will be determined from the results of the many separate-effects experiments already performed and ongoing. While the experimental data summarised above



Fig. 8: Schematic of proposed air oxidation model.



indicated a dependence on alloy composition, the model will for now be limited to standard Zircaloy-4 only. However, the formulation will be sufficiently general to allow a later treatment of advanced cladding materials as well, by user choice of cladding type. The breakaway model parameters for these cladding materials would be determined by analysis of the relevant separate-effects air oxidation data, outside of the present contract. In addition, the new model will be focused on the conditions likely following air ingress in-vessel, rather than on spent fuel pond accident conditions, thus concentrating on the higher temperature ranges considered. This implies that the effect of steam pre-oxidation will use data from such ranges, rather than that resulting from simulated waterside corrosion (which would need a separate treatment). The model is shown schematically in Figure 8 below.

## National Cooperation

This project does not involve cooperation with other Swiss projects.

## International Cooperation

Cooperation with organisations within European countries and Canada generally is performed under the auspices of the SARNET [7]. This includes access to the data from the Institute of Nuclear Research Pitesti, Romania, and Forschungszentrum Karlsruhe, Germany. Access to data from the MOZART programme of separate-effects tests at IRSN Cadarache, France, is obtained through

PSI membership of the International Source Term Programme (IRSN-PSI contract dated 28.3.2006). Access to the ISTC programme is available by contract between PSI and ISTC on a project-by-project basis. The MELCOR code and early access to the results of USNRC programmes is obtained under the Cooperative Severe Accidents Research Programme Agreement (CSARP) between HSK and USNRC, and close contact is kept with the MELCOR developers at Sandia National Laboratories (SNL) regarding code maintenance, development and use. PSI obtains the SCDAPSIM code, maintenance and user support via a licence agreement with Innovative Software Services (ISS), Idaho Falls, USA. SCDAPSIM is a derivative of SCDAP/RELAP5 formerly supported by the USNRC.

## Assessment 2007 and Perspectives for 2008

The project has continued successful progress, keeping up-to-date with the ongoing experimental programmes (notably by FZK and IRSN), considering the latest results that assess the likely boundary conditions defining air ingress into a reactor vessel, and maintaining knowledge of model developments in other codes. The main challenge lies in the interpretation of the copious data, the situation is more complicated than originally envisaged, in particular concerning new material on the effect of nitriding under oxygen-starved conditions, the contrasting effects of pre-oxidation during transient and water-side corrosion (thin layers typical of water-side corrosion appear most vulnerable to nitrogen), and the complicated dependence on temperature due to  $ZrO_2$

phase transitions (c.f. breakaway steam oxidation). Therefore some simplification is necessary concerning model definition, restricting attention to a subset of conditions; namely in-reactor accident sequences (in which some steam oxidation may have already taken place), higher temperatures (including the range of fission product release), and oxidation in steam, air and steam-air mixtures (with nitriding not considered explicitly, noting that ZrN formation itself is not energetic but oxidation of ZrN is). As mentioned above, Zircaloy-4 only is considered now, but the formulation is sufficiently general to allow inclusion of treatments of advanced cladding materials at a later stage outside the present contract, as model options. Similarly, the effect of nitriding per se, considering its safety implications, could be included amongst the objectives of a further study.

Bearing in mind these remarks, the contract is proceeding on schedule. The next stage will be detailed coding of the model and testing against integral data.

## Nomenclature

AEKI	Atomergia Kutatotintezet
CFD	Computational Fluid Dynamics
CSARP	Cooperative Severe Accident Research Programme
EdF	Electricité de France
ERMSAR	European Review Meeting on Severe Accident Research
EU	European Union
FZK	Forschungszentrum Karlsruhe
GRS	Gesellschaft für Anlagen und Reaktorsicherheit
IBRAE	Nuclear Safety Institute of the Russian Academy of Sciences
INR	Institute for Nuclear Research
IRSN	Institut de Radioprotection et de Sûreté Nucléaire
ISS	Innovative Software Services
ISTC	International Science and Technology Centre
ISTP	International Source Term Programme
MCCI	Molten Core Concrete Interaction
PSI	Paul Scherrer Institute
PWR	Pressurised Water Reactor
RPV	Reactor Pressure Vessel
SARNET	Severe Accident Research Network
USNRC	United States Nuclear Regulatory Commission
VVER	Vodo-Vodyanoi Energetichesky Reactor (PWR of Russian type)

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