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MELCOR BENCHMARKING AGAINST INTEGRAL SEVERE FUEL DAMAGE TESTS[1]

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ABSTRACT

MELCOR is a fully integrated computer code that models all phases of the progression of severe accidents in light water reactor nuclear power plants, and is being developed for the U.S. Nuclear Regulatory Commission (NRC) by Sandia National Laboratories (SNL). Brookhaven National Laboratory (BNL) has a program with the NRC to provide independent assessment of MELCOR, and a very important part of this program is to benchmark MELCOR against experimental data from integral severe fuel damage tests and predictions of that data from more mechanistic codes such as SCDAP or SCDAP/RELAP5. Benchmarking analyses with MELCOR have been carried out at BNL for five integral severe fuel damage tests, namely, PBF SFD 1-1, SFD 1-4, and NRU FLHT-2, FLHT-4, and FLHT-5. This paper presents a summary of these analyses, and their role in identifying areas of modeling strengths and weaknesses in MELCOR.

INTRODUCTION

MELCOR is a fully integrated computer code that models all phases of the progression of severe accidents in light water reactor nuclear power plants [1]. It is being developed for the NRC by SNL as severe accident source term analysis tool to be used in Probabilistic Risk Assessment (PRA) studies. Severe accident phenomena that can be modeled in MELCOR include reactor coolant system and containment thermal/hydraulic response, core heatup, degradation and relocation, zircaloy and steel oxidation and hydrogen production, and fission product release and transport. However, the usefulness of MELCOR for risk assessment studies depends on its ability to provide validated models for the severe accident phenomena.

An area in MELCOR that has the largest uncertainty, and that requires the maximum assessment efforts, is in-vessel melt progression. Through the Cooperative Severe Accident Research Program (CSARP), the NRC has conducted several tests related to core degradation and melt progression during severe accident conditions in the Power Burst Facility (PBF) at Idaho National Engineering Laboratories (INEL), the Annular Core Research Reactor (ACRR) at SNL, and the National Research Universal (NRU) reactor at Chalk River Nuclear Laboratories (CRNL), and has been associated with the KfK work in NIELS and CORA out-of-pile facilities. Information on melt progression also became available from the TMI-2 post-test examinations and from the OECD LOFT project (Test FP-2).

BNL has a program with the NRC to provide independent assessment of MELCOR as a severe accident thermal-hydraulic/source term analysis tool, and a very important part of this program is to benchmark MELCOR against experimental data from integral severe fuel damage tests and predictions of that data from more mechanistic codes such as SCDAP or SCDAP/RELAP5. In accordance with a BNL study on experimental data alternatives for benchmarking MELCOR [2], which identified in-vessel phenomenology as an area in MELCOR that needed to be assessed, benchmarking analyses with MELCOR have been carried out at BNL for five integral severe fuel damage tests, namely, PBF SFD 1-1 [3], SFD 1-4 [4], and NRU FLHT-2 [5], FLHT-4 [6], and FLHT-5 [7].

The PBF SFD tests were a series of four integral severe fuel damage (SFD) experiments performed by INEL, to examine the meltdown behavior of a small region of a reactor core under loss of coolant accident conditions. These tests were performed with 0.9 meter long, 32-rod bundles of test fuel and at 68 bars test pressure. The final test, SFD 1-4, with high-burnup fuel, Ag-In-Cd control rods, and on-line aerosol diagnostics, was the most prototypical. These integral tests produced substantial data on core heatup, clad oxidation, fuel melting and relocation, and fission product release, for determining and modeling the early phase of severe accident conditions.

The NRU full-length, high-temperature (FLHT) experiments were a series of four severe damage tests, conducted by PNL, to characterize fuel bundle behavior, including fuel temperature history, hydrogen production, melting and relocation, and fission product release and transport, during the early phase of a severe accident. A stated objective of the tests also was to provide data for the validation of severe accident computer codes. The severity of peak conditions and their duartion increased from one FLHT test to the next, FLHT-5 being the most severe. The FLHT tests being performed with full-length PWR fuel rods, are important for code validation, particularly for clad oxidation and hydrogen generation where length scaling from the shorter PBF and ACRR data may cause some uncertainties.

[1]Work performed under the auspices of the U.S. Nuclear Regulatory Commission.

RESULTS AND COMPARISONS

In all tests, the fuel bundle was surrounded by an insulating shroud, to minimize radial heat losses. The shroud was multi-layered, consisting of zirconium oxide sandwiched between inner and outer zircaloy walls, and an inner zircaloy liner facing the fuel bundle. Bypass coolant flowed around the outer surface of the shroud. Bundle coolant entered the bundle inlet region and flowed up along the fuel rods. It was heated by fission power (representing decay heat in an actual plant), converted to steam, and reacted with the high-temperature zircaloy cladding and liner to form hydrogen. The boilaway transient began when inlet flow was reduced (coupled with a gradual increase in fission heat for tests SFD 1-1 and 1-4). The degraded cooling conditions led to rapid decrease in the bundle coolant inventory, fuel uncovery and dryout, heatup, cladding rupture, and rapid oxidation. With sustained fission power and heat from oxidation, temperatures continued to rise rapidly, resulting in melting and relocation of core material, and the release of hydrogen and fission products. More details on the individual tests can be obtained from the test results reports [8-12].

