ASSESSMENT OF THE REFLOOD OXIDATION MODELS IN SCDAP/RELAP5/MOD3.1[a]

J. K. Hohorst
C. M. Allison

Idaho National Engineering Laboratory
Applied Engineering Development Laboratory
Lockheed Idaho Technologies Company
Idaho Falls, Idaho 83415

Presented at the RELAP5 International Users Seminar
Le Meridien Hotel
Dallas, Texas
March 17-21, 1996

Abstract

Reflooding of a hot damaged core following the start of a severe accident can lead to significant increases in the heating, melting, and oxidation of the core prior to the termination of the accident. These effects have been observed in bundle heating and melting experiments terminated by the addition of water and are postulated to have had a major impact on the accident progression in the TMI-2 accident. Although the detailed mechanisms for these processes are not completely understood, new SCDAP/RELAP5/MOD3.1e models, describing the cracking/spalling of oxidized fuel rod cladding during reflood, and the resulting oxidation of the underlying Zircaloy and relocating liquefied U-Zr-O, provide a reasonable estimate of the experimentally-observed bundle temperatures, hydrogen production, and changes in bundle geometry.

This paper provides a brief description of the new models, selected highlights from code-to-data comparisons, and selected results from a recent set of calculations for TMI-2 using the new models. The potential impact of these new models on other plant calculations is discussed in the concluding portion of this paper.

Introduction

Reflooding of a hot damaged core following the start of a severe accident can lead to significant increases in the heating, melting, and oxidation of the core prior to the termination of the accident. These effects have been observed in fuel bundle heating and melting experiments terminated by the addition of water. The experiments indicate that the transition to accelerated heating occurs when the peak bundle temperature exceeds 1500 K. If reflood occurs when bundle temperatures range between 1500 to 2100 K, the accelerated heating of fuel rods results in limited melting of the fuel rod cladding and the associated flow restriction in portions of the bundle. In this case, the combination of oxidized cladding and rapid cooling can result in the fragmentation of a portion of the fuel and cladding material. If the peak bundle temperatures are above 2100 K when cooling water is added to the hot core region, the accelerated heating and oxidation can lead to increased melting and the formation of a non-coolable cohesive debris bed and molten pool. This is the situation that has occurred in the larger experiments. In addition, this is the process that is predicted to have occurred in early stages of the TMI-2 accident.

Unfortunately, early models of fuel rod cladding oxidation could not predict this behavior. For example, in the OECD International Standard Problem -31 using the CORA-13 experiment performed in 1990[3], none of the participating codes including SCDAP/RELAP5, MELCOR, ICARE, and ATHLET were able to predict the sharp increases in bundle temperature, hydrogen production, and melting occurring during the reflood phase of that experiment. At this time, these codes used standard correlations for Zircaloy oxidation including Cathcart-Pawell[4] and Urbanic-Heidrick[5]. Since that time there has been a substantial effort involved in developing new models to treat this process. In addition, new experimental programs such as the Quench program in Germany[6] have been instituted to help assess those new models. For SCDAP/RELAP5, these new models have been introduced in two different stages[7,8,9]. First, new models describing the spalling or cracking of the protective oxide films during reflood were introduced in SCDAP/RELAP5/MOD3.1. This change moved the total hydrogen production for reflood experiments to within a factor of two. (By contrast, earlier versions of SCDAP/RELAP5 under predicted the total hydrogen production in reflood experiments by nearly a factor of 5. However they were able to accurately predict hydrogen production in experiments without reflood within $\pm$ 20 %[10]) Then, new models describing the oxidation of liquefied fuel rod material, were introduced into SCDAP/RELAP/MOD3.1e. As discussed in this paper, this

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

additional model appears to accurately predict hydrogen production during reflood as well as the temperature increase and melting during this phase of an accident or simulated accident.

This paper provides a brief description of the new models, selected highlights from code-to-data comparisons, and selected results from a recent set of calculations for TMI-2 using the new models. The potential impact of these new models on other plant calculations is discussed in the concluding portion of this paper.

Reflood Oxidation Models

As noted in the introduction the new models that describe the accelerated oxidation during reflood have been introduced into SCDAP/RELAP5/MOD3.1 in two steps. The initial version of SCDAP/RELAP5/MOD3.1, which was released in 1994, contained two bounding correlational-based models to treat the cracking of the oxidized fuel rod cladding. One model, a local model, assumed the protective oxide layer would crack at a given elevation when oxidation-embrittled Zircaloy cladding cooled rapidly to a temperature between 1150 to 1560 K. The other model, a global model, assumed the protective oxide layer would crack over the full height of the fuel rod cladding as soon as water was added. In both cases, enhanced oxidation and heating then occurred due to the oxidation of the hot Zircaloy layer exposed by the cracking of the protective oxide. Mass diffusion of steam to the surface of the cladding was the oxidation-rate limiting process once the oxide was cracked. The flooding rates and heat transfer during the reflood process were described using standard RELAP5 thermal-hydraulic constitutive models.

