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. In order to address limitations in simulation of air ingress scenarios, a new oxidation model has been developed at PSI which captures the transition to linear (breakaway) kinetics. The model was already assessed against data from separate effects experiments, and underwent initial assessment against integral transient data from the PARAMETER and QUENCH air ingress experiments. The model is now successfully implemented into a special version of MELCOR 1.8.6 and has been shown to reproduce the intended oxidation behaviour. In particular it gives the same results as the standard MELCOR model when the new features are not enabled, while the breakaway model yields results consistent with the same model in SCDAP. In parallel, PSI is participating in the OECD Sandia Fuel Project (SFP), in which a series of experiments are being performed by SNL using prototypic materials and full-scale fuel assemblies are 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, recently implemented into MELCOR, is undergoing assessment against the SFP data. The PSI model has calculated very similar results to those obtained with the SANDIA breakaway model.

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 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 wurde von SNL durchgeführt. Es lieferte qualitativ und quantitativ hervorragende Daten für die Verifizierung des am PSI entwickelten Oxidationsmodells. Nach der Implementierung des Modelles in MELCOR wurden diese Versuchsdaten zur Verifizierung herangezogen.

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], 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 recently completed four-year project from 2009-2012 comprises two complementary activities 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 provided 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 present PSI-ENSI collaboration [11], which concentrates mostly on its implementation in MELCOR and SCDAP/Sim, which thus enables validation against air ingress experiments PARAMETER-SF4, QUENCH-10 and -16, and the OECD Sandia Fuel Project (SFP). The second part presents an overview of the SFP project, the experiments therein and the sought-for results. Included in this part is comparison with the PSI and SNL models in MELCOR.

An indication is given of further work that could be carried out, including a possible extension to the zirconium-nitrogen reaction and also generalisation of the model to advanced cladding materials such as Zirlo™ and M5™, that feature in current new reactors.

Part 1: Air oxidation modelling

Review of state of knowledge

Experimental Activities

The status of air oxidation knowledge acquisition and modelling studies during the past several years has been regularly reported in the present series of annual progress statements. During the last two years further separate effects experiments have been performed at KIT [12, 13], concentrating on nitriding of homogenised alpha-Zr(O). Analysis has continued of the latest air ingress bundle transient experiment, QUENCH-16, which was performed in July 2011[14]. It comprised a comparatively minor degree of preoxidation 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. QUENCH-16 thus complemented the earlier experiments CODEX-AIT [15], QUENCH-10 [16] and PARAMETER-SF4 [17]. Collectively these experiments examine the effect of air covering the whole spectrum from very low to high levels of preoxidation. The QUENCH-10 and -16 experiments are the subject of a combined benchmark exercise (QUENCH-air) among several institutes. 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.

Current status of model development

As reported in the 2011 progress statement, full implementation in a developmental version of SCDAP/Sim was successfully completed jointly by PSI and Innovative Software Services (ISS). Mainstream release of the new version is imminent at the close of 2012. The model is now also successfully implemented in a trial version of MELCOR 1.8.6, as a preliminary to implementation by SNL into MELCOR 2.1.

Validation of the PSI model has continued. The new code version has been used for further post-test analyses of PARAMETER-SF4 [18, 19] and QUENCH-10, -16 [20, 21]. The new model successfully reproduced the oxygen consumption (figures 1, 2), the oxidation in the presencs of both steam and air (figure 3) and the results are consistent with SCDAP and MELCOR (figure 4).

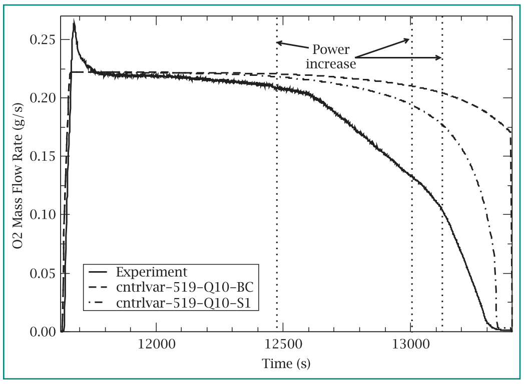

Figure 1: *Oxygen consumption for QUENCH-10. Sample results of QUENCH-10 analysis show the impact of the pre-oxidation state on the PSI oxidation model during the air ingress phase. The base case used nominal power during the steam phase and the S1 case used adjusted kinetics in order to match as well as possible the state of the bundle at the end of pre-oxidation.*

