

SCDAP/RELAP5/MOD3 Code Development^a

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C. M. Allison, L. J. Siefken, E. W. Coryell
Idaho National Engineering Laboratory

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ABSTRACT

The SCDAP/RELAP5/MOD3 computer code is designed to describe the overall reactor coolant system (RCS) thermal-hydraulic response, core damage progression, and fission product release and transport during severe accidents. The code is being developed at the Idaho National Engineering Laboratory (INEL) under the primary sponsorship of the Office of Nuclear Regulatory Research of the U.S. Nuclear Regulatory Commission (NRC). Code development activities are currently focused on three main areas - (a) code usability, (b) early phase melt progression model improvements, and (c) advanced reactor thermal-hydraulic model extensions. This paper describes the first two activities. A companion paper describes the advanced reactor model improvements being performed under RELAP5/MOD3 funding.

Introduction

The SCDAP/RELAP5/MOD3 computer code is designed to describe the overall reactor coolant system (RCS) thermal-hydraulic response, core damage progression, and fission product release and transport during severe accidents up to the point of reactor vessel or system failure^{1,2}. The code is being developed at the Idaho National Engineering Laboratory (INEL) under the primary sponsorship of the Office of Nuclear Regulatory Research of the U.S. Nuclear Regulatory Commission (NRC). The code also includes models developed by the U.S. Department of Energy.

SCDAP/RELAP5/MOD3[7x]^b, created in January, 1991, represents a merger of

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^b The number in brackets, [7x], represents the configuration control number assigned to each code version for quality assurance purposes.

the SCDAP/RELAP5/MOD2 damage progression and fission product transport and deposition models with RELAP/MOD3 thermal-hydraulics. A systematic code developmental assessment effort is now underway for both the RELAP5/MOD3 thermal-hydraulic models and the SCDAP early phase damage progression models^{3,4}. As a result of the assessment completed thus far, SCDAP/RELAP5/MOD3[7x] was frozen in May and released to a limited number of organizations for beta testing and independent assessment. At that time, code improvement activities were also initiated to incorporate code improvements where the assessment had indicated that deficiencies existed. These development activities are currently focused on three main areas - (a) code usability, (b) early phase melt progression model improvements, and (c) advanced reactor thermal-hydraulic model extensions. This paper describes the results of the first two activities. A companion paper⁵ describes the advanced reactor thermal-hydraulic model improvements.

Code Usability Improvements

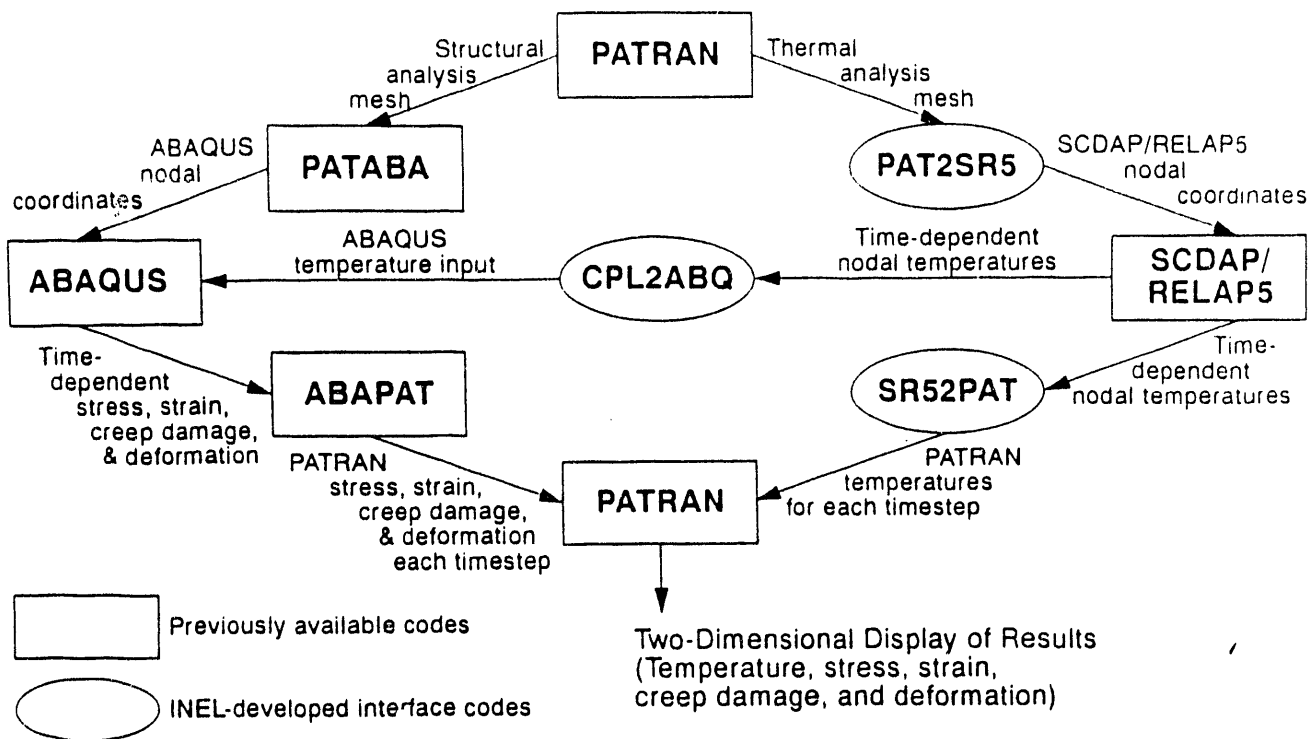
Specific requirements and priorities for code usability improvements were identified from a series of user surveys and the initial results of an independent peer review of the code. These improvements are focused primarily on the reduction of overall analysis costs associated with plant system analysis or the addition of specific user requested features. They include (a) changes to reduce numerical instabilities and water property or other state failures, (b) changes in input/output processing to reduce user errors and to compress output files, and (c) the addition of a data link between SCDAP/RELAP5/MOD3, PATRAN, and ABAQUS.

The changes in the code to reduce numerical instabilities and other code failures have dramatically improved the overall reliability of the code for many types of problems. In addition, in those problems where the code had previously reduced the time steps to unacceptable values to insure code stability, these changes have resulted in substantial reductions in overall run times. The most important changes in this category include (a) a better treatment of the influence of noncondensibles on phase appearance and disappearance, (b) time smoothing options for the explicit

coupling between radiation heat transfer and hydrodynamics models, and (c) elimination of the discontinuities in thermal-hydraulic constitutive models for many types of problems.

