# Development and Assessment Program for the MELCOR Code


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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 effects experiments carried out at KIT. Implementation into MELCOR, and assessment against independent separate-effects and integral data, are underway. 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 are 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 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 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] , 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 1.8.5 [6] has been the main production code until now, while version 1.8.6 [7] has undergone assessment and development at PSI during the last few years. MELCOR is supported by SCDAP-based codes [8], [9], for more detailed treatment of thermal hydraulics and core degradation. The modelling of air ingress in MELCOR is not sufficient to capture all aspects of the phenomena associated with accelerated oxidation in air.

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 [10], namely a review of relevant experimental data and models, and the development and assessment of an improved Zircaloy/air oxidation model intended for use in MELCOR. 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) [11], 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 [12], which concentrate mostly on its implementation within MELCOR. Also included here is an update of the status of the database as a result of continuing experimental efforts. 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 [13], and TOPSAFE2008 [14]. Since then separate effects experiments at KIT [15] have continued, extending the existing database [16] to cover alternative cladding materials and transient temperature conditions. The recent experiments also compare the oxidation behaviour under isothermal and transient conditions. Figure 1 shows the effect of different temperature regimes and shows the finite time required for breakaway to become established.

Results from tests conducted with a thermal step show the different oxidation behaviour below and above 1000 °C. A layered, fragile oxide scale forms in the

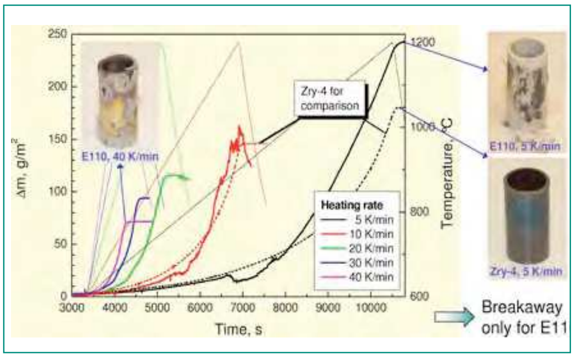


**Figure 1:** *Effect of temperature ramp rate on oxidation in steam – breakaway occurs on E110 at 5 and 10 K/min only [15].*

monoclinic phase regime of $ZrO_2$ at the lower temperature, while a columnar, more robust oxide forms in the tetragonal phase regime at the higher temperature. The increased temperature can partially reverse the breakaway with transition back to quasi-parabolic kinetics. Parallel experimental studies (MOZART) have been performed by IRSN in the frame of ISTP [17]. Recent experiments by AEKI on air oxidation of E110 cladding [18] show that a quasi-cyclic growth and breakaway can occur. Figure 2 demonstrates this dynamic character of the breakaway process.

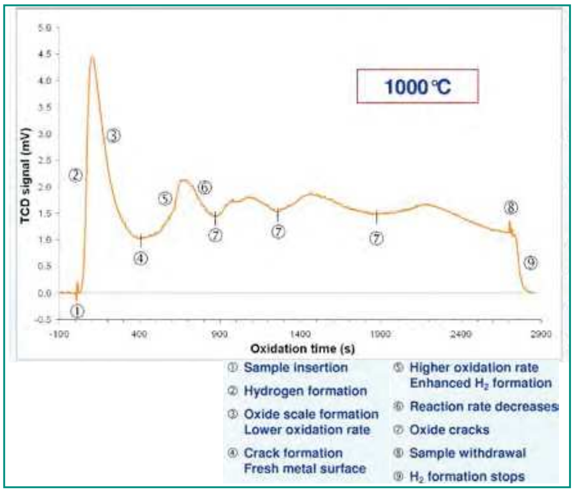


Figure 2: *Cyclic evolution of hydrogen concentration during post-breakaway oxidation [18] of E110 sample at 1000 °C.*

The ITSC PARAMETER air ingress experiment SF4 [19] was conducted during 2009. SF4 was an approximate counterpart to QUENCH-10 [20], 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. Planning support was coordinated between IBRAE Russian Academy of Science, EDF, GRS, Kurchatov Institute, KIT, with PSI as the lead organisation in this effort.

