Code Assessment Program for MELCOR1.8.6

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ABSTRACT

The MELCOR code developed at Sandia National Laboratories (SNL) for the USNRC is used in Switzerland for analysis of severe accident transients in light water reactors. One area of concern is that of air ingress, which can lead to accelerated fuel degradation and enhanced release of fission products, especially the highly radiotoxic ruthenium. Existing oxidation models do not fully represent all the relevant physical processes, and cannot be guaranteed to be conservative. A new model has been developed at PSI which captures the essential features of initial parabolic (protective) kinetics, the transition to linear (breakaway) kinetics. The model has undergone developmental assessment against data from separate effects experiments carried out at KIT. Implementation into the SCDAP and MELCOR codes has been performed, and assessment against independent separate-effects and integral data is in progress. In parallel, PSI are participating in the OECD Sandia Fuel Project (SFP), in which a series of experiments is being performed by SNL using prototypic materials and full-scale fuel assemblies arranged in a simulated dried-out storage pond. The project is providing high quality data with which to assess the capability of models to simulate the air oxidation and its potential to trigger a self-propagating fire in an uncovered spent fuel pond. The PSI model, when implemented into MELCOR, will be assessed against the SFP data.

ZUSAMMENFASSUNG

Das MELCOR-Programm, entwickelt von den Sandia National Laboratory 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 Thema des Lufteinbruchs, welcher zu einer beschleunigten Kernzerstörung und einer erhöhten Freisetzung von Spaltprodukten führen kann, 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. Am PSI wurde deshalb ein Modell entwickelt, welches die Oxidation von Zirkaloy-4 an Luft beschreibt, basierend auf Experimenten des Karlsruhe Institute of Technology. Dieses Modell befindet sich in der abschliessenden Verifizierungsphase. Zusätzlich zu diesen Experimenten ist das PSI auch eingebunden in das OECD Sandia Fuel Project (SFP), welches in einer Serie von Experimenten Daten liefert über das Verhalten von prototypischen Materialien in einem trocken gefallenen Lagerbecken für abgebrannte Brennelemente. Dieses Versuchsprogramm wird von SNL durchgeführt. Es wird qualitativ und quantitativ hervorragende Daten liefern für die Verifizierung des am PSI entwickelten Oxidationsmodells. Nach der Implementierung des Modells in MELCOR können diese Versuchsdaten zur Verifizierung herangezogen werden.

Project Goals

The safety impacts of air ingress on nuclear fuel elements at high temperature have been studied for many years, in accident situations involving failure of the reactor pressure vessel (RPV) lower head, shutdown conditions with the upper head removed [1] and with, or in spent fuel ponds after accidental loss of coolant [2]. 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 high temperatures can lead to increased release of some fission products [3]. The situation is kept under continual review, with experimental and modelling studies performed, notably within the European Union Framework SARNET project [4], and the International Source Term Programme (ISTP) [5], in which PSI takes part.

The MELCOR code 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. Version 1.8.6 [6] is now established as the current production version while MELCOR 2.1 is still undergoing assessment. MELCOR is supported by SCDAP-based codes [7], [8], for more detailed treatment of thermal hydraulics and core degradation. The air ingress model is being implemented in both MELCOR and SCDAP/Sim.

The present three-year project running from 2009 to 2012 comprises two complementary activities being pursued in tandem. The first of these is a continuation of the previous PSI-ENSI collaboration [9]. The model is being implemented in MELCOR to enable simulation of integral experiments and plant or spent fuel transients. In the second activity PSI is participating in the OECD Sandia Fuel Project (SFP) [10], which will provide a prototypic dataset under large scale fuel pond loss of coolant conditions for validation of MELCOR code and air oxidation models. The intended result is an improved tool for plant and fuel pond simulation to support PSA investigations and source term studies.

Work Carried Out and Results Obtained

This section is divided into two parts. The first presents a status of modelling activities during the first year of the present PSI-ENSI collaboration [11], which concentrate mostly on its implementation in MELCOR and SCDAP/Sim, the latter to enable validation against PARAMETER-SF4, an air ingress experiment. The second part presents an overview of the SFP project, the experiments planned therein and the sought-for results. An indication is given of further work that could be carried out, including a possible generalisation of the model to advanced cladding materials such as Zirlo^{TM} and M5^{TM}, that feature in current new reactors.

