

# 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 and the transition to linear (breakaway) kinetics. The model has undergone developmental assessment against data from separate effect experiments carried out at KIT. Implementation into MELCOR, and assessment against independent separate-effect and integral data, are in progress. In parallel, PSI are 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 which arranged in a simulated dried-out storage pond. The project will provide 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.

Das MELCOR-Programm, entwickelt von den Sandia National Laboratorys 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 Karlsruher 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 für die Verifizierung des am PSI entwickelten Oxidationsmodells liefern. Nach der Implementation des Modelles 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 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 2009–2012 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 knowledge and modelling activities dur-

ing 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™ and M5®, 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 TOP-SAFE2008 [13]. Since then separate effects experiments at KIT [14] have continued, extending the existing databases [15] to cover alternative cladding materials and transient temperature conditions. A recent series of experiments [16] investigated the difference in oxidation behaviour between Zry-2 (used in BWRs) and Zry-4 using in most operating Western PWRs. Part of the objective of this work was to complement the SFP experiments. Tests were also performed on samples which had been machined in different ways to replicate the preparation of the heater rods for the SFP experiments. Figure 1 shows the very similar behaviour between the two samples.

During a thermal transient the kinetics are determined not only by the temperature but the time of exposure,

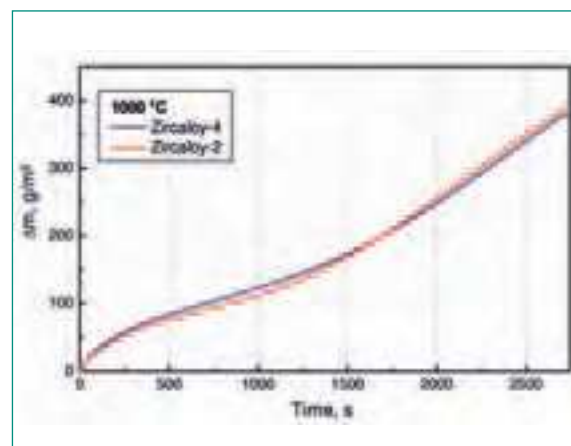


Figure 1: Mass gain during oxidation of Zry-2, Zry-4 in air at 1000 °C [16].

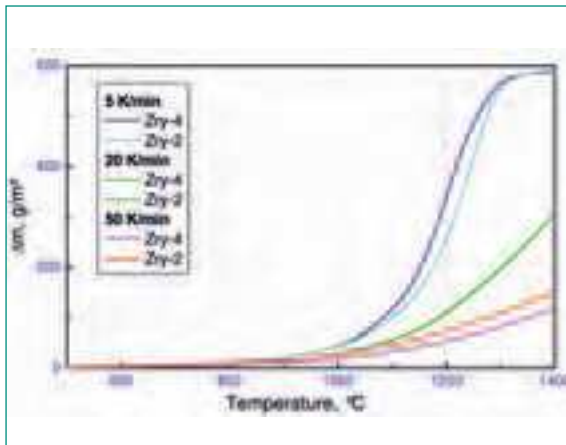


Figure 2: Transient oxidation of Zry-4 and Zry-2 in air at different temperature ramp rates [16].

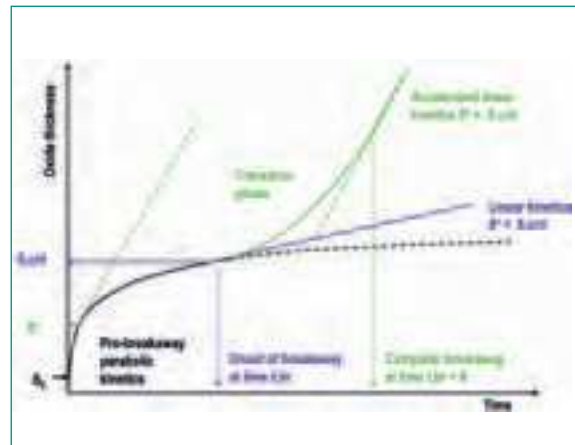


Figure 3: Schematic of accelerating kinetics during transition to breakaway oxidation.

such that the oxidation rate can be greater at a certain temperature if the thermal ramp is slower. Figure 2 shows there is no significant difference between the two forms of Zircaloy during transient oxidation.