After a systematic assessment of these models, an additional model was then added to MOD3.1 to treat the oxidation of the liquefied U-Zr-O moving down the outer surface of the fuel rod cladding. During reflood, molten U-Zr-O is formed during the initial increase in temperature resulting from the oxidation of the hot Zircaloy layer exposed by oxide cracking. This model, based upon the observation of U-Zr-O rivulet and droplet flows in bundle heating and melting experiments, describes the motion of droplets of liquefied U-Zr-O and the resulting oxidation of those drops as shown in Figure 1. As indicated in this figure, the droplets and rivulets of liquefied U-Zr-O are represented as a series of hemispherical droplets relocating down the outer surface of the cladding. The heat transfer between the droplet, coolant, and underlying cladding and fuel and the oxidation of the droplet are considered by the new model.
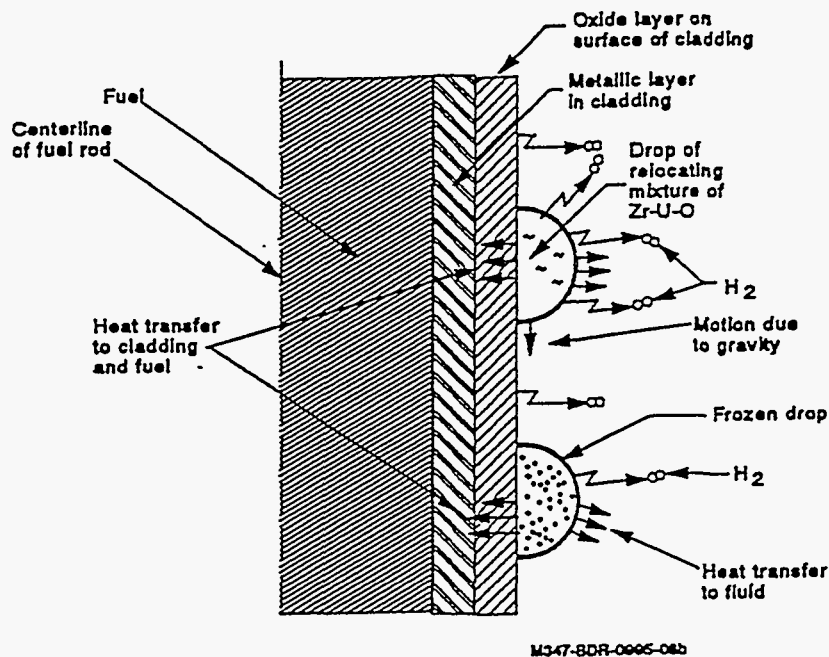
Figure 1 - MOD3.1e U-Zr-O droplet oxidation model.

Highlights of Code-to-Data Comparisons

The assessment of the new reflood oxidation models included the analysis of four experiments from tests performed in the CORA facility (CORA experiments) in Germany[11,12] and the Power Burst Facility (Severe Fuel Damage, SFD, experiments) in the United States[13]. The comparisons included (a) both electrically heated and nuclear heated experiments; (b) bundles with fuel rods only, fuel rod bundles with Ag-In-Cd control rod structures, and fuel bundles with BWR control blade/channel box structures; and (c) initial heating rates varying from 0.5 to 1.0 K/s; (d) peak bundle temperatures between 2100 to 2900 K. The specific features of these experiments are described in the Appendix.

The overall calculated temperature response and heating rates of the experiments are consistent with the measured temperatures in the experiments.