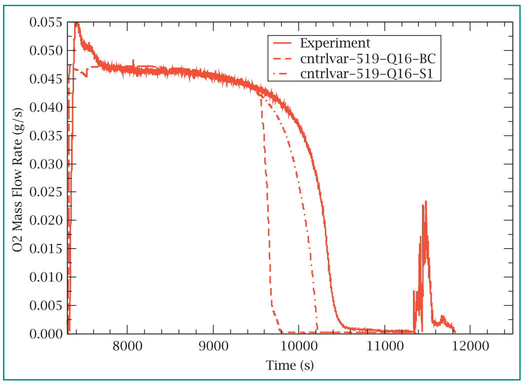

Figure 2: *Sample results of QUENCH-16 analysis showing the effect of the PSI oxidation model during the air ingress phase. The base case calculates breakaway and in the S1 the breakaway model is disabled.*

A feature of QUENCH-16 was the unexpected flow of steam during the nominally dry air phase. The presence of air and steam together provided a fortuitous opportunity to exercise the model in conditions that would be representative of a reactor air ingress event. The model successfully captured the mixed oxidation with both MELCOR and SCDAP.

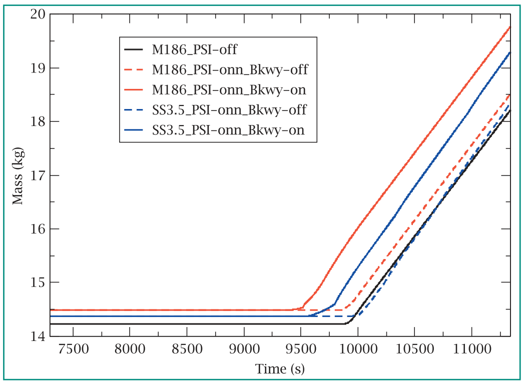

Figure 3: *Simulation of QUENCH-16 mixture air and steam oxidation using SCDAP and MELCOR.*

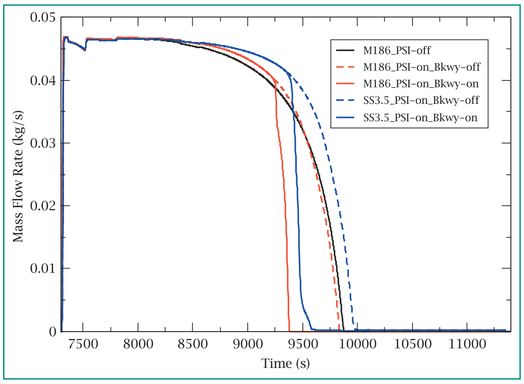

Figure 4: *Comparison of results for oxygen consumption during QUENCH-16 using MELCOR 1.8.6 and SCDAP/Sim3.5 shows very good consistency.*

Results of separate effect tests at KIT revealed a clear effect of oxygen concentration on reaction kinetics, particularly when the air is diluted by other gases. A trial empirical correlation was derived from the results and implemented in a local version of SCDAP in order to explore the influence of low oxygen concentration.

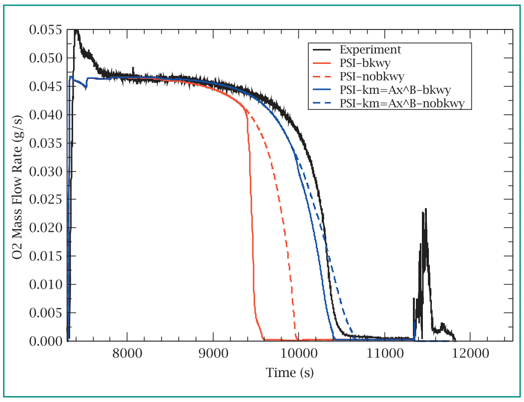

Figure 5: *Effect of low oxygen concentration on rate of consumption in QUENCH-16.*

The limited range of data on the effect of concentration means that the correlation should be regarded as rather heuristic. However, the improved agreement suggests that the topic should be further investigated with a view to including it in the model, especially since low concentrations are more likely in reactor or spent fuel sequences.

Potential model extensions

As mentioned in previous reports, the 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.