The ITSC PARAMETER air ingress experiment SF4 [17] was conducted during 2009. SF4 was an approximate counterpart to QUENCH-10 [18], but with VVER configuration and cladding material (E110). An objective of SF4 was to achieve a significant period of oxygen starvation in order to investigate the nitriding of pre-oxidised cladding, and this was successfully achieved. Post-test analyses were performed by IBRAE, EDF, GRS, Kurchatov Institute, and PSI, using the codes SOCRAT, MAAP-4, ATHLET-CD, ICARE/CATHARE, and SCDAP/Sim, respectively [19]. All of the codes adequately reproduced the steam pre-oxidation behaviour but there was a wide variation in the oxygen consumption rate and location of the starvation front during the air phase. This variation reflects the present status of the air oxidation models, which are still undergoing assessment.

Figure 3 shows some results from a preliminary analysis with SCDAP/Sim. The air oxidation kinetic model is the NUREG correlation currently standard in MELCOR, which overestimates the oxygen consumption. By contrast the steam kinetic correlation gives good agreement with experiment, indicating no significant acceleration in the kinetics following the switch to air. One of the aims of the PSI model is to reproduce the delay or non-occurrence of breakaway during air oxidation of steam pre-oxidised cladding. This work is currently in progress.

### Current status of model development

The model concept, formulation and developmental status were described in some detail in previous reports.

The status was described in a paper presented at the NRC-led CSARP meeting [20]. The acceleration in oxidation rate is modelled by defining two oxide thickness parameters,  $\delta_{crit}$  corresponding to the onset of breakaway, and  $\delta^*$  corresponding to the linear oxidation rate. This modification is indicated schematically in figure 3. The model thus seeks to capture the observed progressive transition.

A much stiffer test of the model is to reproduce the air oxidation behaviour during an integral transient comprising steam pre-oxidation followed by air oxidation. QUENCH-10 exhibited a delayed and partial transition to breakaway, with mild acceleration in kinetics, while SF4 exhibited no obvious accelerated oxidation.

Following discussions, USNRC offered to commission IBRAE to implement the PSI model into a special version of MELCOR 1.8.6. This development is currently in progress, with the additional support of SNL and PSI, ahead of the later planned implementation into MELCOR 2.1. An advantage of MELCOR 1.8.6 is that the source code is available so that PSI and ENSI can access the models and participate more effectively in the assessment process. A closed meeting took place in conjunction with the recent CSARP meeting hosted by USNRC, in which the workscope was defined. As part of the verification, calculations will be performed to demonstrate consistency with the stand-alone model by comparison with selected cases, and simulations of previous transient cases without air to demonstrate compatibility with the standard MELCOR model. In this way the implementation of the new model will be verified.

In parallel, a partial implementation of the PSI model has been performed into a local version of MELCOR 1.8.6. This is restricted to cases where only air is present, and

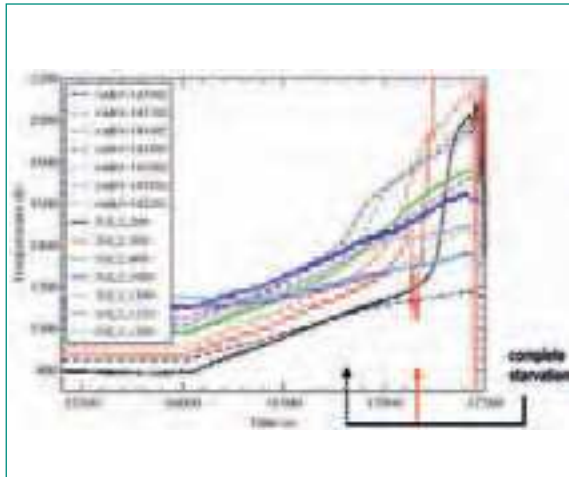


Figure 4: Bundle temperatures during SF4 air phase: comparison between data and SCDAP using MELCOR air kinetic correlation [21].