In most cases, peak bundle temperatures were not measured directly because of the failure of bundle thermocouples in the hottest regions of the bundles. In these experiments, peak temperatures were inferred from post-test metallurgical examinations in combination with the extrapolation of surviving thermocouples in cooler regions of the bundles. One example taken from comparisons with the CORA-17 experiment is shown in Figure 2. This experiment used a combination of electrically heated fuel rod simulators, fuel rods, and BWR control blade/channel box structures[12]. As indicated in the figure, this experiment is terminated by the reflooding of the bundle. The figure shows the calculated and measured temperatures at three elevations. All of thermocouples at these elevations fail near the end of the initial heating and melting phase of the experiments. However, as shown in the figure, thermocouples in cooler regions are consistent with the calculated temperature response of the bundle. In addition, this figure also shows the sharp increase in the bundle temperature resulting from the start of bundle reflood. The bundle had started to cool prior to reflood due to the termination of electrical heating. The calculated temperature spikes show the same trend. These spikes were not predicted with previous versions of the code.
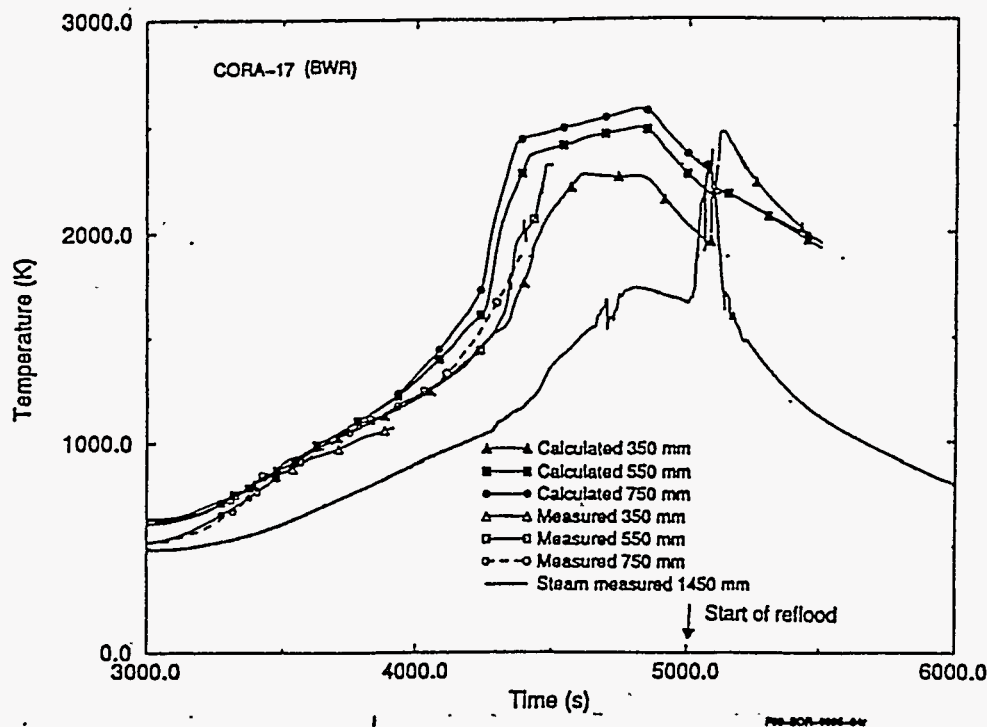

Figure 2. Calculated and measured bundle temperature for the CORA-17 BWR experiment.

A similar trend was observed for the CORA-13 experiment[11]. This experiment also used electrically heated fuel rod simulators but had a PWR Ag-In-Cd control rod and Zircaloy guide tube rather than the BWR structures used in CORA-17. Figures 3 and 4 show the calculated and measured temperatures in the bundle during the entire experiment and an enlarged scale immediately before and during reflood. The thermocouples at the 550 and 750 mm elevations had failed previously so a thermocouple in a cooler region above the bundle is shown for comparison to the calculated temperatures in the hot region of the bundle. This figure shows a comparison where the MOD3.1e U-Zr-O droplet oxidation model is either included or not included, indicating that the new model plays an important role in the ability to predict the continued heating of the bundle even though the electrical heating of the bundle was terminated prior to reflood.
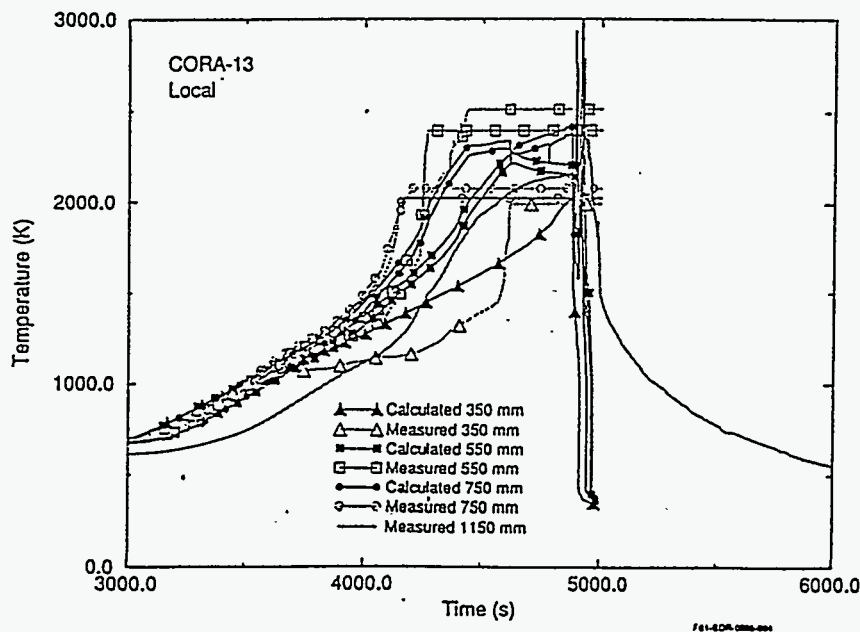