The results of both separate effects and bundle transients show a strong effect of nitriding under oxygen starved consitions. This may be particularly important as the Zr-nitrogen reaction is exothermic, albeit not as much as the oxidation. In addition ZrN appears to be susceptible to breakaway, and also reacts exothermically with steam during reflood.

Finally, there is a case for including the effect of oxygen concentration on the kinetics.

Part 2: OECD SFP Project

The OECD SFP project comprises two large scale experiments (phase I and II) 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 complementary tests on properties of cladding materials.

The PSI model implementation in MELCOR provides the opportunity to make comparison with both the data and SNL model. For phase I figure 6 shows very slight differences in the pre-breakaway temperatures due to the different oxidation kinetics but sufficient to delay the onset of breakaway-induced ignition compared with the SNL model. The pre-breakaway PSI air oxidation kinetics are based on transient oxidation rate data from KIT experiments while those of SNL were from integrated oxidation data from ANL. As well as pre-oxidation kinetics the treatment of breakaway is different in the two models. It is noted that although the SNL calculation gives better agreement with experiment for the timing of breakaway, the good agreement was achieved by SNL adjusting the breakaway parameters to fit the SFP data. The PSI breakaway parameters were as developed using the KIT data and not tuned to the SFP result.

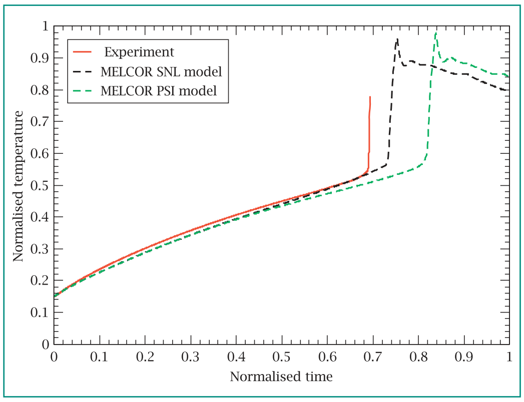

Figure 6: *Measured and calculated cladding temperature at location of first ignition; data, SNL model, PSI model (phase I).*

The SFP phase II full scale experiment was performed in June 2012, representing a spent fuel element with high heat load (Burnup of 45 MWd/kg and 3 month after shutdown) surrounded by 4 much older fuel elements which are represented by unheated assemblies. This geometry is known as cold neighbour configuration. The heat up in this experiment is much faster compared with phase I because of the increased power, despite the relatively high heat transfer to the cold neighbours. After a few hours the oxidation excursion started close to the top of the heated central bundle and like in phase I the oxygen was completely consumed.

The same modelling as in the above phase I calculations again show slightly slower thermal escalation using the PSI model, but the onset of igniton occurs at a similar time in both the PSI and SNL calculations, and also in agreement with the experiment.

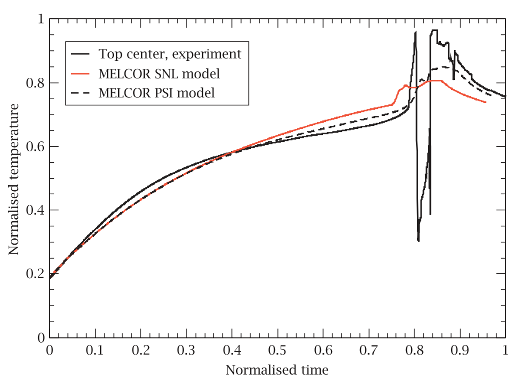

Figure 7: *Comparison of phase II thermal response up to first ignition: Data, MELCOR, PSI model.*

The phase II analyses are reported by Jaeckel [24]. The flame front slowly propagated downward, reaching the bottom of the bundle after about a further 6 hours (figure 8). A problem in the downward propagation of the zirconium fire is that a flat power profile along the heated fuel pins is assumed. The slight temperature-dependence of the heater wire resistance causes the power profile to be peaked at regions with higher temperatures. Due to limitations in MELCOR, qualitative assessment of the effect was made using a constant tilted power profile which resulted in closer agreement with the data.

The radial fire propagation into the peripheral fuel elements was also simulated with MELCOR (figure 9). There was insufficient oxygen to consume all the metallic cladding during this downward propagation, and like in the phase I experiment burning continued for about 4 days at a low air flow rate. As can be seen, the fire spread outwards from the centre at the same time as propagating downward. The first ignition at the radial locations occurred at progressively lower elevations during the the fire spreading.