A typical MELCOR nodalization for the test simulations is shown in Figure 1 [5]. There are 4 control volumes (inlet, fuel bundle, plenum, and environment) and 3 flow paths interconnecting them. The environment is a contrived volume and is assumed very large, allowing the system pressure to stay nominally constant, as in the experiments. The fuel bundle active length is nodalized into several axial segments and 1 radial ring. The shroud is nodalized axially to match the core cells and radially into several layers. Note that for FLHT-5, the test bundle was modeled as a BWR geometry (see Figure 2), to allow the mass of zircaloy in the shroud liner and carriers to participate in oxidation with steam as a canister component [7].

The benchmarking calculations of integral severe fuel damage tests have helped to identify areas of modeling strengths and weaknesses in MELCOR; the most appropriate choices for input parameters; selection of axial nodalization for core cells and heat structures; and workarounds that extend the capabilities of MELCOR. These insights are explored in greater detail, with the help of selected results and comparisons from all five integral tests, as follows.

Temperature Comparisons

Comparisons between predicted and measured clad temperatures for all five tests are shown in Figures 3 to 7. The agreement between MELCOR and the test data appears to be very good in the heatup phase, prior to the onset of accelerated oxidation of zircaloy.

For the first four tests (Figures 3 to 6), MELCOR generally

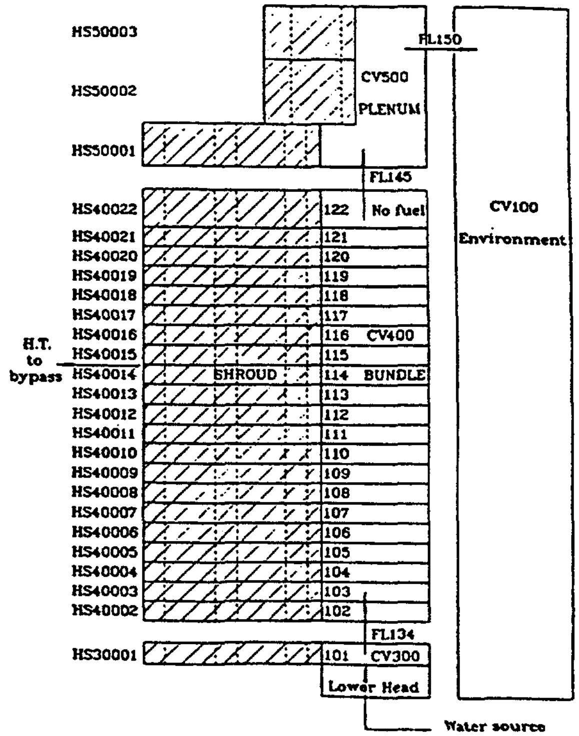

Figure 1. MELCOR Nodalization for the FLHT-2 Test

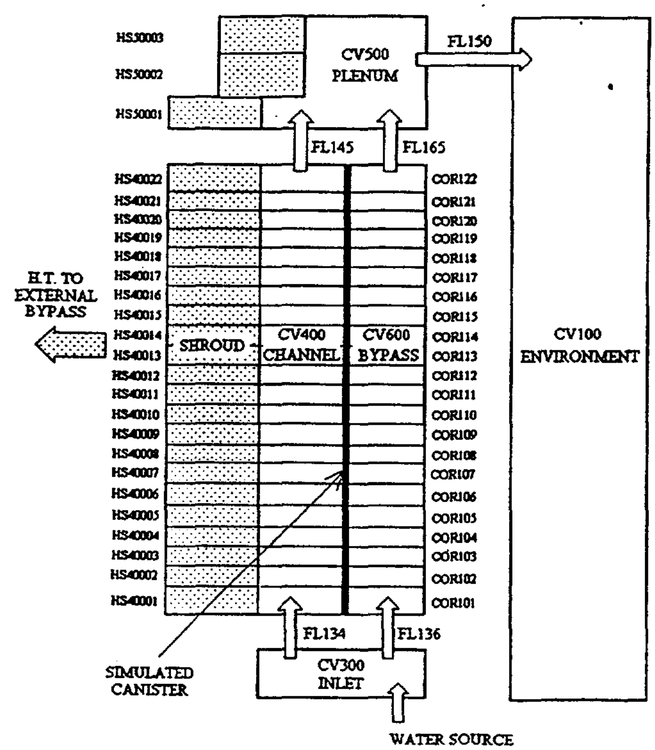

Figure 2. MELCOR Nodalization for the FLHT-5 Test

DISCLAIMER

fails to achieve measured the steep temperature rise prior to thermocouple failure. This could be attributed to several causes. Firstly, following clad rupture, the inner clad surface also gets exposed to steam and hence subject to oxidation. This is not modeled in MELCOR. The effect may not be pronounced for steam-starved conditions, but there could nonetheless be local availability of steam close to the rupture opening. Secondly, the effect of clad ballooning (not modeled in MELCOR) could give rise to local flow reductions and temperature excursions. Finally, zircaloy present in the shroud inner liner, which can react with steam, was not allowed to oxidize in MELCOR as it was not a core component. This effect is not important for steam-starved conditions as in SFD 1-1. But where there is adequate steam supply, this may create divergence in predictions. For FLHT-5, the shroud liner was modeled as a canister of a BWR fuel bundle, and MELCOR predictions of both heatup and temperature escalation are very

