Transactions of the **13th International Conference on Structural Mechanics in Reactor Technology** (SMiRT 13), Escola de Engenharia - Universidade Federal do Rio Grande do Sul, Porto Alegre, Brazil, August 13-18, 1995

Code package SVECHA: Modelling of core degradation phenomena

Veshchunov, M.S., Palagin, A.V., Volchek, A.M., Yamshchikov, N.V., Boldyrev, A.V.
Nuclear Safety Institute, Russian Academy of Sciences, Moscow, Russia

ABSTRACT: The code package SVECHA for the modelling of in-vessel core degradation (CD) phenomena at severe accidents is developed in the Nuclear Safety Institute, Russian Academy of Sciences (NSI RAS). This program package is characterized by the development of detailed physical theory of key processes. The code package SVECHA serves as the basis for the development of mechanistic code SVECHA, which being coupled with thermohydraulic code (also being developed in the NSI RAS) will form a new detailed mechanistic code for the description of severe accidents at nuclear power plants.

1 INTRODUCTION

A recent OECD/CSNI state-of-the-art report (SOAR) (In-Vessel... 1991) on in-vessel core degradation concluded that although the experimental data base and models are adequate in some areas, there are still substantial gaps. This was confirmed by the results of two recent OECD International Standard Problems: ISP 28 (PHEBUS B9 test) and ISP 31 (CORA-13 test). The inadequacies of models being quite common for the majority of existing codes have been recently formulated for SCDAP/RELAP5 code in the Independent Peer Review (1994) and can be summarized shortly as following:

1. Mechanistic models are not included to account for effects of internal pressure, effects of oxidation in strengthening the cladding, effects of oxide cracks in oxidation kinetics, description of oxide-shell failure and mechanistic description of breach formation;
2. The *Zr-U-O* mixture relocation is based on a gravity driven mixture, slug-ring flow. Rivulet, rather than slug flow has been established experimentally;
3. The possibility of melt running down inside the balloon rather than forming a crust on the outer surface ("gap candling") is not considered;
4. There is no proper coupling between the models for the reactions between *Zry*/steam (outside of the cladding) and UO_2 /*Zry* (inside);
5. Additional Zr oxidation during *Zr-U-O* relocation is not modeled;
6. The current models for control rods and spacer grids material interactions are absent or oversimplified.

To avoid such kind of discrepancies more physically grounded approach for the description of CD phenomena is being developed in NSI RAS. The main features of this approach can be shortly characterized as following:

1. Development of detailed physical theory of key processes for the analysis of experimental data;
2. Investigation of qualitatively new physical phenomena occurred in accident conditions on the basis of developed theory;

3. Recommendations for arrangement of additional experiments (or examinations of existing samples) aimed on the revealing of the required details or data collections;
4. Development of code modules on the basis of physically grounded simplifications of the theoretical models;
5. Development of new mathematical methods which allow to implement more sophisticated physical models in the codes;
6. Verification of the modules against separate-effect tests; implementation of the new modules in different integral codes;
8. Benchmarking and sensitivity calculations against integral experiments and comparison with other code systems; analysis of the test results and improvement of the models and codes.

Such an approach increases the predictive power of the qualitative analysis of the complex system behavior and reduces the ambiguity gap in the quantitative results.

The following models are currently under investigation:

1.Fuel - Cladding Oxidation.
2.Dissolution of UO_2 by Molten Zircaloy.
3.Fuel - Cladding Deformation.
4.Relocation of Molten Materials (Candling).
5.Eutectic Interactions and Liquid Phase Formation.

On the basis of these models FORTRAN modules, ready for implementation in different CD codes, are developed. Up-to-now some of the developed modules have been implemented into ICARE2 code (France) and demonstrated satisfactory description of integral Severe Fuel Damage (SFD) tests. Implementation of the modules into the codes ATHLET (Germany) and SCDAP (USA) has been started recently.