Figure 3 - Calculated and measured bundle temperatures for the CORA-13 PWR experiment.
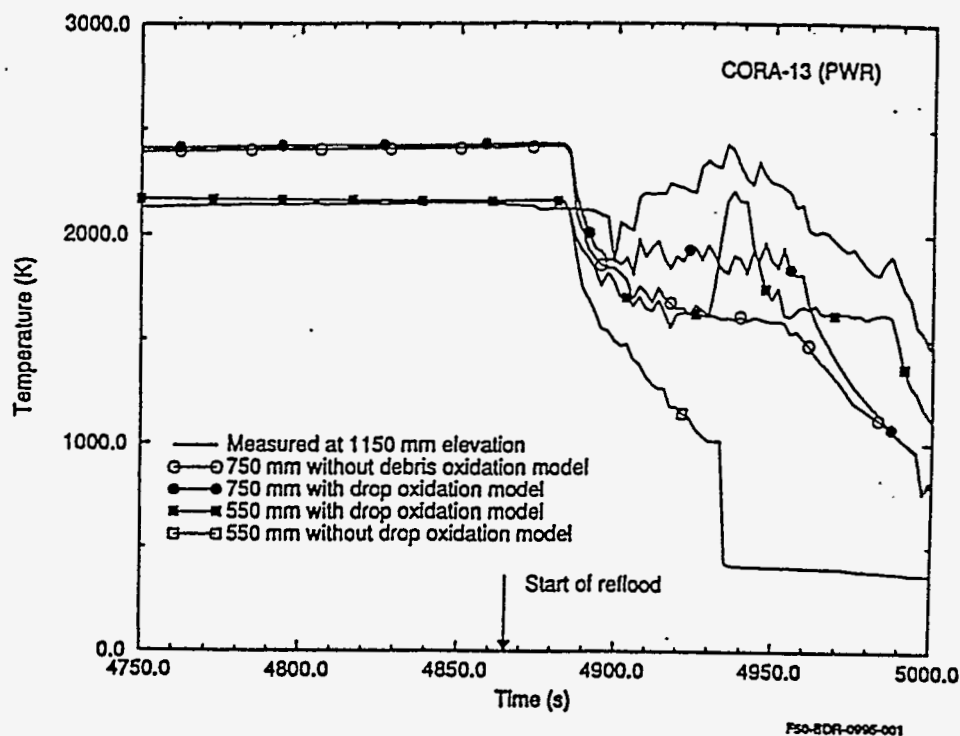
Figure 4. Calculated and measured bundle temperatures during the reflood phase of the CORA-13 PWR experiment.

The predicted total hydrogen production for these experiments was significantly improved by the addition of the new oxidation models. Even though the introduction of the ZrO_2 oxide cracking models into MOD3.1 eliminated much of the variation between calculated and measured hydrogen production for several reflood experiments, the calculated total hydrogen production rates were still consistently below those measured in the experiments[2]. However, with the addition of the MOD3.1e U-Zr-O droplet oxidation model, that systematic bias was eliminated. For example, in the CORA-13 experiment, the total hydrogen calculated for MOD3.1 was 77 g while MOD3.1e calculated 222 g. The measured value was 210 g. For SFD-ST, the measured value was 172±40 g; MOD3.1e calculated 146 g. The MOD3.1 predicted value was 81 g. For these two experiments the discrepancy between calculated and measured total hydrogen for MOD3.1e is now well within the estimated experimental uncertainty in the measurement. The calculated values are between +6% to -15% of the measured values. For comparison, for SFD-ST where an error estimate is provided, the experimental uncertainty is ±23%.

The one notable outlier in the code-to-data comparison was the CORA-17 experiment, the only BWR bundle experiment that included reflood. In this case, the predicted total hydrogen production was still below that measured. The measured value was 150 g, while the predicted value was only 63 g. Although the exact cause for this discrepancy has not yet been established, the experimentalists[11] attribute much of the total hydrogen production to the oxidation of the B_4C. Although the MOD3.1e BWR control blade/channel box

model considers the oxidation of the B_4C, stainless steel, and Zircaloy, there are no specific models which address the possible cracking of the protective oxides or the fragmentation of these structures during reflood.