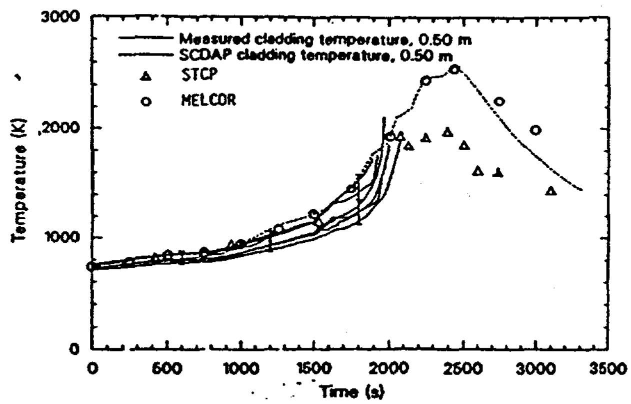

Figure 3. Comparison of measured and calculated clad temperatures, SFD 1-1

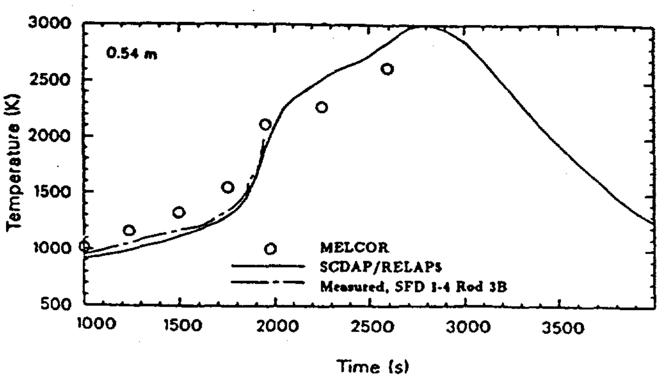

Figure 4. Comparison of measured and calculated clad temperatures, SFD 1-4

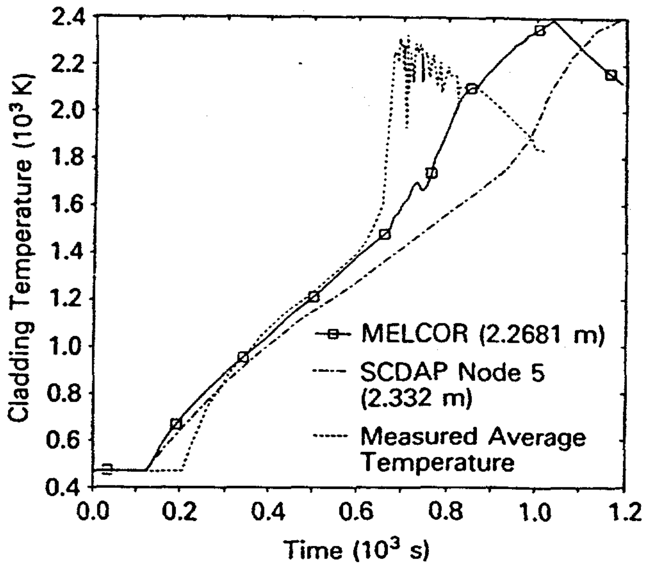

Figure 5. Comparison between calculated and measured temperatures, FLHT-2

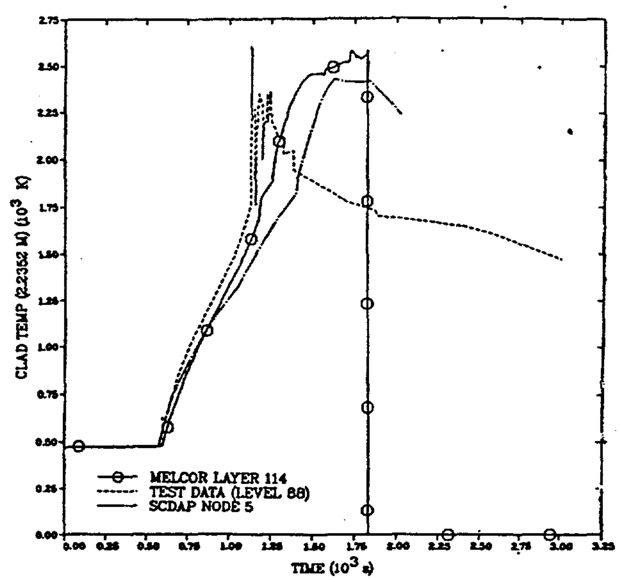

Figure 6. Comparison of calculated clad temperature with test data, FLHT-4

close to the measured values (see Figure 7). The sudden drop of MELCOR calculated cladding temperature in the figures represents clad melting and relocation downwards. SCDAP calculations [13] show temperatures rising to almost 3000K before dropping. This is because the ZrO_2 holdup temperature in SCDAP was artificially specified to be 3000K, in order to minimize the predicted relocation, and increase the predicted hydrogen produced.