Part 1: Air oxidation modelling

Review of state of knowledge

Experimental Activities

The last formal reviews of activities in the experimental area was presented at ERMSAR2008 [12], and TOPSAFE2008 [13]. The status of studies continuing since then has been regularly reported in the present series of annual progress statements. During the last year further separate effects experiments have been performed at KIT [14], concentrating on nitriding of homogenised alpha-Zr(O). The latest air ingress bundle transient experiment, QUENCH-16, was performed in July 2011[15]. It comprised a comparatively minor degree of pre-

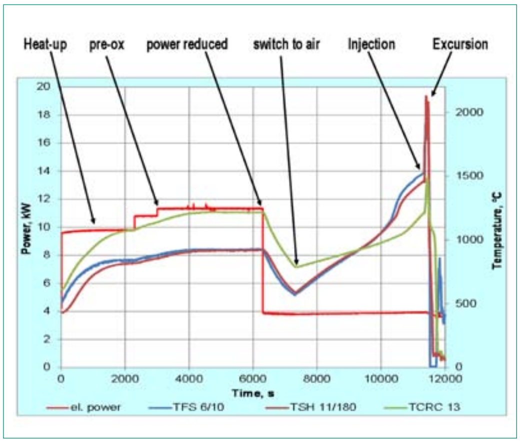


Figure 1: *Sample results of QUENCH-16, indicating the main phases of the experiment, the thermal response during air ingress and the oxidation excursion during reflood.*

oxidation in steam, followed by a low flow rate of air leading to an extended period of oxygen starvation, in order to examine the interaction between nitrogen with the pre-oxidised bundle. The experiment conduct and results are ilustrated in figure 1. QUENCH-16 thus complemented the earlier experiments CODEX-AIT [16], QUENCH-10 [17] and PARAMETER-SF4 [18]. Collectively these experiments examine the effect of air covering the whole spectrum from very low to high levels of preoxidation.

A clearly exhibited feature of QUENCH-16 is nitriding of the cladding, particularly in the upper elevations which were most strongly affected by the oxygen starvation. The oxygen starvation and nitriding lasted about 850 s and may have been the driving force for the strong oxidation excursion during reflood, which did not occur in QUENCH-10 where the starvation period was very short. Pretest analytical support to QUENCH-16 was provided by PSI, using SCDAP/Sim and MELCOR, EDF using MAAP-4 and GRS using ATHLET-CD. Preliminary post-test analyses have been performed [19].

Current status of model development

Validation of the PSI model has continued. A full implementation in a developmental version of SCDAP/Sim has been successfully completed by Innovative Software Services (ISS). The new code version has been used for further post-test analyses of PARAMETER-SF4 [20, 21] successfully reproducing the air ingress thermal transient (figures 2, 3) and oxygen consumption (figure 4). The same version is also being used for the analysis of QUENCH-16, currently in progress.

In parallel with the above work, the model has been implemented into a special version of MELCOR 1.8.6 by the Russian Academy of Science (RAS). The model is identical to the one successfuly implemented in SCDAP. A trial version was provided to PSI for verfication of the implementation. Verification of the model as applied to oxidation in steam has been successfuly carried out, as shown in figure 5. However, the features needed to simulate the heater rods in QUENCH and PARAMETER are not included in this version and so the model cannot yet be fully validated within the MELCOR code. Efforts to rectify this deficiency are in progress.

An initiative is being planned within the European Framework SARNET-2 Programme to per-

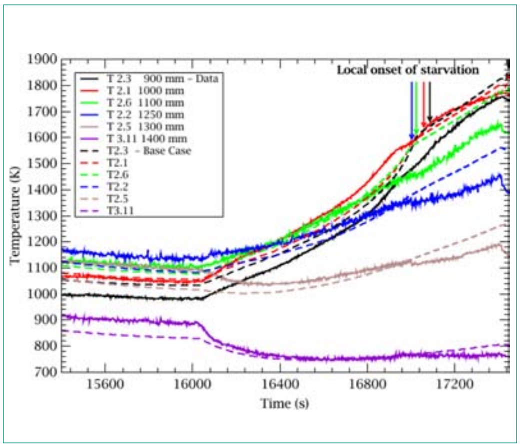


Figure 2:
Thermal response in upper elevations of bundle during PARAMETER-SF4 air ingress phase. Change in slope indicates onset of local oxygen starvation.