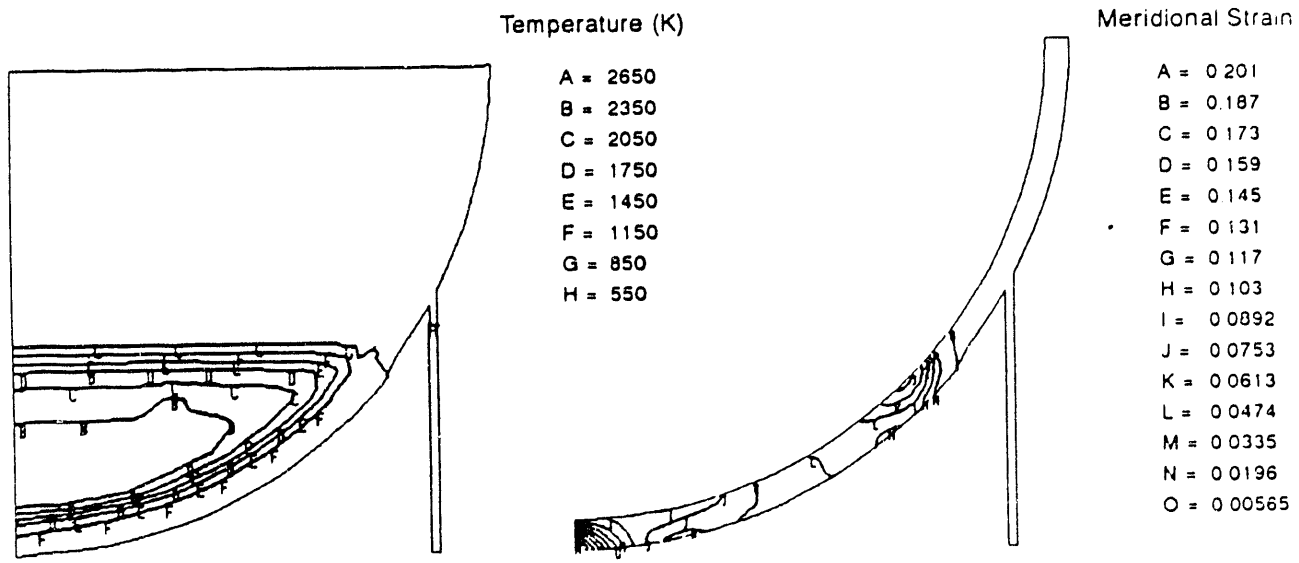
Changes in code input and output have included the (a) conversion of all the input to the RELAP5 free form, numbered card format, (b) addition of extensive input error checking, (c) addition of input range checking and best estimate defaults, (d) addition of options for automatic data compression for restart plot files, and (e) more descriptive output. As a result of the changes in code input, the time required to set up and qualify an input deck has been substantially reduced since a majority of actual and potential errors can be identified in a single input test run. In addition, the code will automatically substitute best estimate default values for selected model input based upon the results of code-to-data comparisons performed as part of the code assessment activities. However, the user can override the default values for sensitivity runs to evaluate the influence of modeling uncertainties on overall calculations. The addition of the restart plot compression options was the most notable change in the output process. These options can reduce the size of the output file and disk storage requirements substantially, in some cases by as much as a factor of 5.

The data link between SCDAP/RELAP5/MOD3, PATRAN, and ABAQUS has been added to the code as a user option. This option was developed to support the NRC's Lower Head Failure Program⁶ and was intended primarily to allow the detailed thermal and structural analysis of the lower head. This option can be used to analyze structures throughout the system, however. An example of the possible application of this link is shown in Figures 1 and 2. In this example, the user uses the general purpose PATRAN code to build the thermal and structural meshes for a detailed 2D analysis of debris and associated lower head structures. The resulting thermal mesh is then used to create the input for the SCDAP/RELAP5/MOD3 detailed COUPLE model using the INEL-developed PAT2SR5 code while the structural mesh is processed for input into ABAQUS. The COUPLE model is then used to perform the detailed thermal analysis of the debris and lower head. This analysis can include (a) time dependent accumulation of debris, (b) 2D heat



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Figure 1. Thermal and structural analysis performed using PATRAN-ABAQUS-SCDAP/RELAP5.



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Figure 2. Two-dimensional display of thermal and structural analysis results.

conduction within the debris bed and associated structures, (c) dryout or quench (rubble bed only), and (d) molten pool formation and growth. The resulting temperature response can then be used in the ABAQUS structural analysis. As shown in Figure 2, PATRAN can then be used to display the results from both the SCDAP/RELAP5 and ABAQUS.

Early Phase Model Improvements

As described in a previous Water Reactor Safety Meeting paper[4] and subsequent report[7], a systematic assessment of the SCDAP/RELAP5 models has been underway since the summer of 1992. That assessment, which has included code-to-data comparisons for SCDAP/RELAP5/MOD3 and earlier versions of the code, has thus far focused upon the early phases of an accident where a wide range of experiment results are available. These early phase code-to-data comparisons have indicated that SCDAP/RELAP5 can describe many of the important features of the experiments. Specifically, it has been concluded that:

1. The thermal response of the early phase experiments, including variations in timing as well as magnitude, could typically be predicted within $\pm 20\%$ with a few outliers in the $\pm 40\%$ range. The ballooning and rupture could typically be predicted to a few percent. The hydrogen production had the worst overall agreement, particularly during bundle reflood, with a variation up to a factor of two. The general trends of the melt relocation, amount of material liquefied and location of the blockage regions, could be predicted but qualitative estimates were still limited by the availability of data.
2. Some features of the experiments could not be adequately predicted including (a) the renewed hydrogen production, heating and melting during reflood, (b) the influence of material interactions between the fuel rod, control rod/blade, and structural materials, (c) flow diversions due to changes in geometry, (d) rivulet and free droplet flow of liquefied fuel rod materials, (e) oxidation of the inside of unpressurized fuel rod

cladding, (f) the oxidation of relocating material or material that has formed a cohesive blockage, and (g) the porosity of frozen melt and the relocation of ceramic fuel rod material.