The difference between measured and predicted temperatures of the saddle, located outside the ZrO_2 insulation layer, is more significant and can be attributed in part to the difficulty in estimating the effective thermal conductivity of the shroud during the high temperature transient.

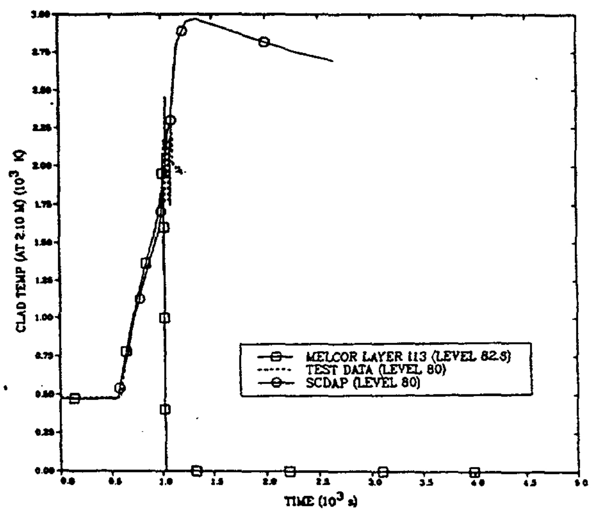

Figure 7. Measured and calculated clad temperatures, FLHT-5

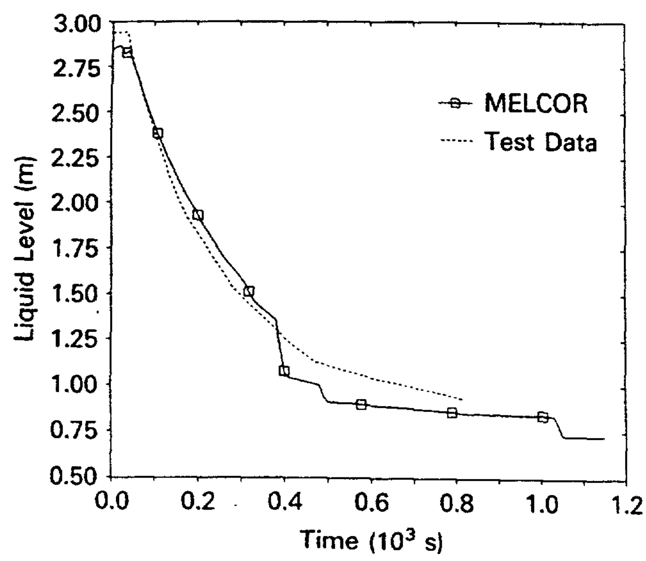

Figure 8. Comparison of calculated liquid level with test data, FLHT-2

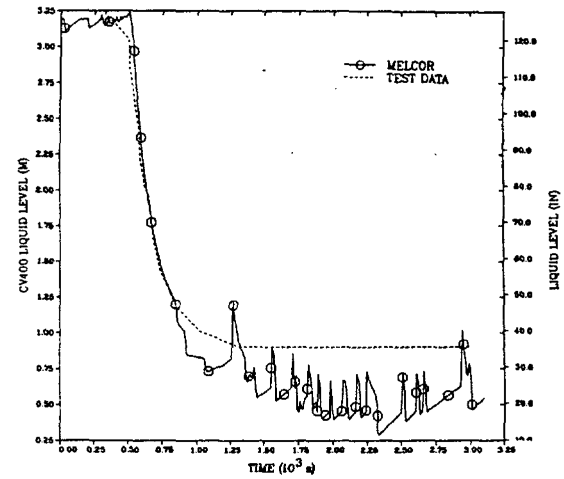

Figure 9. Comparison of calculated liquid level with test data, FLHT-4

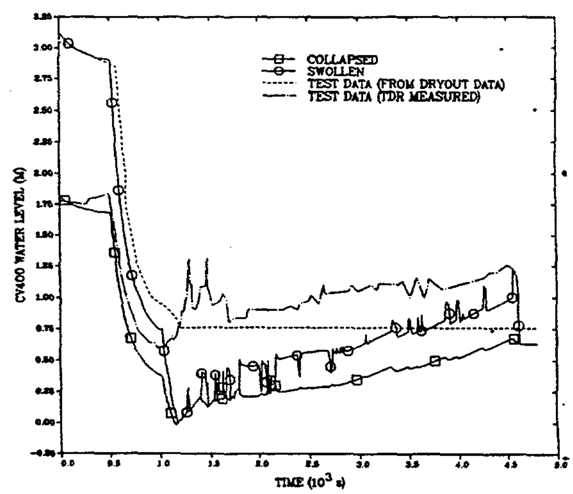

Figure 10. Comparison of calculated liquid level with test data, FLHT-5

The overall temperature behavior is strongly influenced by the calculated liquid level in the bundle region, and the converse is also true. Figures 8 - 10 show MELCOR-calculated liquid levels in the bundle region, compared with the measured levels, for tests FLHT-2, FLHT-4, and FLHT-5, respectively. A contributing factor to uncertainties in liquid level calculations