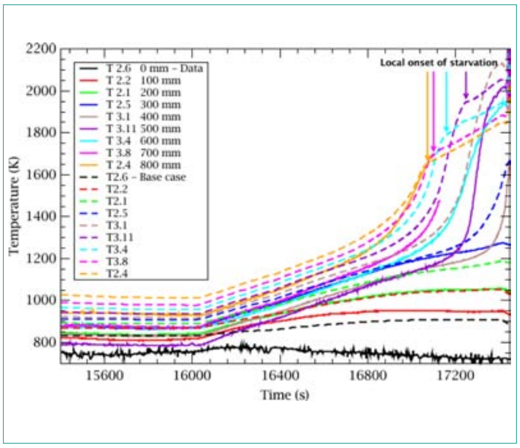


Figure 3:
Thermal response in lower elevations of bundle during PARAMETER-SF4 air ingress phase. Change in slope indicates onset of local oxygen starvation.

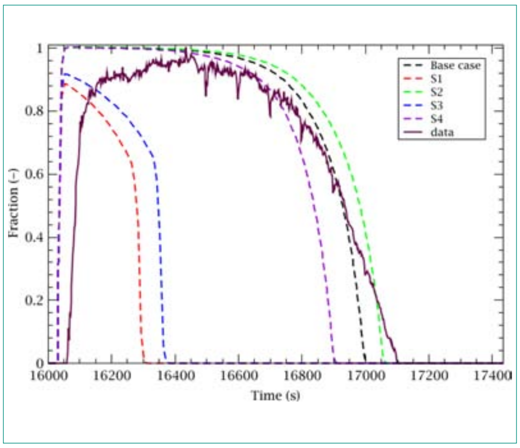


Figure 4:
Oxygen consumption during PARAMETER-SF4 air ingress phase. Base case, S1 and S2 used the PSI model and kinetic parameters; S3 and S4 used the Benjamin correlation (MELCOR default parameters) in conjunction with the PSI model.

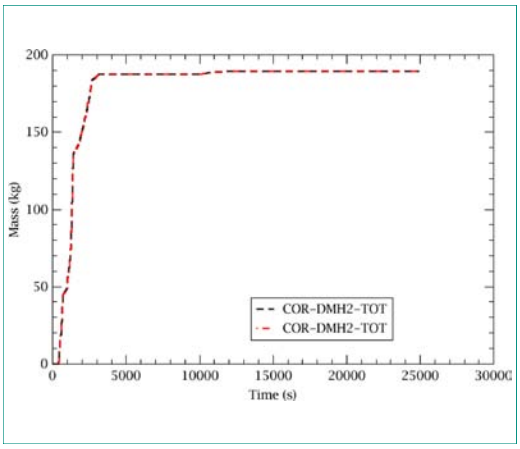


Figure 5:
Verification of PSI model implementation in MELCOR 1.8.6: Sample problem comparison for hydrogen production during steam oxidation.

Figure 6:
Reaction in different atmospheres at 1200 °C: from top (i) bare Zry in nitrogen, (ii) pre-oxiddised Zry in nitrogen, (iii) oxygen-stabilised α-Zry, (iv) bare Zry in oxygen, (v) pre-oxidised Zry in air, (vi) bare Zry in air.

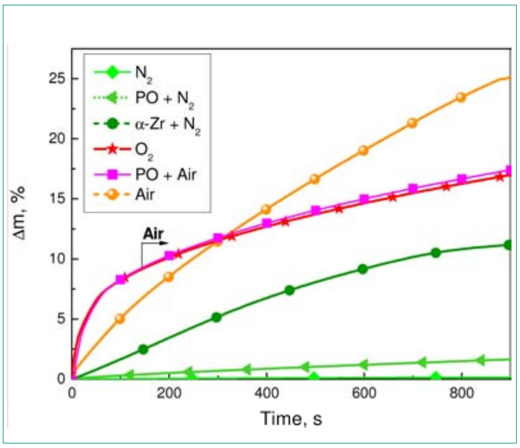


Figure 7:
Calculated and measured cladding temperatures at the 3150 mm elevation. The ignition suggests a breakaway process.