As a result of that assessment, work was started in improving the models where they were shown to be deficient. Of the seven areas noted above, model improvements have been completed for (a) renewed hydrogen production, heating, and melting during reflood, (b) interactions between Inconel spacer grids-Zircaloy cladding and BWR B₄C, stainless steel control blade, Zircaloy channel boxes, and (c) the influence of cold walls upon the flow diversions associated with changes in geometry. Work was started on the interactions between (a) Ag-In-Cd control material, stainless steel, and Zircaloy and (b) rivulet and free droplet flow of liquefied fuel rod materials.

As shown on Figures 3 and 4, experiments performed in the CORA facility in Germany^{7,8,9} have shown that the reflooding of a hot, damaged bundle can have a dramatic influence on the hydrogen production and heating of the bundle. Figure 3 shows the results from a PWR bundle test, CORA-12, while Figure 4 shows the results from two BWR bundle tests, CORA-16 and CORA-17. CORA-12 was an electrically heated bundle with a 25 rod array consisting of fuel rods, electrically heated fuel rod simulators, and Ag-In-Cd control rod. The power in the bundle was increased linearly with time until indicated temperatures exceeded the melting point of Zircaloy, at a time of ~4900 s, the power was then decreased, resulting in the initial cooling of the bundle. Then at ~5100 s, the bundle was quenched. The resulting spike in the hydrogen and temperatures at 50 and 1250 mm where bundle thermocouples were still operational is obvious. The same trend was shown in the CORA-17 experiment. In this case, the bundle was composed of BWR structures, fuel rods, electrically heated fuel rod simulators, Zircaloy channel, and B₄C control blade segment. By way of contrast, the hydrogen production for the CORA-16 test is also shown. Both CORA-16 and CORA-17 were subjected to the same heatup and melting transient. However, the bundle in CORA-16 was slowly cooled while the CORA-17 bundle was quenched.