Table 1. Comparison of Calculated Total Hydrogen and Test Data

	HYDROGEN PRODUCED (g)			
	Experiment	MELCOR	SCDAP or SCDAP/RELAP5	STCP
PBF SFD 1-1	64 ± 7	67	89	60
PBF SFD 1-4	86 ± 12	86	87	--
FLHT-2	42 ± 2.5	43	39.7	--
FLHT-4	175 - 240	119	110/125	--
FLHT-5	220 - 340	158	168	--

Table 2. Comparison of Calculated Clad Rupture and Test Data for PBF SFD Test 1-1

	Criterion	Rupture Time(s)	Axial Location (m)
Experiment		1538 - 1632	0.30 - 0.69
MELCOR	T_{fail} = 1173K	1370	0.46 - 0.57
SCDAP	Mechanistic	1290	0.46 - 0.55
STCP	T_{fail} = 1173K	1755	

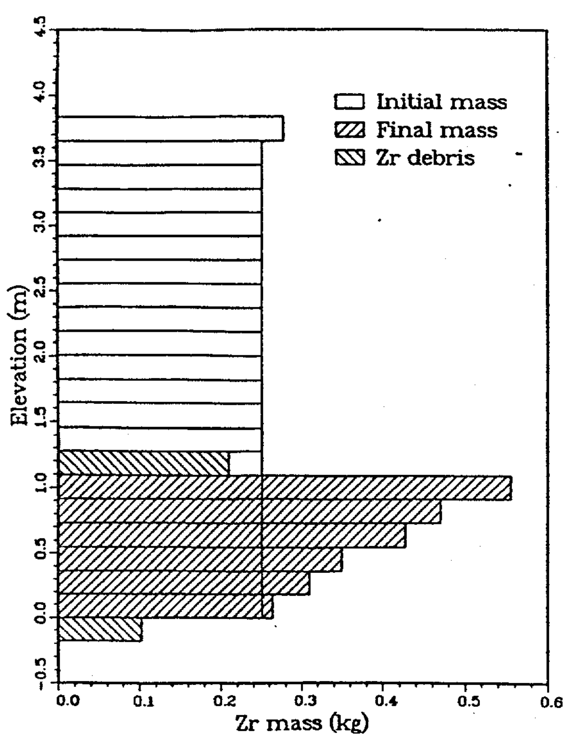

Figure 11. Fuel mass relocation calculated by MELCOR, FLHT-4

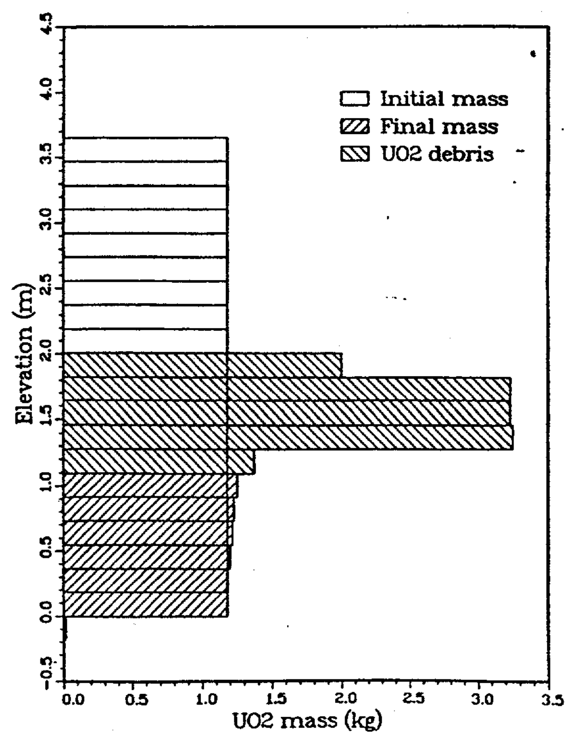

Figure 12. Zircaloy mass relocation calculated by MELCOR, FLHT-4

Table 3. Comparison of Measured and Calculated Release Fractions of Fission Products

Element	Experiment SFD 1-1	MELCOR (CORSOR)	SCDAP
Xe, Kr	0.06 ± 0.03	0.53	0.04
I	0.12 ± 0.02	0.53	
Cs	0.094 ± 0.014	0.53	
Element	**Experiment SFD 1-4**	**MELCOR (CORSOR)**	**FASTGRASS**
Noble Gas	0.23 - 0.52	0.57	0.63
I	0.24 ± 19%	0.57	
Cs	0.51 ± 15%	0.57	
Te	0.03	0.03	
Element	**Experiment FLHT-4**	**MELCOR (CORSOR)**	**SCDAP**
Noble Gas	0.25 - 0.55	0.67	0.12
Element	**Experiment FLHT-5**	**MELCOR (CORSOR)**	**SCDAP**
Noble Gas	Best estimate ~0.50	0.53	0.20