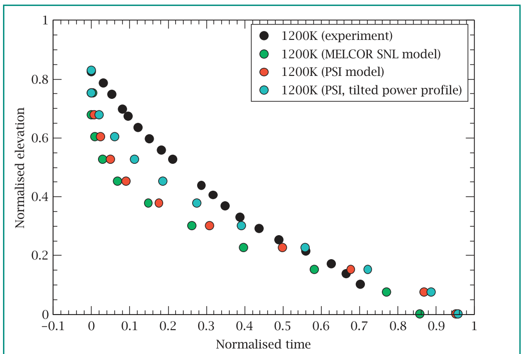

Figure 8: *Calculated and measured downward propagation of flame front in fuel bundle in phase II experiment inclusive calculations with the PSI air oxidation model.*

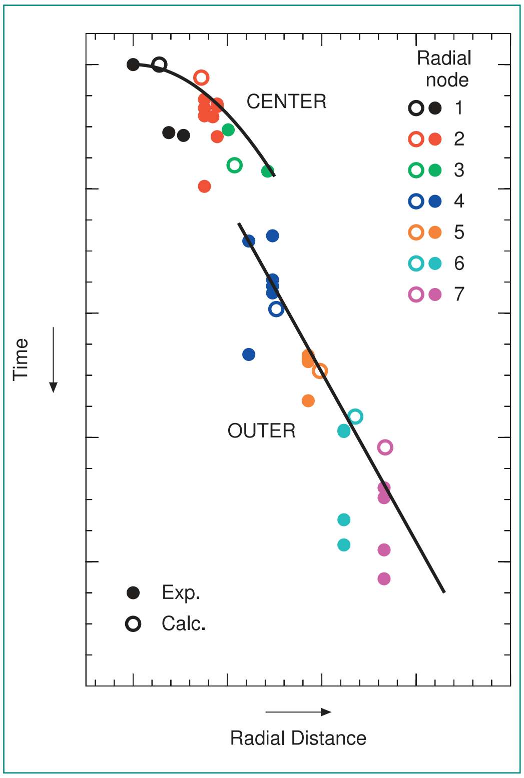

Figure 9: *Radial fire propagation into the peripheral fuel elements. The colours indicate the radial node in the MELCOR model.*

In phase II the gas composition at the fuel bundle outlet was measured during the entire experiment. A very important finding was the strong nitrogen consumption during the downward propagation of the fire, followed by release of nitrogen during the upward propagation as the zirconium nitride was reoxidised. The nitriding reaction of zirconium in the oxygen-starved region may deliver as much heat as the oxidation by oxygen. The reoxidation is also exothermic.

The final benchmark report of the SFP phase II experiment will be released in February 2013. The present analysis forms the basis of PSI contribution to the benchmark. Work continues on this topic.

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 until 2013. 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 isssues 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 (including application of the PSI model to MELCOR) 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 2012 and Perspectives for 2013

Progress has continued, with full implementation into MELCOR and further assessment using data from integral transient experiments with air ingress. Detailed assessment and refining of the model continues into 2013.

A benchmark has been conducted 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 outcome of the exercise will be reported at the final SARNET conference.

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

Following the findings from SFP Phase II and QUENCH-16, there is a strong case for including a model for ZrN reactions. Possible further development is inclusion of the effect of low oxygen concentration.

As OECD SFP approaches completion, SNL have proposed a follow-on programme. There are clear prospects for ongoing experimentation in the area.

Publications

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- *L. Fernandez-Moguel,* Preliminary analysis of air ingress experiment QUENCH-16 using RELAP/SCDAPSim3.5 and MELCOR 1.8.6, 21st International Conference Nuclear Energy for new Europe, Lyubljana, September 2012.
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- *P. Vryashkova (INRNE) and L. Fernandez-Moguel,* Modelling of air oxidation in QUENCH-16: effect of oxygen concentration, 18th International QUENCH Workshop, Karlsruhe Institute of Technology, Germany, November, 2012.
- *B. Jaeckel and A. Rydl,* MELCOR activities at PSI: SFP program, first results and air oxidation, CSARP Meeting, Bethesda, Maryland, USA, September 2012.
- *B. Jaeckel,* Analysis of SFP Phase 2 Experiment using MELCOR, TM-42-12-12, November 2012.

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
KIT	Karlsruhe Institute of Technology (formerly FZK)
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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