2 FUEL - CLADDING OXIDATION

The progress of a severe accident is strongly influenced by the *Zr*/steam and *Zr*/fuel reactions. The former produces significant additional heat and hydrogen. The temperature of the core may as result rise sufficiently for remaining unoxidized *Zr* to melt. This liquefied cladding can dissolve a substantial quantity of fuel, forming an eutectic, which may then relocate downwards. Two different approaches for modeling of pellet-cladding oxidation were used previously:

1. Simulation of the oxidation processes by the parabolic law for growth of different layers width.
2. Physical modeling, using diffusion equations of oxygen in different layers and mass balance conditions on the interphase boundaries.

An advantage of the first approach is its simplicity and quick calculation. However, it works well in the simplified isothermal conditions, and is valid for unlimited steam supply and semi-infinite *Zr* substrate. Problems of physical consistency arise if the approach is used directly to model complete oxidation of finite-thickness fuel clad and under possible steam-starved conditions. Calculations demonstrate that in the transient temperature regime this approach fails as well.

The second approach (e.g. code PECLOX) is much better physically grounded and provides better agreement with experiment. A serious disadvantage of this approach for numerical realization is connected with large computation time and memory consumption.

2.1 *Physical model*

The proposed model (Volchek 1993) is free from the disadvantages of these two approaches. This model is based on the solution of the oxygen diffusion equation in the multilayred structure (up to 7 different layers) of different phases formed in the course of the UO_2 /*Zr*/steam interactions. PDE describing real diffusion processes are reduced

to ODE. This mathematical procedure is well physically grounded. The proposed model being rather accurate and simple, allow to take into account the following physical phenomena, occurred in the course of UO_2 /Zr/steam interactions and not accounted in the framework of the correlation approach:

1. Coupling of *Zr*/steam (outside) and Zr/UO_2 (inside) interactions;
2. Cladding internal oxidation;
3. "Chemical thinning" (and even complete disappearance) of the oxide layer in the conditions of limiting steam supply ("starvation");
4. Tetragonal-to-cubic phase transition in ZrO_2 at transient temperature regimes;
5. Oxidation of *Zr-U-O* mixture during relocation.

Currently the model is coupled with "FUEL-CLADDING DEFORMATION" model (described in section4); this allows to account selfconsistently:

6. Effects of strengtening the cladding due to oxidation;
7. Effects of oxide cracks in oxidation kinetics.

2.2 *Numerical module, verification and applications*

On the basis of this model FORTRAN module is developed. Proposed mathematical procedure leads to a great simplification of calculations, which become comparable (in computation time and memory consumption) with empirical correlation approach. The accuracy of these calculations is rather high and comparable with more sophisticated and time consuming methods (i.e. PECLOX code).

A number of verification tests performed on the base of P.Hofmann's experiments for transient temperature conditions which can be described selfconsistently by the present module coupled with "FUEL-CLADDING DEFORMATION" module (section 4) only with account of oxide cracks effects.

The simplicity, relatively high degree of accuracy and fast running of developed module allows to implement it in different code systems. The module has been implemented into ICARE2 computer code (France) and validated against integral SFD tests CORA-13 and PHEBUS B9+. Currently implementation of the module into codes ATHLET (FRG) and SCDAP (USA) is in development.

3 DISSOLUTION OF *UO2* BY MOLTEN ZIRCALOY

Dissolution of UO_2 by molten Zircaloy is an important chemical process influencing many physico-cheemical processes during core melt progression in severe accidents. Once as-received Zircaloy cladding starts to melt at about 1760C, the interaction between solid UO_2 and molten *Zr* becomes more active and leads to a partial dissolution of fuel in the liquid phase. Therefore, liquefaction and relocation of UO_2 must be assumed about 1000~K below the melting point of the fuel (2850C). This limits the possibility of stopping the high-temperature transient before an uncontrolled core meltdown occurs and has a strong impact on fission product release.