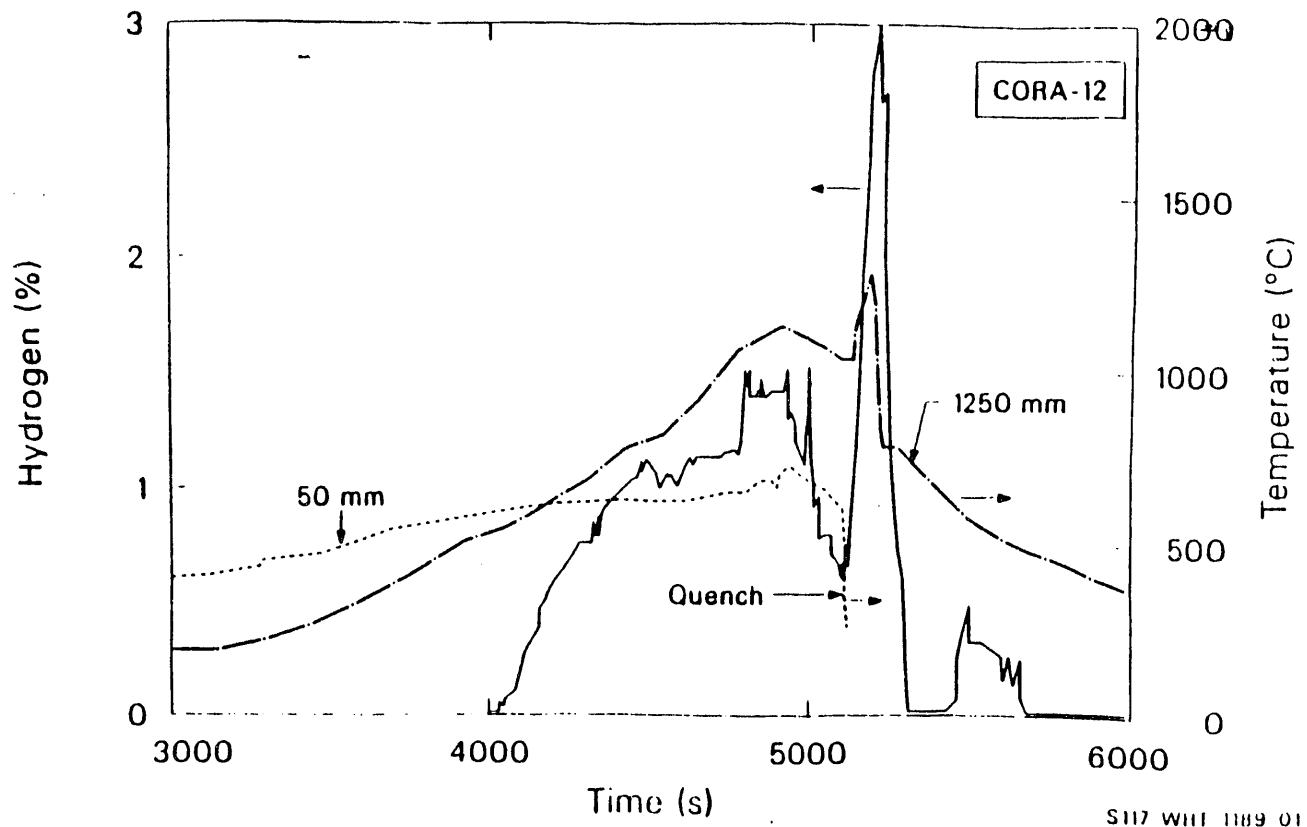


Figure 3. Measured CORA-12 PWR bundle test hydrogen generation rate and

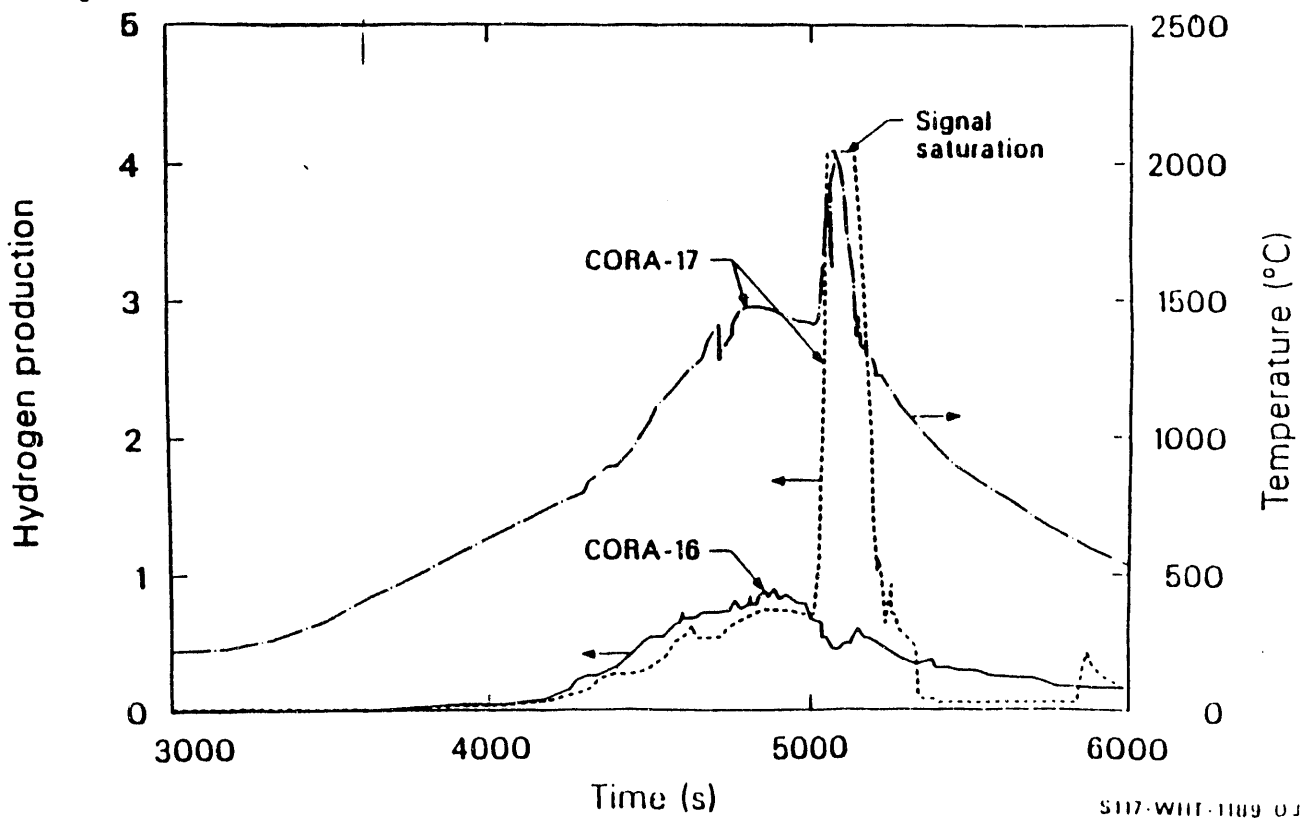
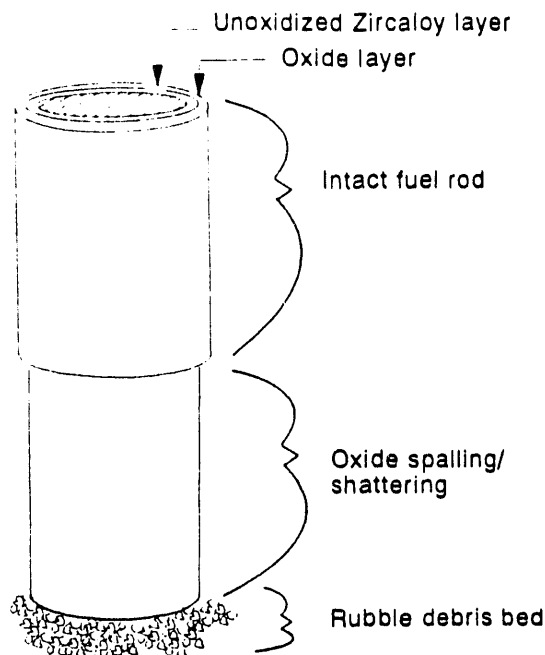


Figure 4. Comparison of measured CORA-16 and CORA-17 BWR bundle hydrogen generation rate and temperatures.

However, during the analysis of these experiments, it was found that the existing SCDAP/RELAP5 models could not predict such a rapid increase in oxidation during reflood. In fact, the models consistently underpredicted the oxidation during the reflood phase of the experiments by nearly a factor of two. In the original models, it was assumed that, during reflood, the fuel rods would shatter, exposing unoxidized Zircaloy and forming a loose rubble debris bed, if two basic criteria was satisfied. First, the cladding was sufficiently oxidized that the cladding had become embrittled using a criteria developed by Kassner and Chung¹⁰. That is, the remaining, relatively oxygen free (<0.9 wt %), beta layer of the Zircaloy cladding had a thickness less than 0.1 mm. Second, the fuel rods were cooled below 1270 K where it was expected that the oxide was no longer ductile due to a phase transition in the ZrO_2 .

Consequently, the SCDAP/RELAP5 models were changed using the basic concepts illustrated in Figure 5. It was still assumed that the fuel rods would shatter using the same criteria as before. However, an additional region was added where the protective oxide could spall or shatter leaving a fresh unoxidized surface of metallic Zircaloy. The region would form, based upon an analysis of the available data, if the cooling rate was greater than 2 K/S and the temperature of the oxide fell below 1560 K. In addition, a vapor limited diffusion model was added using a heat/mass transfer analogy to limit the maximum rate of oxidation when the hot metallic surface was exposed to steam. Although a detailed assessment of this model has not been completed, results of verification testing¹¹ indicates that the predicted trends are correct.