Applications of the New Models to TMI-2

Although SCDAP/RELAP5/MOD3.1 was able to predict many of the important trends associated with the accident at TMI-2[14], there were two areas where the calculations appeared to be deficient. First, the system pressure response after 125 minutes was underpredicted. This period included the initial heatup and melting of the core and the partial reflood during the B-pump transient at 174 minutes. Second, the molten pool formed in the core did not spread all of the way to the core former wall prior to the operation of the High Pressure Injection system and the complete reflooding of the core. As a result, the molten pool did not drain through the former wall into the lower plenum. Although these deficiencies could be partially attributed to the uncertainties in the thermal-hydraulic boundary conditions, it appeared that both deficiencies could be related to the underprediction of the oxidation and heat generation during reflood. Thus, the application of the new reflood models to TMI-2 appeared to be a good way to test this theory.

Representative MOD3.1e calculated results are shown in Figures 5-7 for the set of calculations that gave the best overall agreement with the pressure response during the B-pump transient. Figure 5 shows the calculated and measured pressure response. Figure 6 shows the predicted collapsed water level, while Figure 7 shows the peak core temperatures. The pressure history between 125 minutes and 174 minutes is still underpredicted. However, this trend appears to be related to the uncertainties in the heat removal to the secondary and the manner in which the steam generators are being modeled rather than the uncertainties in initial core heatup and melting. Sensitivity studies on the water level to account for the uncertainties in core make up flows resulted in some variations in the pressure during this period but resulted in totally unrealistic core temperatures and damage histories in the most extreme cases.

A comparison between the MOD3.1e and earlier MOD3.1 indicated that the MOD3.1e predicted slightly lower pressures during the initial heating and melting of the core and a significantly higher pressure during the B-pump transient as shown in Figure 8. The pressure difference show on this figure is the MOD3.1e calculated pressure minus the MOD3.1 calculated pressure. MOD3.1e predicted a pressure increase within 1 MPa of the measured data during the 2B-pump transient and the release of 440 Kg hydrogen up through this period. MOD3.1e also predicted more hydrogen than did MOD3.1, approximately 3% more prior to the B-pump transient and more than double during the transient itself. This increase is due to a longer period of sustained oxidation and hotter temperatures in the central core region. As a result, MOD3.1e predicts that the molten pool created through the end of the B-pump transient is more than a factor of two larger than that predicted by MOD3.1.
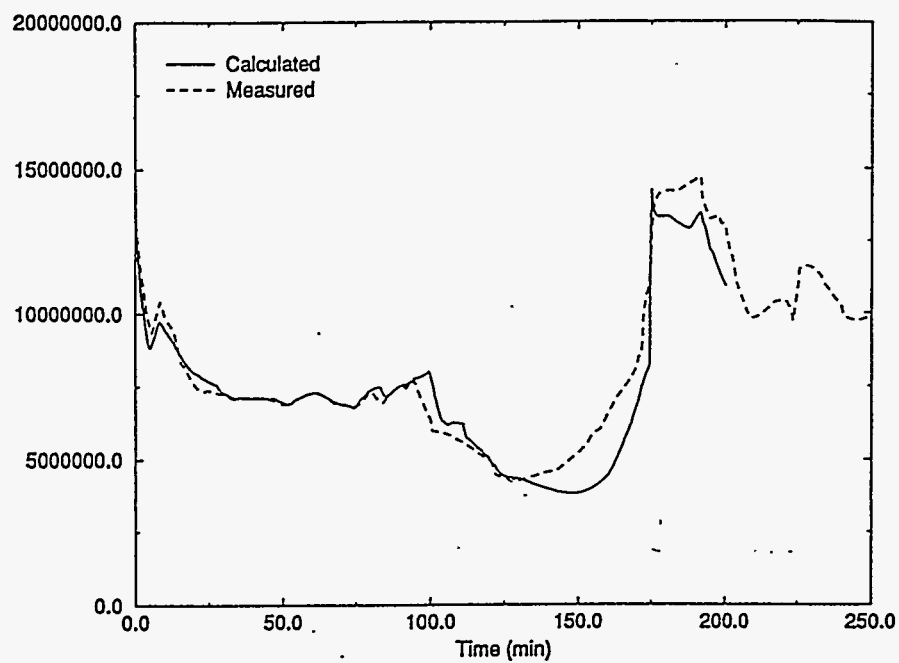
Figure 5. Best estimated MOD3.1e calculated system pressure compared to the measured TMI-2 pressure.
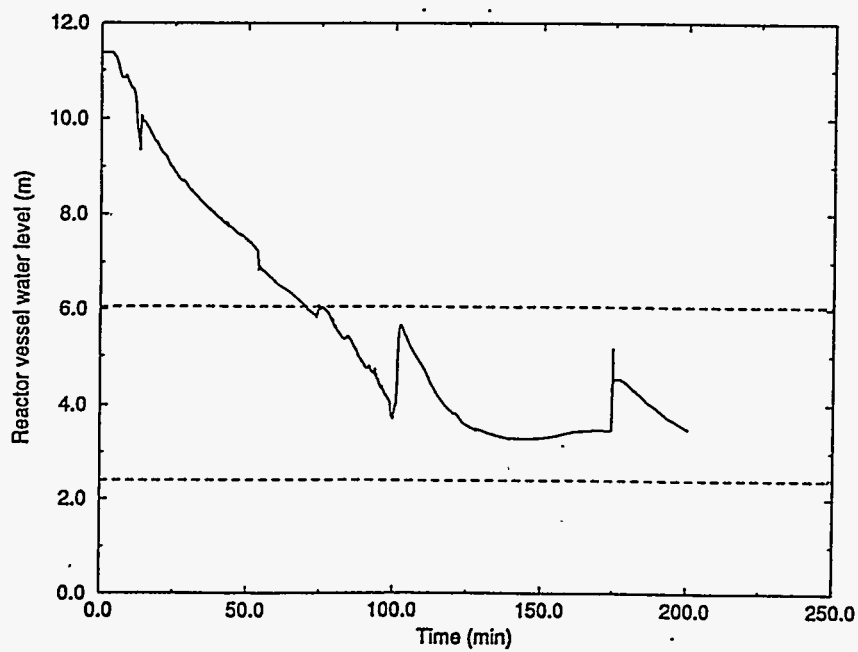