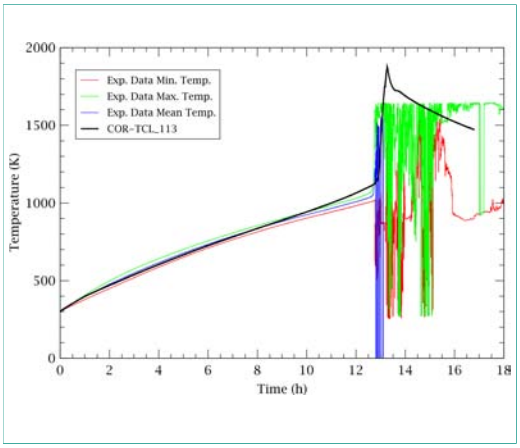


Figure 8:
Calculated and measured oxygen partial pressure at the assembly outlet, showing sudden increase in consumption.

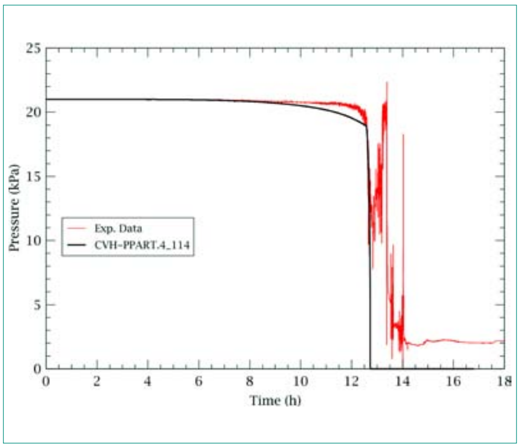
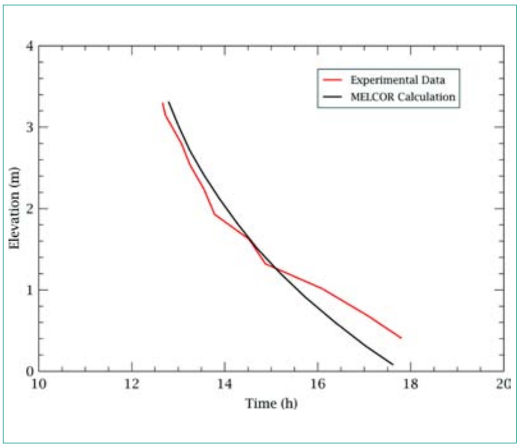


Figure 9:
Calculated and measured downward propagation of flame front in fuel bundle; the change in slope in the experiment is attributed to disruption of geomtery.



form a benchmark exercise using the air ingress experiments QUENCH-10 and -16. The aims of the exercise are to compare the various air oxidation models that have been developed and implemented by PSI, GRS and IRSN, and to assess the improved capabilities compared with previously existing models.

Potential model extensions

It was mentioned previously that results of separate-effects tests performed at FZK and IRSN also show a dependence on cladding type of oxidation in steam, oxygen and air. There is therefore a case for extending the model to other zirconium-based cladding alloys.

QUENCH-16 shows clearly the role of nitrogen, not only as a catalyst for the oxidation, but also as an active ingredient . This observation, together with findings from separate effects tests [14] show that formation of zirconium nitride (ZrN) occurs in the absence of oxygen and is particularly strong if the cladding has been preoxidised. The extent of nitriding is illustrated in figure 6. The Zr-nitrogen reaction is exothermic, although not as much as the oxidation. ZrN appears to be susceptible to breakaway, and also reacts exothermically with steam during reflood. There is a case for extending the model to include this reaction. However, the kinetics of this reaction and competition with the oxidation are unclear; the task would be challenging.

Part 2: OECD SFP Project

The OECD SFP project comprises two large scale experiments on full length, commercial 17 × 17 pressurized water reactor (PWR) fuel assembly mock-ups to provide data for the severe accident codes. There are also complementatry tests on properties of cladding materials.

The first full scale experiment was performed in March 2011, on a single fuel assembly allowed to heat up under simulated decay heat in a naturally convecting flow of dry air. The heating took place very slowly over a period of about 12 hours, until a maximum temperature of about 1150 K when oxidation began to occur near the top of the bundle. Locally the temperatures increased more rapidly and almost all of the oxygen was consumed. The change in temperature slope and rapid increase in oxygen consumption suggests a possible breakaway oxidation process. The flame front slowly propagated downward, reaching the bottom of the bundle after about a further 6 hours. There was insufficient oxygen to consume all the metallic cladding during this downward propagation, and burning continued for about 4 days at a low air flow rate.