The CORA, and other separate effects, experiments performed in Germany¹² also show that grid spacers have a pronounced impact on the relocation and freezing of liquefied material and relocation of loose debris. As shown in sketches of the end state of several CORA experiments, Figure 6, the grid spacers act as barriers to the relocation of liquefied material and loose debris. In addition, Inconel spacer grids can also chemically interact with the Zircaloy cladding to form relatively low melting temperature alloys. These interactions can occur quickly as the temperatures are increased with complete liquefaction of the material in



Model Features

- Thermal hydraulics
 - RELAP5 reflood and quenching correlations used
- Vapor limited diffusion of steam to surface
 - Mass transfer coefficient calculated using heat/mass analogy
- Shattering of oxidized cladding
 - Cooling rate ≥ 2 K/s
 - β -layer ≤ 0.1 mm
 - $T_{\text{debris}} \leq T_{\text{ox}} \leq 1560$ K

Figure 5. Features of the new reflood and oxide shattering model. M155-BDR-1092-004

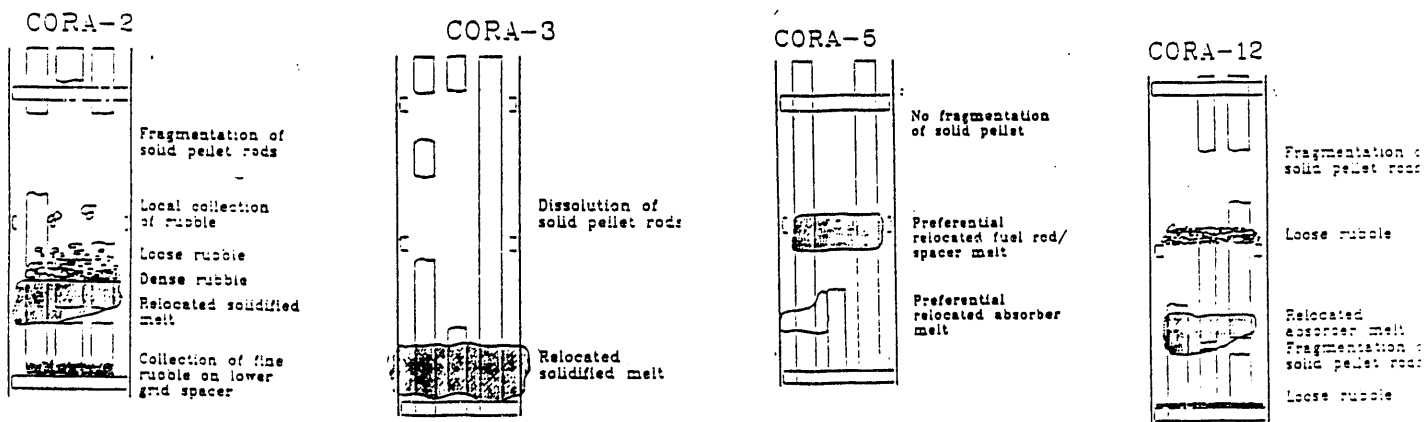
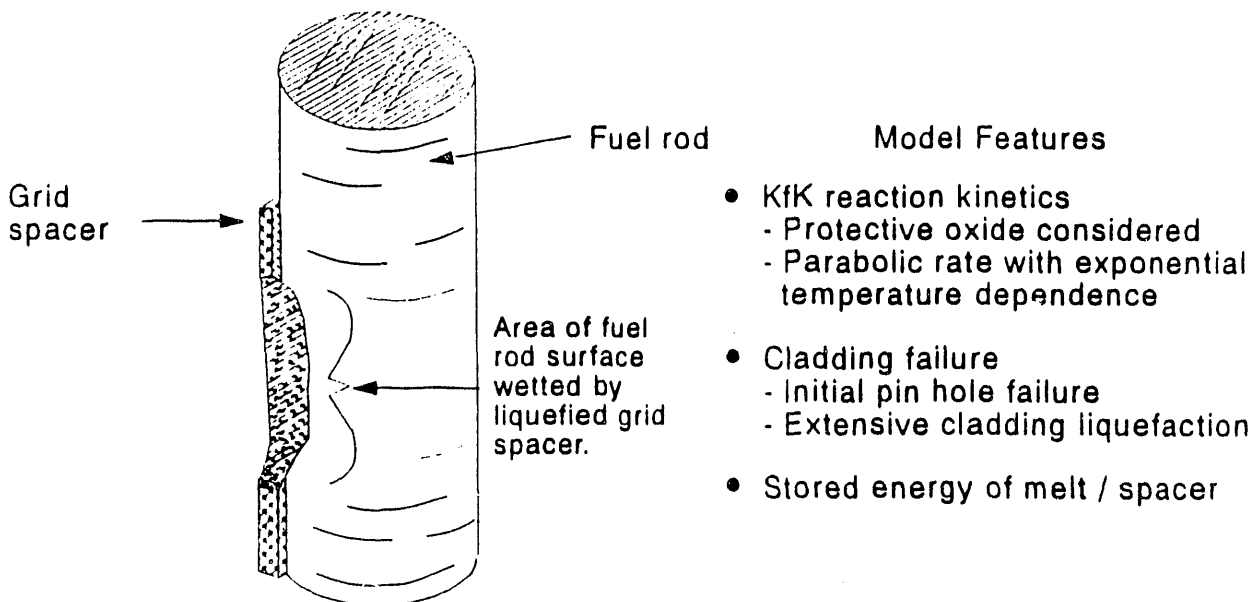


Figure 6. Influence of grid spacers in selected CORA experiments.

the location of the interactions at a temperature near 1500 K.

To account for these effects, the spacer grid models in SCDAP/RELAP5 were modified to account for the stored energy associated with the grid as well as the interactions between Inconel and Zircaloy. These models are described in detail by Siefken¹³. However, the key features of the models are shown on Figure 7. The Inconel spacer grid model is the most elaborate due to the incorporation of reaction kinetics correlations that define the rate of chemical interactions between the grid and the adjacent cladding. These correlations use a parabolic rate equation with exponential temperature dependence. These correlations also account for the rate limiting effect of an initial protective oxide layer. The interactions are assumed to proceed initially with the formation of a pin hole failure in the cladding at the point of contact between the spacer grid and cladding. The interactions will then spread from that point radially until the grid is completely liquefied. Both Zircaloy and Inconel spacer grids can also act as barriers to the downward relocation of liquefied or loose debris. In this case, the thermal mass of the grid



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Figure 7. Features of the new Inconel spacer grid-Zircaloy cladding interaction model.

spacers are included in the event that the grid, adjacent cladding, and overlying debris or melt continue to heat up and eventually relocate downward. Initial assessment of the new model using the results from the CORA-7 experiment¹⁴ indicates that the new model results in a prediction of melt relocation behavior in much better agreement with the test.