## Model development and assessment in other codes

The status of model development was recently summarised in a paper to ERMSAR2009 [21]. The codes differ in the level of detail, corresponding with their overall philosophy. All the codes consider breakaway effects. Development has continued at a low level of effort during the past year, with the introduction of models for oxidation and nitriding within ATHLET [22] and ICARE/CATHARE [23]. The ATHLET model has been validated against the KIT separate effects tests with pure nitrogen, but a model for nitriding of pre-oxidised cladding has yet to be developed.

The treatment in MAAP4 [24] follows the code's philosophy of fast-running, simplified modelling in keeping with PSA level 2 studies. Linear or parabolic behaviour may be selected for the post-transition behaviour.

An *ad hoc* model for breakaway was developed by SNL based on a Larson-Miller time to failure approach and empirically fitted to the Argonne separate effects test data [25] at temperatures up to 800 °C. It was included as a trial model in MELCOR 1.8.6 and later versions, but there is little published documentation or validation.

## Current status of model development

The model concept, formulation and developmental status were described in some detail in the 2008 report [10]. The model development and testing have been

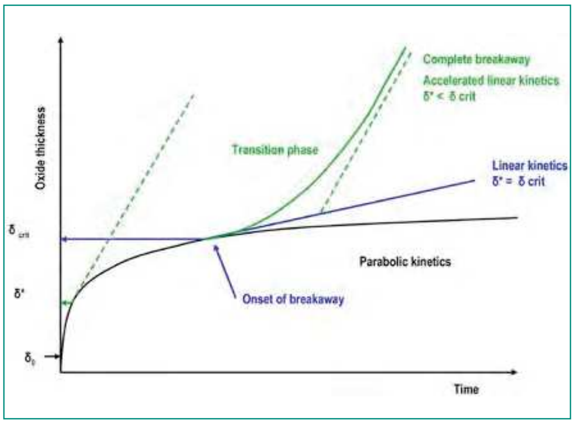


Figure 3: *Schematic of accelerating kinetics during transition to breakaway oxidation.*

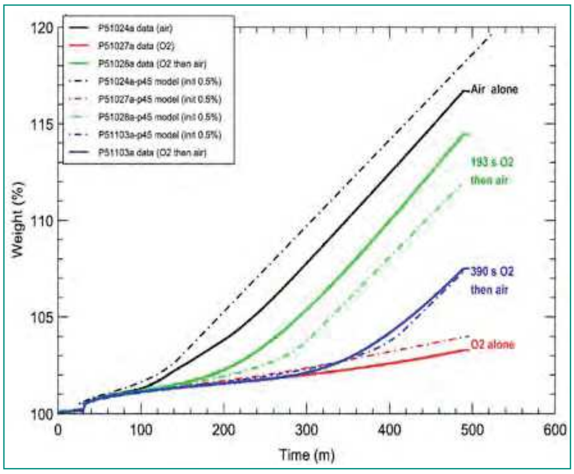


Figure 4: *Comparison of PSI model with KIT test results in oxygen and air (T = 800 °C) [10].*

completed with some modification of the treatment of breakaway. The status was described in a paper presented at a workshop on high temperature behaviour of fuel held in Moscow [26] and at the NRC-led CSARP meeting [27]. 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. The effect of this modification is indicated schematically in figure 3 and enables the observed acceleration to be captured, as shown in figure 4. This seeks to capture the progressive transition demonstrated by the KIT results.

The model is now being implemented in MELCOR. 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 the 2008 progress report it was stated the model would be implemented into MELCOR 2.1 which is still undergoing development. However, the new code version is not yet mature enough to warrant introduction of the new model. In the meantime the model is being implemented into MELCOR 1.8.6, which is likely to remain the target production version for some time. Implementation in MELCOR 2.1 will be performed later, ideally by SNL. It is anticipated that PSI will complete the implementation in MELCOR 1.8.6 in the near future and will participate in the implementation in MELCOR 2.1.

The next stage of validation effort will perform assessments against independent separate effects data from other sources, chiefly IRSN MOZART tests, and integral transient tests, QUENCH-10, PARAMETER SF4, OECD SFP and possibly CODEX AIT. Integral simulations will be performed with full MELCOR code, to give confidence in application to reactor and fuel pond transients.