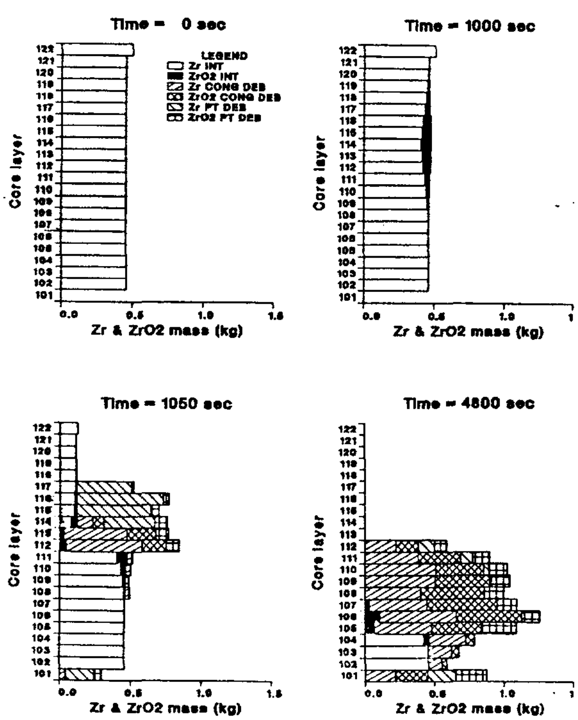

Figure 13. MELCOR-calculated relocation of Zr and ZrO_2, FLHT-5

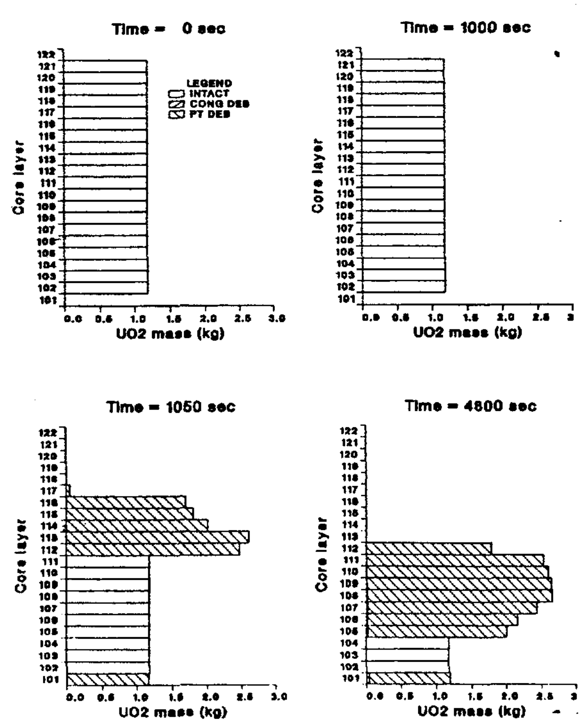

Figure 14. MELCOR-calculated relocation of UO_2, FLHT-5

is that the actual bundle flow was never constant, whereas MELCOR input (for convenience) assumed it to be constant.

Oxidation and Hydrogen Production

MELCOR calculates oxidation of both zircaloy and steel by solid-state diffusion through the oxide layer using standard parabolic kinetics, with appropriate rate constant expressions, and limited by steam availability. For zircaloy, the rate constant is evaluated from the correlation by Urbanic and Heidrick. The shift to rapid oxidation is modeled to occur at 1853K. This temperature can be changed via sensitivity coefficient, and was changed to 1700K based on experimental observations for FLHT-4 and FLHT-5.

Table 1 shows comparisons between experimental and calculated values of total hydrogen production for all five integral experiments. MELCOR calculations show good agreement with test data for PBF SFD1-1, SFD1-4, and FLHT-2, and poor agreement for FLHT-4 and FLHT-5. The poor agreement for the FLHT-4 test could be attributed to the following: (i) There was less zircaloy mass available for oxidation in MELCOR, since the liner, being a heat structure, was not allowed to oxidize; (ii) MELCOR does not model clad ballooning, and allows no oxidation on the inside of the clad after it fails, and (iii) MELCOR calculates more relocation than in the test, bringing zircaloy to cooler regions of the bundle, where oxidation is suppressed. For FLHT-5, the predictions were significantly improved (by about 55-60 %) by including the shroud liner as a canister component that could participate in oxidation. But the overprediction of relocation by MELCOR included significant relocation of the liner material, so that much less zircaloy from the liner was able to oxidize, as compared to the experiment. The better predictions for SFD1-1 and FLHT-2 tests can be partially attributed to less severe conditions in the tests resulting in almost no relocation, both observed and calculated. For SFD1-4, with a shorter length fuel bundle, and more severe conditions, there was significant relocation and the formation of blockages both calculated and observed in the test.

Changes in Bundle Geometry

The first indication of bundle geometry changes is clad ballooning. There is no explicit model for clad ballooning in MELCOR. Clad rupture is modeled to occur when the clad temperature at an axial cell exceeds a user-specified threshold temperature. This temperature has a default value of 1173K.

Table 2 [3] shows comparisons of measured (SFD 1-1) clad rupture times and location and MELCOR, SCDAP, and STCP predictions. Based on this comparison, the default value of 1173K, while not mechanistic, is adequate and need not be changed unless appropriate data is available for a given application.

For SFD1-4, MELCOR calculates 40 percent of fuel relocated during the transient [4]. This is a strong function of the assumed holdup temperature for the oxide shell in MELCOR (2600K in this case). An assumed holdup temperature of 2650K resulted in almost no relocation. The value of 2600K was selected based on observations of the SFD tests [14]. This sensitivity to user-input quantities clearly demonstrates the need for the user to be knowledgeable about the modeled phenomena.