BWR heating and melting experiments in the Annular Core Research Reactor (ACRR)^{15,16} and in the CORA facility^{7,8,9,17} also showed that the interactions between the B₄C control material, stainless steel cladding and sheath material, and the channel box Zircaloy dominated the initial liquefaction and relocation of the BWR control blade and channel box. However, these structures were originally modeled using two separate component models. A B₄C/stainless steel control rod/blade component was used to represent the BWR control blade while a general slab model was used to represent the channel box. Because of this approach, the interactions between the control blade and adjacent channel box could not be properly addressed. To resolve this problem, a new component model has been added to the code which represents the BWR specific combined channel box and control blade geometry. This model was developed by Oak Ridge National Laboratory¹⁸ and includes (a) a representation of the control blade and channel box segments adjacent to the control blade and open interstitial gap, (b) interactions between the B₄C, stainless steel cladding and sheath, and the Zircaloy channel box, (c) oxidation of the stainless steel, Zircaloy, and B₄C, and (d) liquefaction and relocation of the component structures. The model allows for different flow conditions in the interstitial region and fuel assembly using the RELAP5 thermal-hydraulics models and correlations.

The analysis of the LOFT FP-2 test with SCDAP/RELAP5^{19,20} provided the first indication that the flow diversion due to changes in core geometry could be important even during the initial change in geometry due to fuel rod ballooning. As shown in Figure 8, which shows the calculated and measured temperatures in the central fuel assembly of the LOFT core, calculations either including or not including the influence of flow diversions due to fuel rod ballooning tended to bound the measured temperature response of the assembly, but resulted in a substantial change

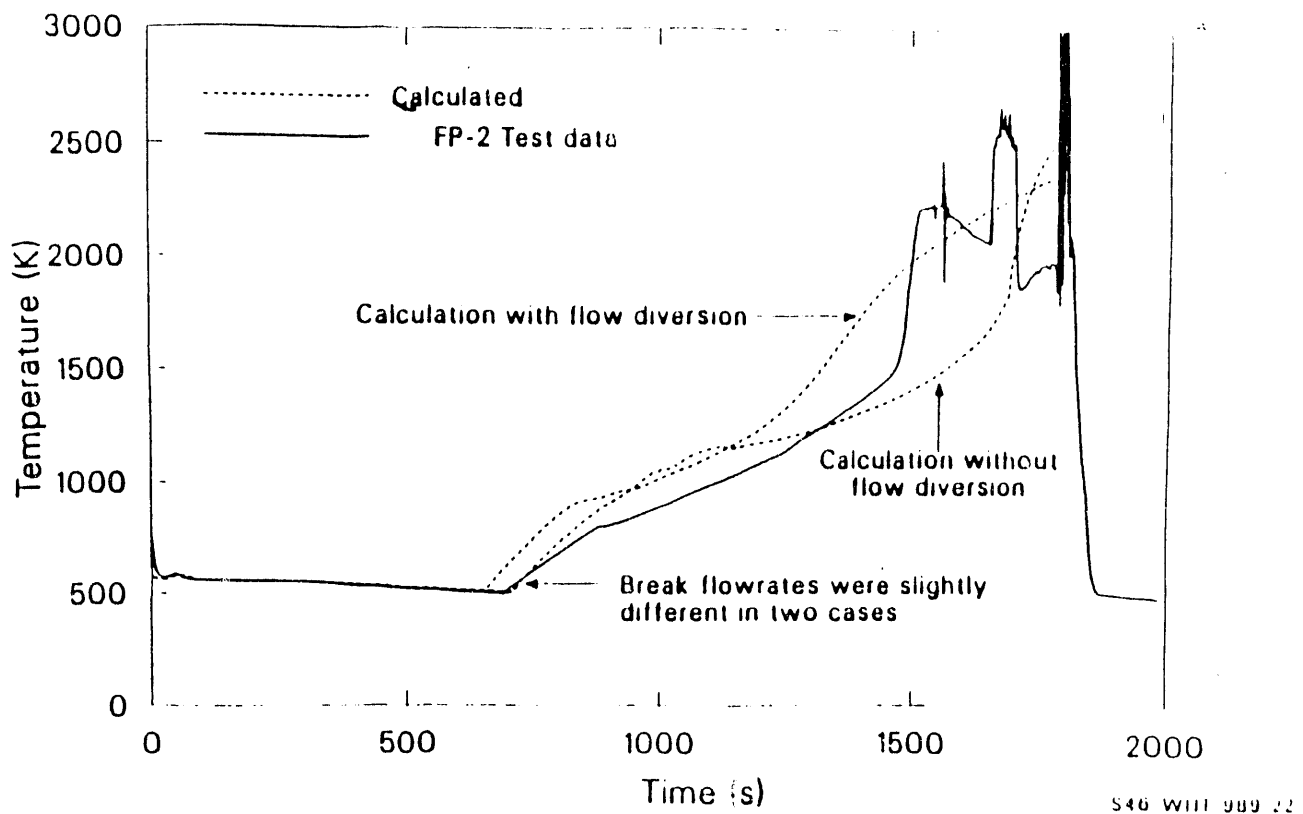


Figure 8. Calculated and measured temperatures for the LOFT FP-2 core central fuel assembly.

in the predicted temperatures. Further analysis indicated that the insulated shroud surrounding the central assembly had a substantial impact on the predicted behavior of the core. As shown in the schematic of the left hand side of Figure 9, the initial calculations were performed using a two flow channel core model due to limitations in coupling between the SCDAP/RELAP5 radiation heat transfer and hydrodynamics models. As a result, the radial temperatures in the central fuel assembly, fuel rod ballooning, and melt relocation were predicted to be relatively uniform across the assembly. The resulting predicted flow diversion was then from the central assembly to the outer assemblies. Yet, the experimental results showed that the fuel rod temperatures adjacent to the unheated shroud were significantly lower than those in the inner part of the assembly. As a result, as shown in Figure 10, the peak rod temperatures, and associated formation of blockages due to the melting of the assembly were concentrated in the center of the assembly.