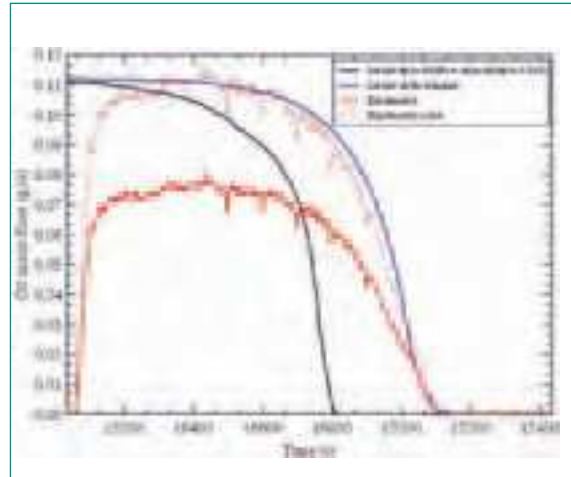


Figure 5: Oxygen consumption during SF4 air phase: comparison between data and SCDAP with standard steam and MELCOR air kinetic correlations [21].

hence cannot simulate sequences involving steam-air mixtures or steam pre-oxidation. It is intended to apply the version to the SFP experiments which are conducted in the complete absence of steam.

In addition to implementation in MELCOR, Innovative Software Systems (ISS) are implementing the PSI model into a version of SCDAP/Sim. First results of assessment against PARAMETER-SF4 confirm the previous result that the transition to breakaway did not occur to any significant degree during the time period of air flow.

Figure 4 compares the calculated and observed bundle temperatures during the air phase, showing the premature increase in temperatures when the standard MELCOR correlation is used. This is reflected by the early occurrence of total oxygen consumption, shown in figure 5. Also shown is the result using the steam correlation, which shows good agreement with experiment [21].

In previous progress reports it was stated the model would be implemented into MELCOR 2.1 which is still undergoing development. However, the new code version was not then mature enough to warrant introduction of the new model. That situation still applies but MELCOR 2.1 will probably be ready some time in 2011. A successful implementation in MELCOR 1.8.6 will provide excellent preparation for implementation in 2.1. Assessment against data from integral transient tests, QUENCH-10, PARAMETER SF4, OECD SFP and possibly CODEX AIT is underway.

### Potential model extensions

The 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 need to extend the model to Zirlo™ and M5® cladding, as these could feature in reload fuel in existing plant, and very likely in new build in Switzerland. Extension to E110 cladding would make use of Russian data feasible, especially from the PARAMETER SF4 experiment that extends the integral test database.

A spent fuel pond would typically involve lower temperatures than the in-vessel cases. Larger differences amongst cladding types are seen at lower temperatures, as evidenced by the FZK and IRSN data referenced above, and also by the Argonne experiments which were targeted at spent fuel pond conditions. Such extensions, with implementation into MELCOR, would help assure high quality PSA results and help formulate prevention and mitigation strategies for spent fuel pond events.

## Part 2: OECD SFP Project

The objective of the proposed OECD SFP project is to perform a highly detailed thermal-hydraulic characterization of full length, commercial 17 × 17 pressurized water reactor (PWR) fuel assembly mock-ups to provide data for the direct validation of MELCOR or other appropriate severe accident codes. The proposed PWR characterization will be similar to that successfully conducted for the BWR study and will lead to two full-scale PWR fire tests where the zirconium alloy cladding is heated in air to ignition. The first test will study the heating and oxidation-induced ignition of a single assembly. The second test will study also the response of neighbouring