During the FLHT-4 test, much of the fuel bundle metal components including the liner above 1.5m elevation was molten, but there was no indication of substantial relocation to lower bundle regions. In contrast, MELCOR calculated severe material relocation. Figures 11 and 12 [6] shown the UO_2 and zircaloy mass relocated, respectively, as calculated by MELCOR. The severe material relocation calculated by MELCOR could also be one of the reasons for the lower hydrogen production. For FLHT-5, MELCOR calculated severe material relocation (see Figures 13 and 14), area reduction, and also a period of 250 sec during which there was complete flow area blockage. The relocation caused early termination of oxidation, hence lower cumulative hydrogen produced. This deficiency also plagued the SCDAP code predictions of the test, in spite of artificially specifying a hold-up temperature of 3000K to minimize downward relocation of material.

Fission Product Release from Fuel

The release of fission products from fuel is modeled in MELCOR using either the original CORSOR or CORSOR-M formulation. Depending on user choice, these release rates can be modified to be a function of the surface-to-volume ratio (S/V) of the material compared to the ratio in the CORSOR experiments. Both models are based on the same experimental data using irradiated fuel. It can be expected, therefore, that agreement with data for fresh fuel will be poor and much better for irradiated fuel. This was confirmed by comparisons of MELCOR calculations using CORSOR and data for test SFD 1-1 which used fresh fuel and test SFD 1-4 that used irradiated fuel. These are shown in Table 3. In FLHT-2, there were no measurements of fission product release. For FLHT-4, MELCOR (1.8.1) somewhat overpredicts and SCDAP somewhat underpredicts the noble gas release. For FLHT-5, there is a large band of uncertainty in the measurements of noble gas release, with a best estimate of ~0.50. MELCOR (1.8.2) calculations using CORSOR are closer to the best-estimate values from the experiment than SCDAP.

MELCOR 1.8.2 also has two CORSOR-Booth models (for high-burnup and low-burnup fuels) available to the user [15]. Both these new models were used and found to predict much lower noble gas releases than measured data and the predictions from CORSOR.

Effect of Axial Nodalization

In the MELCOR core model, the bundle region is divided into concentric radial rings and axial segments that define core cells. Each cell may contain one or more components such as fuel pellets, cladding, etc.; and a lumped parameter approach is used for each component within a cell. For the FLHT-2 test simulation, besides the reference case with 20 axial segments in the bundle active region, three sensitivity cases with 5, 10, and 30 segments were also calculated. Comparisons of cladding temperatures are shown in Figure 15. Predicted values for hydrogen produced were 41g (20 segments), 27g (10 segments), and 26g (5 segments), compared to the measured value of 42g. The case with 20 segments appears to give predictions that are closer to experimental data, compared with the coarser nodalizations. The calculations with 30 segments gave results that were very close to the 20 segments case and are not shown here. Hence, the choice of 20 axial segments in the active length was justified for the reference case, and was retained for all subsequent test simulations.