Theoretical study of this complicated phenomena is carried out (Veshchunov 1990, Veshchunov and Volchek 1992). It is demonstrated that depending on dimensions of molten cladding part two different mass transfer mechanisms through the liquid phase can take place. Correspondingly, two different models for dissolution process are proposed: diffusion and convective.

3.1 *Diffusion model*

The diffusion model describes dissolution kinetics on the basis of diffusion mass transfer equations in the phases with account of an appearance and growth of two-phase (solid and liquid) region at the boundary between solid UO_2 and liquid (Zr,U,O) phases. It is

shown analytically that diffusion mass transfer through this two-phase region can be described by effective (temperature-dependent) diffusion coefficient. Its value estimated from measurements turns to be several orders of magnitude smaller than corresponding value in pure liquid phase and, thus, determines the rate of dissolution process.

3.2 *Convective model*

The convective model, developed by Veshchunov and Hofmann (1994a), describes dissolution kinetics on the basis of convective mass transfer equation in the liquid phase and diffusion equation in the solid UO_2.

The results of different experiments (P.Hofmann, D.Olander, P.Hayward) performed in conditions of convective mixing of molten Zircaloy inside UO_2 crucibles, are rather controversial and, thus, do not allow to choose unambiguously an empirical kinetic correlation which could be used in numerical simulations. The proposed convective model resolves the apparent discrepancy between the empirical results of different groups and provides practical recommendations for application of measured correlations for fuel rods, resulted in a certain renormalization (by a factor 2.5 for Hofmann's correlation) of UO_2 issolution rate, measured in crucibles.

The model self consistently describes both stages of dissolution process, observed experimentally: incubation, or saturation (exponential rate), and post-incubation, or precipitation (parabolic rate). It shows that a rather quick saturation of the liquid phase due to UO_2 dissolution is reached at the first (incubation) stage, and after that, a more slow dissolution process, accompanied by precipitation of ceramic phase and described by parabolic time law takes place. It resolves the discrepancy of existing codes, in which Hofmann's or Olander's parabolic correlation are used for the description of incubation (exponential!) stage, at which saturation is reached, instead of post-incubation stage which should be described by renormalized parabolic correlation.

Currently general model for simultaneous dissolution of UO_2 and ZrO_2 by molten Zr in oxidizing atmosphere is in development. It is demonstrated that in coditions of convective mixing of the melt, an additional supply of oxygen to the melt from ZrO_2 and dissolution of this layer change the kinetics of UO_2 dissolution process significantly.

3.3 *Numerical module, verification and applications*

FORTRAN module is developed on the basis of the diffusion model. It is coupled with Fuel-Cladding Oxidation module and describes simultaneous dissolution of ZrO_2 pellets and ZrO_2 layer, which is competitive with Zr oxidation process. FORTRAN module based on the proposed convective model is currently in development.

Benchmarking calculations for the diffusion model were performed against D.Olander's measurements in special conditions (provided diffusion mass transfer through the liquid phase: experiment with UO_2 disk) and demonstrated satisfactory agreement with experimental data.

The developed diffusion module is implemented in ICARE2 code and validation studies against integral tests are in development.

4 FUEL CLADDING DEFORMATION

Once liquid *U-Zr-O* eutectic has formed, it is assumed to be held in place by the oxide crust until this crust fails. The position and timing of the oxide layer breach depending on the thickness and mechanical properties of this layer are calculated by fuel cladding deformation model. This model also describes the reduction in flow area and the increase in cladding surface area available for oxidation due to ballooning and oxide shell

cracking and is disscused in detailes in the report "Mechanical behavior simulation of oxidized fuel cladding" presented at this Conference (Division C).

On the base of this model computer program in FORTRAN 77 is carried out. This program is coupled with Fuel-Cladding Oxidation module and allows to take into account an influence of cladding geometry change and oxide layer cracking on oxidation kinetics.