Figure 7 shows the measured and calculated temperature histories in the upper part of the bundle, showing excellent agreement for the initial heat up and ignition. Figure 8 compares the consumption of oxygen, via the outlet partial pressure; the measured residual oxygen is believed to be due to bypass of the air through cooler locations. The downward flame propagation rates is shown in figure 9, again showing good agreement until a departure at about 15 hours, believed to be due to the effect of disruption of the flow paths due to the heater rod degradation.

National Cooperation

This project does not involve cooperation with other Swiss projects.

International Cooperation

Cooperation with organisations within European countries and Canada generally was performed under the auspices of SARNET [4] which finished at the end of September 2008. The 7th Framework follow-on project, SARNET2 started early in 2009 and continues for another 4 years. There is a close technical link between work packages WP5 (core behaviour and cooling) and WP8 (source term), via the potential impact of oxygen on ruthenium volatility. The ongoing QUENCH programme is supported also by the German Nuclear industry to address oxidation issues arising from the switch to improved cladding alloys.

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 which provides access to results of those IRSN experiments which are not encompassed within SARNET2. The MELCOR code and early access to the results of USNRC programmes are obtained under the Cooperative Severe Accidents Research Programme Agreement (CSARP) between ENSI 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 ISS, Idaho Falls, USA. SCDAPSIM is a derivative of SCDAP/RELAP5 formerly supported by the USNRC. Access to data from the OECD SFP project is obtained under the terms of the project.

Assessment 2011 and Perspectives for 2012

Progress has continued, with implementation into special versions of MELCOR and SCDAP/Sim, and assessment using data from air ingress experiments. Detailed assessment and refining of the model continues into 2012.

A benchmark is planned within the European Framework SARNET-2 Programme using the air ingress experiments QUENCH-10 and -16. The aims of the exercise are to compare the various recently developed air oxidation models, and to assess the improved capabilities compared with previously existing models.

The second large scale test in the SFP project will examine radial progression of a flame across adjacent bundles. It will examine also the impact of rod pressurisation and the consequent cladding deformation on the flame propagation analysis of the SFP experiments will continue. The new model, when fully assessed in MELCOR 1.8.6 will be implemented in a mainstream version of MELCOR 2.

Possible further developments are inclusion of the formation of ZrN and its reaction with steam.

Publications

- *J. Birchley and L. Fernandez-Moguel,* Simulation of Air Oxidation during a Reactor Accident Sequence: Part 1 – Phenomenology and Model development, Ann. Nucl. Energy, 40, 163–170, January 2012.
- *L. Fernandez-Moguel and J. Birchley,* Simulation of Air Oxidation during a Reactor Accident Sequence: Part 2 – Analysis of PARAMETER-SF4 Air Ingress Experiment using RELAP/SCDAPSIM, Ann. Nucl. Energy, 40, 141–152, January 2012.

- *L. Fernandez-Moguel,* Analytical support to air ingress experiment QUENCH-16, 17th International QUENCH Workshop, Germany, Karlsruhe Institute of Technology, November, 2011.
- *J. Birchley,* Air oxidation of Zircaloy: Phenomenology and modelling, 17th International QUENCH Workshop, Karlsruhe Institute of Technology, Germany, November, 2011.
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Nomenclature

AEKI	Atomergia Kutatotintezet
ANL	Argonne National Laboratories
CSARP	Cooperative Severe Accident Research Programme
EdF	Electricité de France
ERMSAR	European Review Meeting on Severe Accident Research
EU	European Union
GRS	Gesellschaft für Anlagen und Reaktorsicherheit
IRSN	Institut de Radioprotection et de Sûreté Nucléaire
ISS	Innovative Software Services
ISTC	International Science and Technology Centre
ISTP	International Source Term Programme
KIT	Karlsruhe Institute of Technology (formerly FZK)
PSI	Paul Scherrer Institute
PWR	Pressurised Water Reactor
RAS	Russian Academy of Science
SARNET	Severe Accident Research Network
SNL	Sandia National Laboratories
USNRC	United States Nuclear Regulatory Commission
VVER	Vodo-Vodyanoi Energetichesky Reactor (Russian PWR)

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