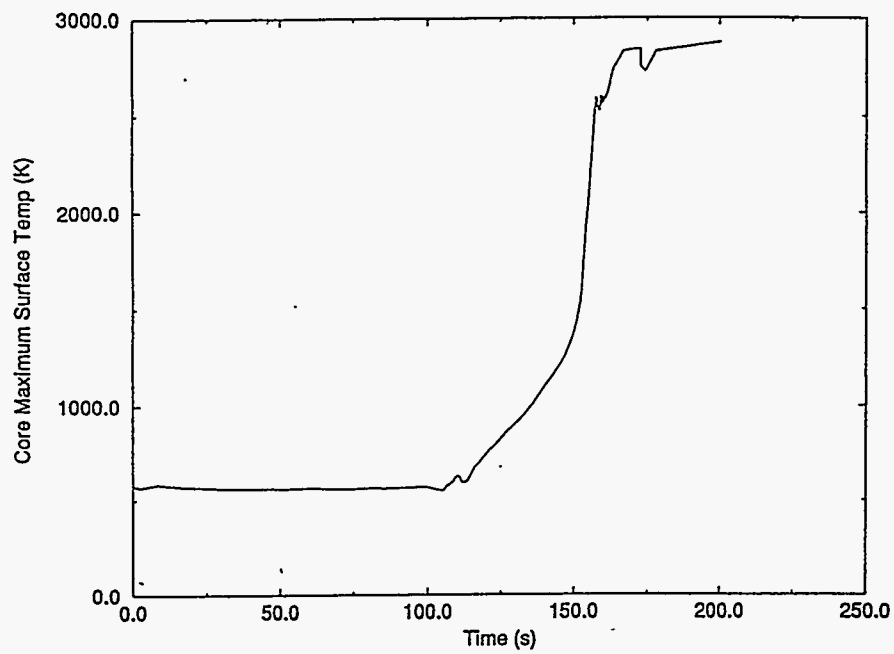Figure 6. MOD3.1e best estimate predicted collapsed liquid level.

