ABSTRACT

ASTEC and ICARE/CATHARE computer codes, developed by IRSN (France) (the former with GRS, Germany), are used in RRC KI (Russia) for the analyses of accident transients on VVER-type NPPs. The latest versions of the codes were continuously improved and validated to provide a better understanding of the main processes during hypothetical severe accidents on VVERs.

This paper describes modelling improvements for VVERs carried out recently in the ICARE2 common part of the above codes. These actions concern the important models of fuel rod cladding mechanical behaviour and oxidation in steam at high and very high temperatures. The existing models were improved basing on the experience in the field and latest literature data sources for Zr+1%Nb material used for manufacture of VVERs fuel rod claddings.

Best-fitted correlations for the Zr alloy oxidation through a broad temperature range were established, along with recommendations on model application in clad geometry and starvation conditions. A model for the creep velocity was chosen for the clad mechanical model and some cladding burst criteria were established as a function of temperature.

The verification of modelling improvements was carried out on several types of tests:

- Separate Effect Tests,
- Integral bundle tests: CORA-VVER, QUENCH, CODEX-CT, PARAMETER-SF (the latter performed in the frame of the International Science Technological Centre or ISTC),
- Paks-2 cleaning tank incident (analysis done in the frame of the corresponding OECD/CSNI project).

The comparison of updated code results with experimental data demonstrated very good numerical predictions, which increases the level of code applicability to VVER-type materials.
1 INTRODUCTION

Main models of ASTEC and ICARE/CATHARE computer codes, developed by IRSN (France) (the former with GRS, Germany) were developed to provide analyses of physical processes during hypothetical severe accidents on NPP and primary concerns western type of core elements and materials, such as for instance, Zircaloy-4 (Zry-4) cladding alloys. The latter versions of the codes were continuously improved and validated by RRC KI, Russia, to provide better understanding of the main processes during hypothetical severe accidents on VVERs.

The current paper is devoted to main ICARE2 modeling improvements for VVERs, carried out in 2006-2007 with particular attention to following items:
- Development of best-fitted correlations for Zr1%Nb oxidation database,
- Modelling improvement of the clad mechanical model.

These improvements have been implemented in both above codes since ICARE2 is now the core degradation module of the new series of versions ASTEC V2.

The short description of most important modelling concepts is accompanied by the presentation of verification work that was done on Separate Effect Tests (SETs), integral bundle tests (CORA-VVER, QUENCH, CODEX-CT, PARAMETER), and on the Paks-2 cleaning tank incident simulations. Main attention here is paid to the Paks-2 simulations, based on the ICARE/CATHARE code with VVER modelling improvements, performed in the frame of the technical collaboration between NSI RRC “Kurchatov Institute” (Russia) and IRSN (France) that should be regarded as a common NSI/RRC-KI and IRSN contribution to OECD- IAEA Paks Fuel Project.

2 MODIFICATION OF ZR ALLOY OXIDATION MODEL

Code assessment against in-pile and out-of-pile integral severe fuel damage (SFD) experiments proved the validity of basic modelling principles and provided adequate cross verification of different oxidation “laws” for Zr alloys, expressed by separate experimental groups as sets of parabolic rate coefficients correlations. Basing on the experience of ICARE/CATHARE code assessment [1], it may be concluded that, as a rule, code predictions of transient sequences fairly well agree with experimental data for Zry-4 alloys. The latter ICARE2 modification of oxidation module (see [2]) allowed establishing best-fitted correlations for Zr-4 alloys through all temperature ranges.

An ICARE2 application of widely used Zr1%Nb correlations for VVER safety analyses showed their difficulties with oxygen mass balance at low temperatures and their poor predictions at higher ones (T > 1800 K). At the same time literature sources present alternative data that in some aspects certainly differ from the set of Zr1%Nb oxidation coefficients present in ICARE2 database. Therefore it was decided to improve physical relevance of the ICARE2 modelling (namely the ZROX sub-module) and to provide best-fitted correlations for Zr1%Nb alloys in the whole temperature range (see [3]).

The work consisted in three parts. Firstly, available experimental material was critically reviewed. It was found that reliable experimental data correspond mainly to the low temperature region and to the concerned oxygen uptake by the claddings. The measurements of oxide scale growth can be regarded only qualitatively due to peculiarities of Zr1%Nb alloys and large scattering of experimental results at low temperatures.

Nevertheless some assumptions can be taken about similar properties of oxide scales in Zry-4 and Zr1%Nb oxidation experiments: namely oxide scales for both alloys have the same diffusion coefficients. Such assumption can be confirmed by latest examination of oxide scale composition and absence of lesser constituents of the alloy (see [4]).
The second task was based on physically grounded evaluation of most likely oxidation rates and diffusivities on the basis of available data by well-known methods of diffusion analyses:

- With above assumption about oxide scale, the diffusion analysis method allowed to obtain evaluation of oxide scale growth and oxygen diffusivity in metallic phases at low temperatures;
- Further calculations with the same assumptions concern high temperature region and let to establish a set of oxidation coefficients through all temperature range including transition region from low to high temperatures;
- Oxidation rates increase smoothly within transition to the high temperature range, which started approximately at 1900 K.