### Potential model extensions

The separate-effects tests performed at KIT 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 KIT 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 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 5.

At the first meeting of the Programme Review and Management Board of the OECD SFP project, Paris, July 2009, the US NRC promised to provide basic information before the end of 2009 regarding how MELCOR calculations were set up for the BWR cases, in particular how the nodalisation was done.

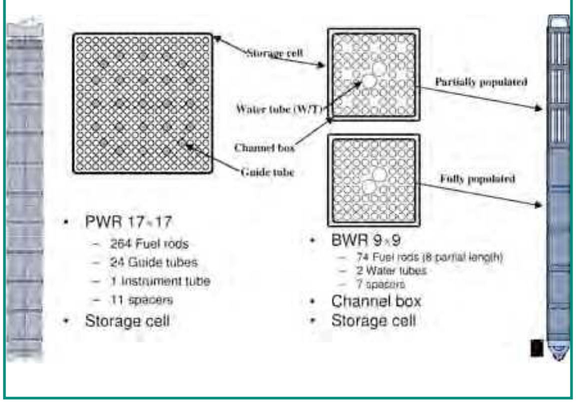


Figure 5: *Schematic of BWR and PWR geometry differences [17].*

## 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 will continue for another 4 years. The provisions of SARNET allow access to the data from the Institute of Nuclear Research Pitesti, Romania (referenced in previous reports), 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 [28] 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 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 2009 and Perspectives for 2010

Progress continued at a low level of effort, concentrating mainly on the implementation into MELCOR. Separate, though closely related effort on planning support to the PARAMETER SF4 air ingress experiment was significant, involving close coordination between several organisations and leading to the successful conduct of a very challenging experiment.

Interpretation of the results of the separate-effects experiments on which the new PSI model is based, especially concerning transition to breakaway has been more difficult than expected. The model exhibits a degree of sensitivity to the exact values used to specify the conditions for onset of breakaway and rate of transition, and this reflects the apparent stochastic nature of the process. This difficulty is worsened in tests at higher temperatures, i.e. above 1200 °C, where a significant oxidation heat results in locally elevated temperatures. Adjustments may be needed when the model is assessed against independent data, including integral experiments.

Concerning implementation into MELCOR, USNRC have indicated [29] that MELCOR 1.8.6 is frozen, while version 2.1 is the current version undergoing beta-testing and subject to minor model development. In any case implementation of a new PSI model will require active cooperation with the USNRC and Sandia National Laboratories to decide on division of the work, testing, documentation, quality assurance and other matters. Thus some negotiation will be needed for implementation to proceed. It is stressed that if the model is to be used in the long term, it is necessary that SNL adopt the model as part of MELCOR 2, and maintain its implementation status.

The OECD SFP project is in the early phase of design work and acquisition of experiment parts. The test plan for Phase 1 on axial heating and fire propagation within a single fuel assembly will be issued by Sandia National Laboratories and commented by the Programme Review Group before 2009. The delivery of the BWR test Final Report, the BWR test data files, including assembly geometry data, possibly also MELCOR input deck, was expected to complete before the end of 2009. The OECD SFP Phase 1 Quick Look Report will be delivered in the second quarter of 2010 and the final Phase 1 Test Report at the end of 2010. The test plan for Phase 2 on radial heating and burn propagation will be issued at the end of 2010. The second Programme Review Group and Management Board meeting was scheduled for the week of 19th of April 2010 at SNL.

## Publications

PSI authored papers concerning modelling of air oxidation of Zircaloy presented at the Moscow workshop on fuel behaviour [26] and the NRC-led CSARP meeting [27]. A detailed contribution was also made to the SARNET final report on corium matters [30], which is now published.

## Nomenclature

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| **AEKI** | Atomergia Kutatotintezet |
| **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 |
| **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 |
| **SARNET** | Severe Accident Research Network |
| **USNRC** | United States Nuclear Regulatory Commission |
| **SFP** | Sandia Fuel Project |
| **VVER** | Vodo-Vodyanoi Energetichesky Reactor (Russian PWR) |

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