Because of this result, the coupling between the radiation heat transfer

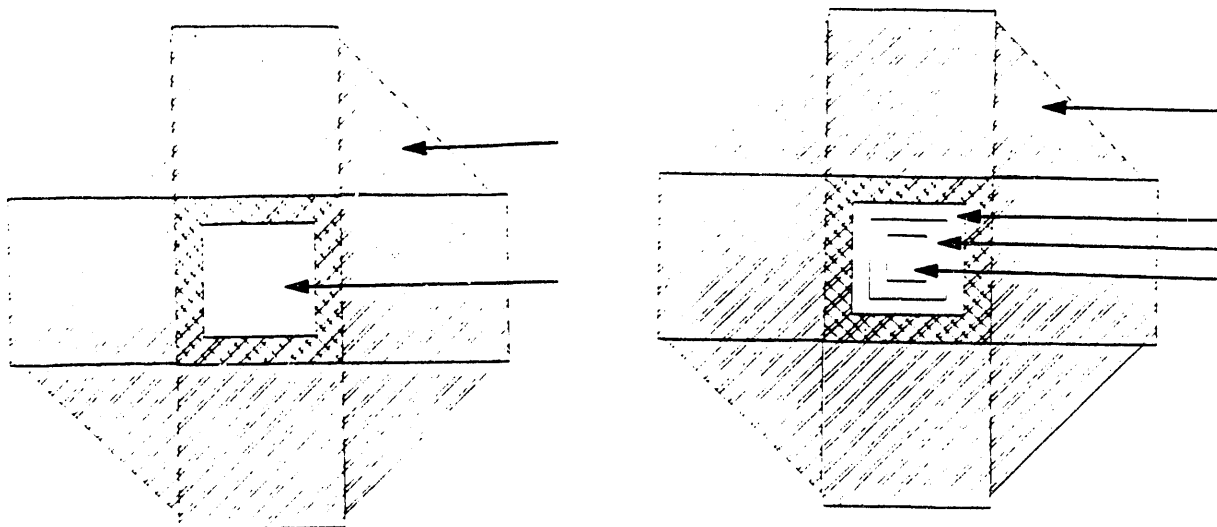
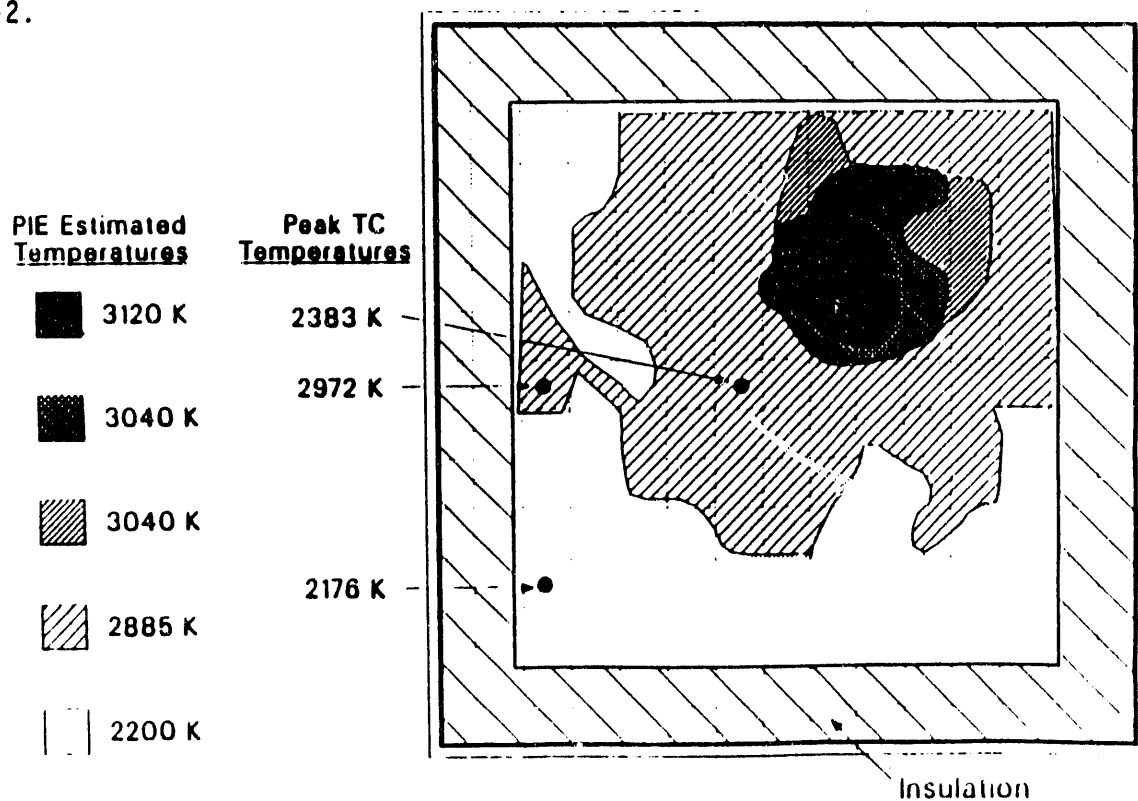


Figure 9. Flow channel representations used for the analysis of LOFT FP-2.



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Figure 10. Estimated peak bundle temperatures from LOFT FP-2.

and hydrodynamics models was modified to allow multiple flow channel within a single radiation enclosure. Initial analysis with these changes and using a more representative set of flow channels in the central assembly indicated that such a radial nodalization more accurately predicted the temperature distribution, fuel rod ballooning, and melting-induced blockage near a cold wall. In the case of the LOFT analysis, the more detailed representation of the flow channels and fuel rod behavior in the central fuel assembly resulted in a reduction in the average flow blockage and associated flow diversion to the outer assemblies as shown in the right hand schematic of Figure 9. Additional LOFT calculations are currently underway to better quantify the influence of the new modeling capability.

The CORA and earlier single rod heatup and melting experiments in the German NEILS facility^{1,22} also clearly identified that the initial relocation of fuel rod materials associated with the dissolution of UO_2 by molten Zircaloy occurs as rivulets and free falling droplets. Figure 11, taken from tests conducted in NEILS in Helium, shows the initial formation of rivulets of liquefied fuel rod material. Although the presence of steam, as shown in Figure 12, confused the image of the process, more recent CORA experiments also show the formation of rivulets and free falling drops in the presence of steam once significant amounts of liquefied material have been formed. This is shown in figure 13, which is a composite of data developed from videos taken for PWR and BWR experiments in CORA⁸. Because of the graphic evidence from recent CORA experiments, work has been started on modifying the existing film flow models that are used to treat the relocation of liquefied fuel rod material.

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Figure 11. Fuel rod melting in single rod tests conducted in the German NEILS facility in helium.