Thirdly, the applicability of the considered improvements was demonstrated by assessment against representative high temperature experimental transients. This part of work is based on experiments of two types: transient separate effect tests and bundle VVER tests (see Section below). The conclusion was a good agreement between calculated and measured values on hydrogen production and final oxide thickness.

The next Figures 1 and 2 present the comparisons for oxygen mass gain and oxide scale growth with basic experimental data and Zry-4 values. Best-fitted oxygen mass gain coefficient for Zr1%Nb in Figure 1 quite well agrees with VNIINM (Russia, [5]) and NFI (Czech Republic, [6]) data at low temperatures. At high temperatures (T> 1800 K) VNIINM correlations should be corrected to include the transition region 1800 < T <1900 K and higher oxidation rates at T > 1900 K. Compared to Zry-4 best-fitted correlations [2], Zr1%Nb mass gain rates are lower, as it was observed experimentally.

![Figure 1: Comparison of oxygen mass gain rates](image-url)
3 IMPROVEMENT OF CLAD MECHANICAL BEHAVIOUR MODEL

Modeling of creep velocities

According to previous RRC KI literature research and comparative analyses, creep velocities were investigated by a number of experimental groups from different countries. Some of these groups, apart from experimental measurements, suggested the physical treatment of experimental results basing on specific form of creep velocity equation. A number of literature sources (with the suggested models within the temperature range 823 – 1500 K) were accounted for (see for example [7], [8]).

The comparison of the correlations led to conclude that the modelling approach developed by the first group (called below as MIPhi model [7]) was the better one. The reasons for the choice were the following:

- MIPhi model concerned all three metallic phases and intermediate two-phase region;
- MIPhi model covered the widest temperature range, while the other ones remained valid only in the range of specific experiments and led to large uncertainty out of it;
- Classical form of basic MIPhi model is useful for the implementation into the codes.

In accordance, NSI RRC KI and IRSN jointly decided to improve the physical relevance of the ICARE2 modelling (namely the CREEP sub-module) on the basis of the MIPhi model.

The classical form of creep velocity is defined by specific formulas depending on the temperature range:
\( \alpha - \text{Zr phase (T < 883 K)} \)

\[
\delta \in 9 \div 32 \text{ MPa} \quad \dot{\varepsilon} = 7.1 \cdot 10^5 \cdot \delta^{2.2} \cdot \exp \left( -\frac{28900}{T} \right) \]
\[
\delta \in 32 \div 90 \text{ MPa} \quad \dot{\varepsilon} = 26 \cdot \delta^{3.1} \cdot \exp \left( -\frac{28900}{T} \right) \]
\[
\delta > 90 \text{ MPa} \quad \dot{\varepsilon} = 2 \cdot 10^9 \cdot \exp(0.05 \cdot \delta) \cdot \exp \left( -\frac{28900}{T} \right) \tag{1}
\]

\( \beta - \text{Zr phase (T > 1173 K)} \)

\[
\dot{\varepsilon} \in 1 \div 12 \text{ MPa} \quad \dot{\varepsilon} = 9.1 \cdot 10^{-2} \cdot \delta^{3.5} \cdot \exp \left( -\frac{13200}{T} \right) \]
\[
\delta > 90 \text{ MPa} \quad \dot{\varepsilon} = 7.0 \cdot 10^{-2} \cdot \delta^4 \cdot \exp \left( -\frac{14440}{T} \right) \tag{2}
\]

\( (\alpha + \beta) - \text{phase region (883 < T < 1173 K)} \)

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<th>883&lt;T&lt;1070 K</th>
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**Modelling of cladding burst**

In course of the previous NSI RRC KI research program it was shown that according to available data the dependence of critical burst strain on such parameters as temperature or pressure ramp cannot be established. Therefore a simple criterion was recommended and presented in [4], where critical burst strain depends only on temperature. This true hoop strain at burst \( \delta_b(T) \) was expressed by specific formulas, depending on the cladding irradiation state:

unirradiated
\[
293 < T < 723 \text{ K} \quad \delta_b(T) = 2016.268 - 5.2948 \cdot T + 0.00627 \cdot T^2 - 2.8233 \cdot 10^{-6} \cdot T^3
\]
irradiated
\[
493 < T < 723 \text{ K} \quad \delta_b(T) = 4178.356 - 12.894 \cdot T + 0.0154 \cdot T^2 - 6.5545 \cdot 10^{-6} \cdot T^3 \tag{5}
\]
\[
973 < T < 1190 \text{ K} \quad \delta_b(T) = 1.1614 \cdot 10^5 \cdot \exp(-0.0065753 \cdot T)
\]
\[
1190 < T > 1493 \text{ K} \quad \delta_b(T) = 7.612 \cdot 10^3 \cdot \exp(-0.004283 \cdot T)
\]

An additional new feature of Zr1%Nb mechanical behaviour was also implemented into ICARE2 modelling to cover the case when radial deformation can spread through the entire domain between fuel rods. Such situation is realized when some condition for outside cladding radius is realized:

\[ \ln(r/r_0) > EP \quad \text{(user-defined parameter, default value of 0.45)} \] \tag{6}

Afterwards only the ballooning of the cladding is stopped in simulations. At the same time the internal pressure can be further changed (increased), so that burst conditions possibly will be satisfied later. The option can be useful to model close to full blockage areas, which seems to be characteristic for Zr1%Nb claddings with much larger deformations than in case of Zry-4. An application of this option is shown below for the simulation of Paks-2 incident.