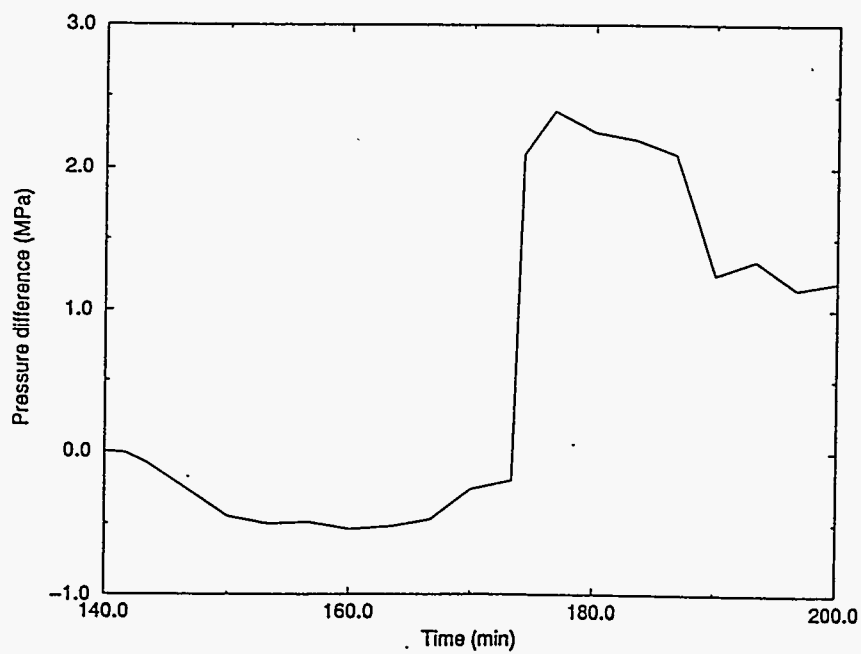Figure 7. MOD3.1e best estimated predicted peak core temperatures.

Figure 8. Predicted pressure difference between MOD3.1 and MOD3.1e.

Potential Impact of Reflood Oxidation on Plant Calculations

The comparison of SCDAP/RELAP5/MOD3.1e calculations directly with results from bundle heating and melting experiments with reflood, and by inference to the TMI-2 results, indicates that the new models now much more accurately predict the accelerated oxidation, heating, and melting during the reflooding of the PWR fuel assemblies. Previous calculations which only considered the oxidation of the intact fuel rod cladding, underpredicted the hydrogen production during bundle reflood in the experiments by as much as a factor of five. The oxidation of BWR assemblies may still be significantly underpredicted during reflood since comparable models have not yet been added to treat oxidation of molten Zircaloy or the cracking and spalling of protective oxide films on BWR channel boxes during reflood. The results from CORA-17 would indicate that this effect may contribute as much as a factor of two to the total hydrogen production.

The specific impact of the new reflood oxidation models on plant calculations using SCDAP/RELAP5 will depend upon the specific features of transients being analyzed. However, the implementation of the new models will result in increased hydrogen production, heating, and melting rates once Zircaloy melting temperatures are reached. This increase will occur independently of the reflooding of the core because of the addition of the new model to treat the oxidation of liquefied U-Zr-O. In addition, the new models can result in dramatic increases in the rate of oxidation, heating, and melting during reflooding of the core. Since the total amount of oxidation is limited by the complete consumption of the Zircaloy and by formation of cohesive debris, the magnitude of these increases are anticipated to diminish with time.

Since the process of oxide cracking and the oxidation of liquified material is not considered in the behavior of BWR channel boxes and control blades, it is clear that such models should be incorporated into future versions of SCDAP/RELAP5. In addition, since other severe accident codes such as MAAP 3B[16], MAAP 4[17], and MELCOR[18] do not currently consider these effects, it is likely that these codes will underpredict the maximum hydrogen production rates, total hydrogen, and the extent of damage for those transients where water is injected into the core.

References

1. SCDAP/RELAP5/MOD3.1 Code Manual, Volumes 1-5, NUREG/CR-6150, EGG-2750, Idaho National Engineering Laboratory, June, 1995.

2. SCDAP/RELAP5/MOD 3.1 Code Manual, Volumes 1-5, Revision 1, NUREG/CR/6150, INEL-95/0609, (Formerly EGG-2720) Idaho National Engineering Laboratory, November, 1995.

3. M. Firnhaber et al, ISP-31 OECD/NEA-CSNI International Standard Problem No. 31, CORA-13, Experiment if Severe Fuel Damage, Comparison Report, GRS-106, KfK 5287, NEA/CSNI/R (93) 17, July, 1993.

4. J. V. Cathcart et al, Zirconium Metal-Water Oxidation Kinetics IV, Reaction Rate Studies ORNL/NUREG-17, 1977.

5. V. F. Urbanic and T. R. Heidrick, "High Temperature Oxidation of Zircaloy-2 and Zircaloy-4 in Steam", Journal of Nuclear Material, Vol. 75, pp. 251-261, 1978.

6. P. Hofmann and V. Noack, "Experiments on the Quench Behavior of Fuel Rod Segments, First International Quench Workshop, Karlsruhe, Germany, October 4-6, 1995.

7. C. M. Allison and J. K. Hohorst, "SCDAP/RELAP5 Code Development and Assessment", 24th Water Reactor Safety Informational Meeting, Bethesda, Md. October 1995, (to be published in proceeding of the meeting).