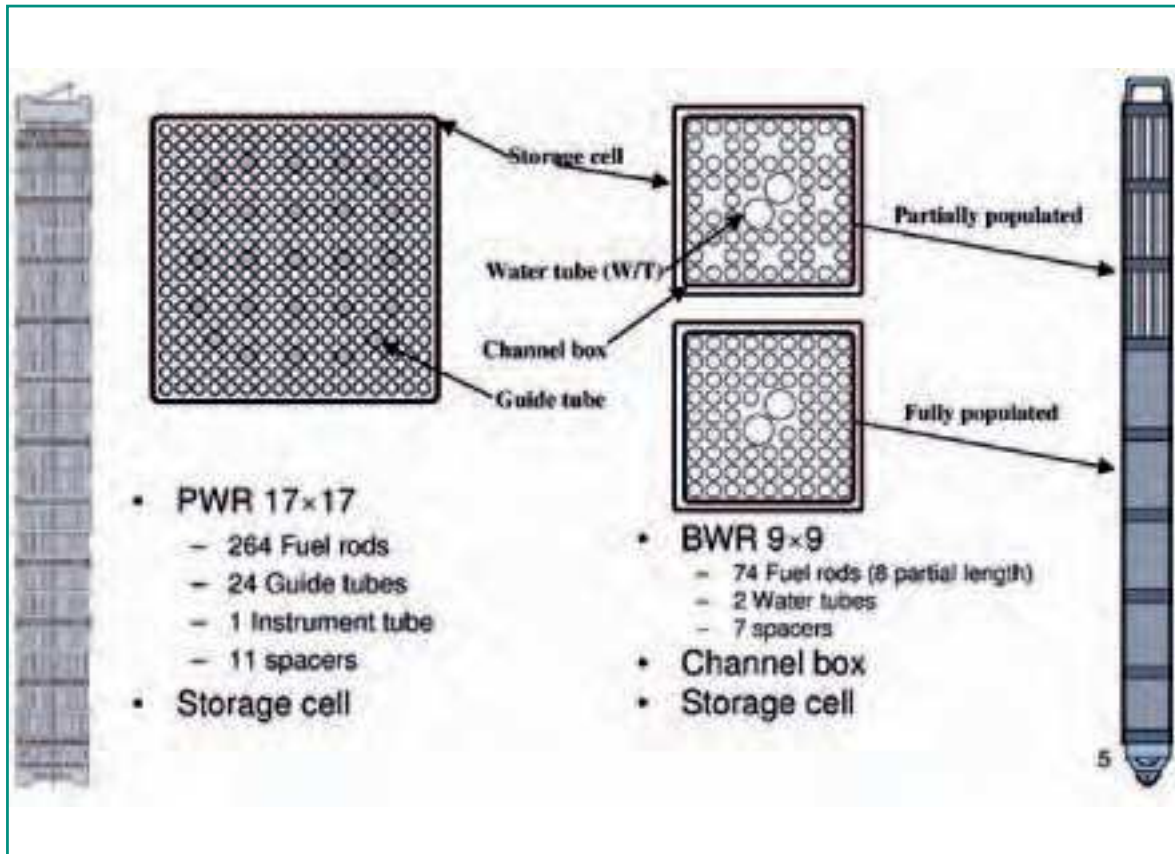


Figure 6: Schematic of BWR and PWR geometry differences [10].

assemblies and will include the impact of ballooning on propagation of the ignition front. The PWR experimental design and data analysis will be closely coupled with MELCOR modelling as was done in the previous BWR study. The BWR and PWR assembly configurations are significantly different, as shown in figure 6. In the frame of the OECD SFP project SNL have developed a special version of MELCOR 1.8.6 for the modelling of

spent fuel pool accidents. This version was distributed to the SFP participants in December 2010 together with the input decks for the BWR and PWR spent fuel pool experiments. A preliminary breakaway model for the air oxidation was included, based on the ANL air oxidation tests [22] and tuned to the SNL BWR spent fuel test data. First calculations for the impact of the breakaway model on the air oxidation were executed and results are compared with experimental data in figure 7, giving a clear qualitative indication the impact of breakaway on the thermal behaviour. The experiments for the PWR fuel geometry will be executed in 2011.