Proceedings of the International Conference Nuclear Energy for New Europe, Bled, Slovenia, Sept. 14-17, 2009
4 VERIFICATION OF MODELLING IMPROVEMENTS

The improvements of Zr1%Nb oxidation and mechanical behaviour ICARE2 models were verified against several types of tests and showed very good agreement with experimental measurements. The following tests were used for verification:

- Separate Effect Tests (see, for example [9]);
- Integral bundle tests (see, for example [10]);
- Paks-2 cleaning tank incident that occurred in April 2003 at Paks NPP (Hungary) (severe damage of 30 fuel assemblies after tank dry out due to incorrect positioning of several assemblies, the ICARE/CATHARE analysis was carried out in the frame of the corresponding OECD/CSNI project, see [11]).

The next Figures 3 and 4 present the main results of Paks-2 incident simulation.

Figure 3: Simulation of Paks-2 fuel rod cladding evolution

Figure 4: Final axial distributions of main SFD parameters in Paks-2 Zr1%Nb claddings
The comparison of different ICARE/CATHARE calculations revealed an essential influence of Zr cladding creep and oxidation modelling on the whole accident transient. The effect is obviously a consequence of Zr oxidation enhancement with the substantial increase of oxidation surface (see Figure 4). Comparison of two code calculations with CREEP module (for Zry-4 and Zr1%Nb) shows that the simulation with new model of Zr1%Nb properties leads to results that differ from Zry-4 ones in following aspects:

- Earlier beginning of temperature escalation;
- Higher temperatures of the fuel rod claddings and assemblies;
- Shift of maximum of cladding oxidation to higher elevations;
- Substantial delay of cladding burst.

The latter item seems the most essential as it allows direct comparison with observation during the transient: the release of fission product gases started approximately in the facility at 18600 seconds, which was considered as first instant of fuel rod cladding burst. The Zr1%Nb choice for alloy type in the modified ICARE2 code leads to the instant 18767 seconds (see Figure 3), which is quite compatible with available observations.

All simulated peculiarities of Zr1%Nb mechanical behaviour with respect to Zry-4 can be explained accounting their main characteristics, such as higher creep velocities (at fuel rod gap pressures more than 1 atm and temperatures more than 1000 K) and higher maximum hoop strain. Due to relatively short period of cladding ballooning, the latter characteristic seems the most important for further applications.

5 CONCLUSIONS

The following general conclusions can be drawn from IRSN/RRC KI activity on ICARE2 modelling improvements for VVERs.

Zr1%Nb oxidation database improvement

- The uncertainty in predictions of Zr1%Nb oxidation rates is substantially decreased with application of new best-fitted correlations for Zr1%Nb oxidation;
- The verification of evaluated parabolic correlations showed their applicability to different types of accident transients (CORA-VVER, QUENCH-12, etc.).

Mechanical modelling improvement

- The modification of CREEP module allowed to properly account for the specificity in Zr1%Nb cladding ballooning and burst;
- The verification against Separate-Effect-Tests generally agrees with the experiments within the range of experimental errors;
- Compared to Zircaloy cladding:
  - the Zr1%Nb cladding experiences burst at higher hoop strain (up to 150%),
  - as a rule the creep velocity of Zr1%Nb cladding is higher than the Zry-4 one.

Application to Paks-2 incident

- It revealed the peculiarity of application of updated CREEP model with substantial influence of mechanical behaviour model on transient and cladding ballooning up to inter-rods dimensions;
- It showed the difference in predictions between Zr1%Nb and Zry-4:
  - earlier beginning of temperature escalation,
  - higher temperatures of the fuel rod claddings and assemblies,
  - shift of cladding oxidation maximum to lower elevations,
  - substantial delay of cladding burst.
- The analysis was confirmed by direct comparison with observations during the transient, when new Zr1%Nb model predicts the time of first fission product release within an error lower than 1% (less than 200s.).
In summary, knowing that, beyond its classical use in ICARE/CATHARE, the ICARE2 mechanistic code is now also used as core degradation module in the new series of ASTEC versions, the new ICARE2 modeling updates for VVERs can be therefore recommended for VVER simulations with both ASTEC V2 and ICARE/CATHARE V2 in a wide range of accidents scenarios. In that frame, the report [12] presents a simulation of one of full range accident scenarios for VVER-1000 large break LOCA with the two codes.

REFERENCES