8. D. H. Hagrman et al, SCDAP/RELAP5/MOD3.1 Code Manuals, Volume 4 - MATPRO-A Library of Material Properties of Light-Water-Reactor Accident Analysis, NUREG/CR-6150, EGG-2720, June 1995.

9. L. J. Siefken et al, "Oxidation of Reactor Core during Fuel Rod Meltdown", Proceeding of the 7th International Meeting on Nuclear Reactor Thermal Hydraulics, NURETH-7, NUREG/CP-0142, Vol. 3, pp 1851-1862, September, 1995.

10. C. M. Allison, "SCDAP/RELAP5 Code Development", 21st Water Reactor Safety Informational Meeting, Bethesda, Md. October 1993.

11. S. Hagen et al, Results of SFD Experiment CORA-13 (OECD International Standard Problem 31), KfK 5054, February 1993.

12. S. Hagen et al, "Comparison of the Quench Experiments, CORA-12, 13, and 17", First International Quench Workshop, Karlsruhe, Germany, October 4-6, 1995.

13. A.D. Knipe et al., PBF Severe Fuel Damage Scoping Test -- Test Results Report, NUREG/CR-4683, August, 1986.

14. S. Hagen, L. Sepold, P. Hofmann, and G. Schanz, Out of Pile Experiments of LWR Severe Fuel Damage Behavior Tests, CORA-C and CORA-2. KfK 4404, September, 1988.

15. J. K. Hohorst et al, "TMI-2 Analysis using SCDAP/RELAP5/MOD3.1", INEL-94/0157, November, 1995.

16. "MAAP, Modular Accident Analysis Program: MAAP3.0B Users Manual", Fauske & Associates, 1990.

17. "MAAP4, Modular Accident Analysis Program, Users Manual", Electric Power Research Institute, Palo Alto, CA., May, 1994.

18. "MELCOR 1.8.3 Reference Manual", Sandia National Laboratory, Albuquerque, NM., July, 1994.

Appendix - Description of Heating and Melting Experiments with Reflood

Three small bundle heating and melting experiments looking at the effects of reflood on a hot degraded core were performed in the CORA facility at Forschungszentrum, Karlsruhe (FzK)[11,12,14]. The CORA-12 and CORA-13 tests were small PWR configured bundles containing PWR control material and the CORA-17 test was a small BWR configured bundle containing a B_4C-stainless steel control blade situated inside a Zircaloy channel box. The two small bundle PWR experimental bundles consisted of 25, 1.0 m in length, rods (16 heated simulator rods, 7 unheated fresh fuel rods and two Ag-In-Cd control rods). Flow conditions, initial heating rates and experimental procedures were the same for both experiments up to the initiation of core reflood. Power to the CORA-12 bundle was terminated and the bundle allowed to cool approximately 300 s before reflood water was introduced into the core region resulting in the formation of a thicker oxide layer on the cladding. Most of the bundle Zircaloy in this experiment was completely oxidized when reflood of the bundle started. Reflood cooling of the CORA-13 experimental bundle started approximately 40 s prior to the termination of power to the simulator rods. The cladding on the CORA-13 unheated and heated fuel rods was only partially oxidized prior to the start of reflood. The CORA-17 small BWR bundle contained 16, 1.0 m in length, rods (10 heated simulator rods and 6 unheated fresh fuel rods). 5 heated and 3 unheated rods were situated on each side of a Zircaloy channel box containing a B_4C-stainless steel control blade representing the tip region of a commercial BWR control blade. The BWR experiment used slower steam and argon flow rates. Bundle conditions at the start of reflood in the CORA-17 experiment were similar to those in CORA-12, most of the bundle Zircaloy was completely oxidized when reflood water was introduced. The slower steam and argon flow rates along with the slower heating rate during the oxidation transient, observed in the CORA BWR experiments, resulted in the production of a thicker oxide layer on the fuel rod cladding. The CORA experiments were chosen for assessment and verification of models in SCDAP/RELAP5 due to the availability of experimental data for comparison purposes. Complete descriptions of these experiments have been presented at numerous meetings and in published papers.

PBF SFD-Scoping Test experiment

The Scoping Test bundle consisted of 32 0.9 m long fresh fuel rods surrounded by an insulating shroud[13]. Prior to the high temperature transient the fuel was trace-irradiated (91 MWd/T) to achieve a suitable fission product inventory. This experiment differed from the CORA reflood experiments, which used a constant steam supply and electrical heating, in that it included a boildown transient to initiate the heating and melting phase of the simulated accident and fission heating to drive the simulated accident transient.