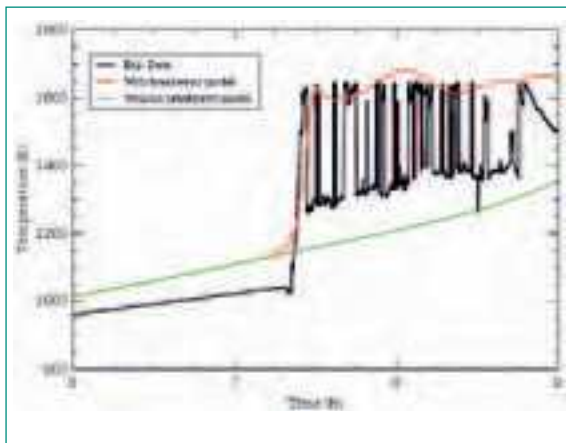


Figure 7: Breakaway-induced ignition of cladding during air oxidation: comparison of data with model, with and without breakaway.

## 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 7<sup>th</sup> 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. 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 Innovative Software Services (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 2010 and Perspectives for 2011

Progress has continued, concentrating mainly on the implementation into MELCOR and SCDAP/Sim, and on post-test analysis of PARAMETER SF4 air ingress experiment. This latter work was coordinated by IBRAE into a benchmark exercise by which the different codes and models could be cross-compared. Detailed assessment and refining of the model continues into 2011.

USNRC have made a very positive and welcome initiative in arranging for the PSI model to be implemented into MELCOR 1.8.6, going beyond the previously declared position that the modelling in 1.8.6 was frozen.

The OECD SFP project has completed the design work and the first experiment will be conducted early in 2011. A decision was made to fabricate the cladding using Zry-2 instead of Zry-4, to avoid difficulties of limited availability of other cladding alloys and to benefit from the previous experience of fabricating the heater rods for the BWR experiments. In conjunction with this decision, KIT performed comparison experiments on samples of both materials to confirm that Zry-2 would adequately replicate the behaviour.

## Publications

PSI authored papers concerning modelling of air oxidation of Zircaloy presented at the NRC-led CSARP meeting [20] and the QUENCH workshop [21].