The module was implemented into ICARE2 computer code (France) and validated against integral SFD tests CORA-13 and PHEBUS B9+. The implementation into SCDAP code is in development.

5 RELOCATION OF MOLTEN MATERIALS (CANDLING)

Once the clad oxide is breached, the process of relocation of materials (downward flow of ceramic melts and liquefied eutectic mixtures) begins. As the mixture flows, it will affect the heat transfer, possibly causing the formation of frozen track. The influence of this process upon the global core behavior during the accident is conditioned by the fact that it results in a change of flow cross sections or a blockage of the cooling channels, further fuel rod heatup and extended core degradation.

In the existing codes the description of the candling process is usually based on the assumption of one-dimensional axysimmetrical film flowing down. The SVECHA candling model dealing with droplike and rivulet flows is described in detailes in the report "SVECHA Candling model for Melt Relocation Process" presented at this Conference (Division C).

On the base of this model computer program in FORTRAN 77 is carried out. Detailed physical consideration of the candling process allows to determine the characteristic size of the liquid elements and thus to decrease sufficiently the dependence of the results of calculation on the nodalization scheme.

A number of verification tests performed on the basis of integral SFD tests CORA-13 shows good agreement with experimentally measured blockage distributions along the fuel rod.

The module has been implemented into ICARE2 computer code (France) and validated against integral SFD tests CORA-13 and PHEBUS B9+. The implementation into SCDAP code is in development.

6 EUTECTIC INTERACTIONS AND LIQUID PHASE FORMATION

Models for physico-chemical interactions between more important core components: *Zr*/stainless steel (SS); *Zr/(Ag,In,Cd)*; *Zr*/Inconel; *Zry*/B_4C; SS/B_4C are currently under investigation. All of these reaction pairs have relatively low eutectic temperatures and, therefore, their interactions are of concern in a severe accident, since relocation of the resulting fragments or melts and formation of local blockages cause further heatup of the core. Separate-effect tests have been performed in different laboratories (KfK, Germany; JAERI, Japan; KI, Russia) in parallel to the integral out-of-pile and in-pile experiments and serve to explain the complex material interactions in the integral tests and the TMI-2 accident by the resulting multi-phase system at room temperature.

New physical models are developed for the description of interaction kinetics measured in these separate-effect tests. A new approach for theoretical study of diffusion processes in multi-component and multi-phase reaction zones, observed experimentally is developed (Veshchunov and Hofmann 1994b). On the base of the proposed theory experimental data obtained by different groups are compared and revised. The models being based on first-principle equations are well physically grounded and, thus, can be used for the description of material interactions in complex transient (accident) conditions.

FORTRAN modules based on the proposed model are currently in development.

REFERENCES

In-Vessel Core Degradation in LWR Severe Accidents: A State of the Art Report to CSNI, January1991, NEA/CSNI/R(91)12.

SCDAP/RELAP5 Independent Peer Review, 1994, Los Alamos National Laboratory, LA-12481.

Veshchunov, M.S.1990. On the kinetics of UO2 interaction with Zircaloy at high temperatures. *J.Nucl.Mater.*, 174: 72-75.

Veshchunov, M.S.& P.Hofmann 1994a. Dissolution of solid UO2 by molten Zircaloy, *J.Nucl.Mater.* 209: 27-40.

Veshchunov, M.S.& P.Hofmann 1994b. Modeling ob B4C interaction with Zircaloy at high temperatures, *J.Nucl.Mater.*,210: 11-20

Veshchunov, M.S. & A.M.Volchek 1992. On the kinetics of UO2 interaction with molten Zircaloy at high temperatures. *J.Nucl.Mater.*, 188:177-182.

Volchek, A.M. 1993. On the modeling of the PELLET/CLADDING/STEAM interactions in the framework of the oxygen diffusion theory", Preprint NSI-13-93.