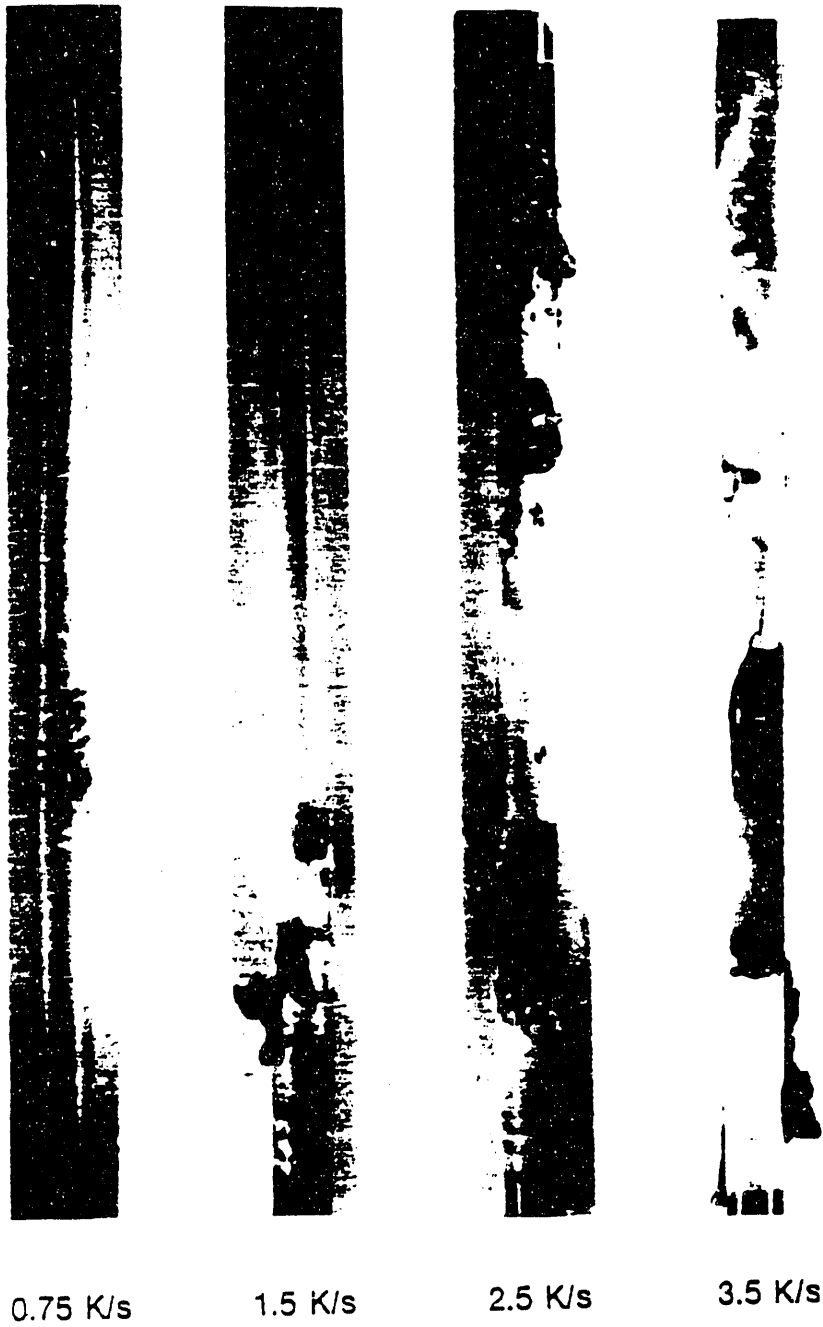
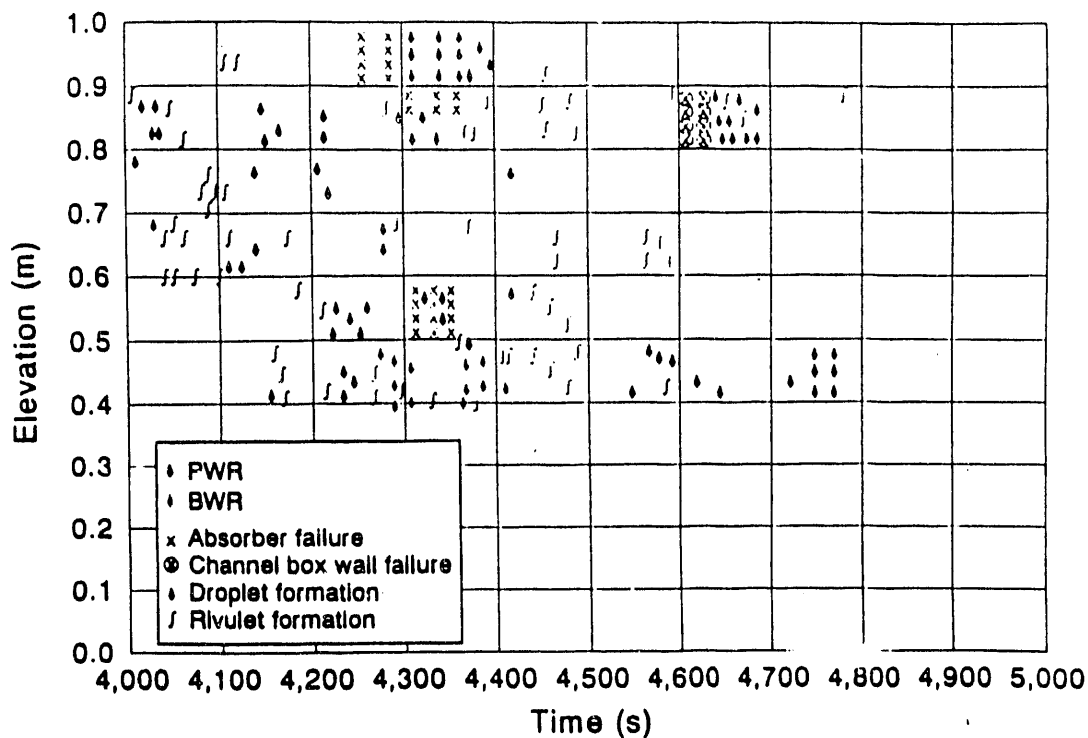


Figure 12. Fuel rod melting in single rod tests conducted in the German NEILS facility in steam.



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Figure 13. Composite of rivulet and free droplet melt relocation from CORA PWR and BWR tests.

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