## Nomenclature

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

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## References

- [1] *D. A. Powers, L. N. Kmetyk and R. C. Schmidt*, «A Review of Technical Issues of Air Ingression during Severe Reactor Accidents», USNRC NUREG/CR-6218, SAND94-0731, Sandia National Laboratories, September 1994.
- [2] *V. L. Sailor, K. R. Perkins and J. R. Weeks*, «Severe Accidents in Spent Fuel Pools in Support of Generic Issue 82», USNRC NUREG/CR-4982, BNL-NUREG-52093, Brookhaven National Laboratories, July 1987.
- [3] *A. Auvinen, G. Brillant, N. Davidovich, R. Dickson, G. Ducros, Y. Dutheillet, P. Giordano, M. Kunstar, T. Kärkelä, M. Mladin, Y. Pontillon, C. Séropian and N. Vér*, «Progress on Ruthenium Release and Transport under Air Ingress Conditions», Nucl. Eng. and Design, Volume 238, Issue 12, pp 3418–3428, December 2008.
- [4] *European Commission*, «SARNET (Severe Accident Research NETwork) Network of Excellence», in the EU 6<sup>th</sup> Framework programme «Nuclear Fission: Safety of Existing Nuclear Installations», contract number FI6O-CT-2004-509065, 2004.
- [5] *B. Clément and R. Zeyen*, «The Phebus Fission Product and Source Term International Programmes», Proc. Int. Conf. on Nuclear Energy in New Europe 2005, Bled, Slovenia, 5–8 September, 2005.
- [6] *R. O. Gauntt et al.*, «MELCOR Code Manuals – Version 1.8.6», USNRC NUREG/CR 6119 Rev. 3, SAND2005-5713, Sandia National Laboratories, September 2005.
- [7] *L. Siefken et al.*, «SCDAP/RELAP5/MOD3.2 Code Manual», USNRC NUREG/CR-6150 Rev. 1, INEL-96/0422 Rev. 1, Idaho Falls National Engineering Laboratories, November 1997.
- [8] *Innovative Systems Software*, «RELAP/SCDAPSIM/MOD3.4 Code Manual», Idaho Falls, USA, 2003.
- [9] *J. Birchley and Y. Liao*, «Development and Assessment Program for the MELCOR Code», Contribution to ENSI 2009 Annual Research and Experience Report – Erfahrungs- und Forschungsbericht 2009, ENSI-AN-7201, ISSN 1661-2892, April 2010.
- [10] *OECD/NEA*, «Agreement on the OECD-NEA SFP Project: An Experimental Programme and Related Analyses for the Characterization of Hydraulic and Ignition Phenomena of Prototypic Water Reactor Fuel Assemblies», January 2009.
- [11] *U. Schmocker, P. Meyer, J. Mesot and J-M Cavedon*, «MELCOR further development in the area of air ingress und Beteiligung an den OECD NEA Projekt SFP», ENSI-PSI MELCOR Assessment Vertrag, December 2008.
- [12] *M. Steinbrueck, M. Grosse, L. Sepold, J. Stuckert, J. Birchley, T.J. Haste, A.V. Goryachev, Z. Hózer, N. Vér, A.E. Kisselev, M.S. Veshchunov, V.I. Nalivaev, V.P. Semishkin*, «Status of Studies on High-temperature Oxidation and Quench Behaviour of Zircaloy-4 and E110 Cladding Alloys», The 3<sup>rd</sup> European Review Meeting on Severe Accident Research (ERM-SAR-2008), Nesseber, Bulgaria, 23–25 September 2008.
- [13] *M. Grosse, L. Sepold, M. Steinbrueck and J. Stuckert*, «Comparison of the Severe Accident Behaviour of Advanced Nuclear Fuel Rod Cladding Materials», Proc. TOPSAFE, Dubrovnik, Croatia, 30 Sept.–3 Oct 2008, European Nuclear Society, ISBN 978-92-95064-06-5, 2008.
- [14] *M. Steinbrueck*, «Separate-effects tests on high-temperature oxidation of zirconium alloys in various atmospheres», International Scientific and Technical Meeting «Computational and Experimental Studies of LWR Fuel Element Behaviour under Beyond Design Basis Accidents and Reflood Conditions», Moscow 27–28 July, 2009.
- [15] *M. Steinbrueck*, «Oxidation of Zirconium Alloys in Oxygen at High Temperatures up to 1600 °C», Oxidation of Metals, Volume 70, pp. 317–329, 2008.
- [16] *M. Steinbrueck, M. Jung and M. Walter*, «Separate-effects tests on the investigation of high-temperature oxidation behavior and mechanical properties of Zircaloy-2 to be used in the SFP PWR tests.» A report prepared in the framework of the OECD/NEA SFP Project, Karlsruhe Institute of Technology, 2010.
- [17] *T. Yudina*, «Comparison results of pretest PARAMETER-SF4 Numerical Modelling», 15<sup>th</sup> International QUENCH Workshop, Forschungszentrum Karlsruhe, 3–5 November, 2009.
- [18] *T. Yudina*, «Comparison results of pretest PARAMETER-SF4 Numerical Modelling», 15<sup>th</sup> International QUENCH Workshop, Forschungszentrum Karlsruhe, 3–5 November, 2009.
- [19] *T. Yudina*, «Pre- and posttest calculations of PARAMETER-SF4 test», 15<sup>th</sup> International QUENCH Workshop, Forschungszentrum Karlsruhe, 16–18 November, 2010.
- [20] *J. Birchley and Y. Liao*, «Modelling of Zircaloy Oxidation in Air» (abstract only) Cooperative Severe

Accident Research Programme (CSARP) meeting, Bethesda, Maryland, USA, September 2010.

[21] *J. Birchley and L. Fernandez-Moguel*, «Post-test analysis of PARAMETER-SF3, -SF4» 15<sup>th</sup> International QUENCH Workshop, Forschungszentrum Karlsruhe, 16–18 November, 2010.

[22] *K. Natesan and W. K. Soppet*, «Air Oxidation Kinetics for Zr-based Alloys», USNRC NUREG/CR-5846, ANL-03/32, June 2004.