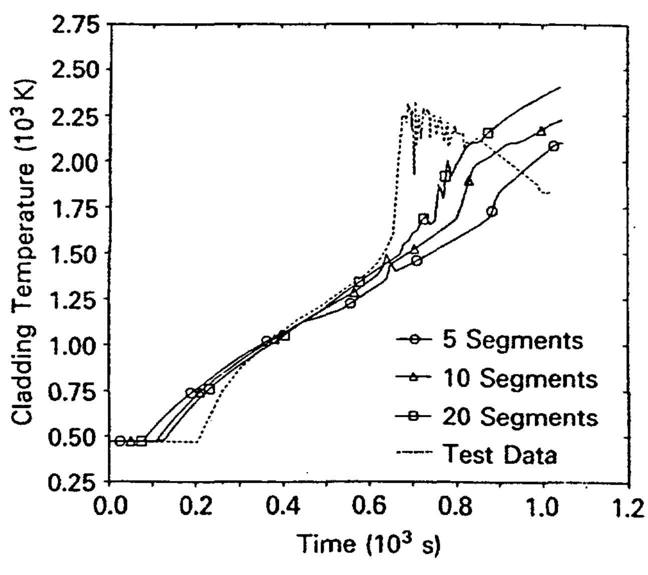

Figure 15. Impact of bundle nodalization on calculated clad temperatures, FLHT-2

Effect of Maximum Allowable Timestep

The maximum and minimum allowable timestep sizes are specified on MELCOR input. MELCOR calculates its system timestep based on directives from the various packages, but it cannot take timesteps greater than the maximum timestep or smaller than the minimum timestep. The selection of Δt_{max} and its impact on the calculational behavior of the code had been an area of lingering uncertainty in the use of earlier versions of MELCOR. For example, when the PBF SFD 1-1 calculation using MELCOR version 1.7.1 was performed with Δt_{max} = 10 s, 5 s, and 2 s, the results were seen to diverge rather than converge with the selection of Δt_{max} = 2 s [16]. In the FLHT-2 simulation using MELCOR version 1.8DN, the impact of Δt_{max} was found to be very small [5]. A similar exercise was attempted for the PBF SFD 1-4 test using version 1.8DN, but in each case, the calculation terminated due to a fatal code error. The impact of Δt_{max} was examined for the FLHT-4 simulation using MELCOR 1.8.1, by varying Δt_{max} from 0.5 s to 5.0 s. The case with 0.5 s gave the best clad temperature predictions, but earlier relocation, and less hydrogen and fission product release. The calculations appeared to converge with the selection of smaller Δt_{max}, prior to relocation. The FLHT-5 test was simulated using the recently released MELCOR version 1.8.2, which has corrections to mitigate numerical sensitivities. The effect of Δt_{max} was examined once again by varying Δt_{max} from 0.1 s to 5.0 s. The impact was insignificant for levels and clad temperatures. For hydrogen production, the maximum deviation was 8 % compared with 14 % for FLHT-4 using MELCOR 1.8.1. For noble gas releases, the maximum deviation was 10 %, compared to 16 % for FLHT-4 using MELCOR 1.8.1. While there was no convergence in going to a smaller Δt_{max}, there was a noticeable improvement in Δt_{max} sensitivity for MELCOR 1.8.2 [7].

Workarounds

Experience with the code has allowed the use of several innovative inputs or "workarounds" that were successful in extending the capabilities of MELCOR [16]. Most of them were used during MELCOR benchmarking analyses. For example, one can sometimes speed up a calculation if a problem control volume is eliminated without loss of physics. Initially, the MELCOR input model for the PBF SFD 1-1 test had a bypass volume, which received heat from the bundle region via the insulating shroud. During MELCOR simulation of the test, the timestep was severely restricted by Courant stability limitations. This problem was traced to the bypass volume which had very high flow through it. To improve timestep behavior, the bypass volume was replaced by a user-specified heat transfer coefficient (H_{ex}) on the outer surface of the shroud. The value of H_{ex} was selected based on actually calculated values of H_{ex} from the code. Sensitivity calculations showed the results to be insensitive to this parameter over a substantial range (5,000 - 15,000 W/m^2-K). That was expected, since the insulating shroud constitutes the largest resistance to heat transfer. This workaround increased the calculational Δt by more than a factor of 50. A similar effect was also achieved in integral plant calculations by eliminating unimportant control volumes.

Another more recent workaround was to model the FLHT-5 test train as a BWR geometry, which allowed the mass of zircaloy in the shroud inner liner, carriers, and clad of one unfueled rod, to be modeled as a canister component and hence participate in oxidation with steam, as in the experiment. This was a modeling change from earlier simulations which treated the test train as a PWR geometry, in which the liner, being treated as a heat structure, could not participate in oxidation. The impact of this modeling change was to increase predicted cumulative hydrogen production by about 55-60%.

CONCLUSIONS

The benchmarking calculations of integral severe fuel damage tests performed by BNL have helped to identify areas of modeling strengths and weaknesses in MELCOR, the most appropriate choice of input parameters and nodalization, and workarounds that allow the analyst to extend the capabilities of MELCOR. Examples of workarounds include eliminating unimportant control volumes, without loss of physics, to speed up calculations, and representing heat structures surrounding the core as BWR canisters to enable them to oxidize as in the test. These and other insights were explored in the paper, with the help of selected results and comparisons with test data and other calculations, for all five integral tests.

The benchmarking analyses were performed for different tests using different versions of MELCOR. In general, the earlier versions of the code had a difficulty in adequately simulating the sharp temperature rise associated with the autocatalytic oxidation of zircaloy in steam. However, as the simulation of FLHT-5 has shown, using MELCOR 1.8.2 appears to have significantly reduced that deficiency.

The PBF SFD tests were operated under steam starved conditions, hence the inability of MELCOR to model oxidation of the inner liner did not cause any problem in the prediction of the oxidation and hydrogen production compared to the experiment, which was, in fact, quite good. However, for FLHT-4 and especially FLHT-5, the hydrogen production was severely underpredicted by both MELCOR and SCDAP. For FLHT-4, one of the reasons for the poor prediction by MELCOR was that there was less zircaloy available to oxidise in steam, since MELCOR does not model the oxidation of heat structures, and the zircaloy inner liner and hard-line carriers were modeled as heat structures. The other reason is that the relocation model in MELCOR is logical-based, rather than rate-equation based, and was found to overpredict the relocation of core material to cooler regions of the bundle where oxidation is predicted to stop. For FLHT-5, the first limitation of the code was removed via innovative input, that is, by modeling the liner and hard-line carriers as a canister component of a BWR reactor core. However, while this workaround improved hydrogen production significantly (by about 55-60 %), the hydrogen generation was predicted to terminate early and was hence still substantially underpredicted. This can be attributed to the code predicting early and severe relocation to cooler regions of the bundle, where oxidation is suppressed. The massive relocation predicted by MELCOR also led to complete blockage of the bundle flow area for a period of 250 s, during which no hydrogen was predicted to form. This is contrary to post-test visual examination of the test bundle which showed evidence of relocation over the bundle region, but no massive relocation and complete blockage anywhere.

Another observation from the FLHT-5 test simulation is that the relocated material in MELCOR included the liner, while the experiment showed oxidation of the liner but almost no relocation. The liner was predicted to relocate along with the core material because it was mmodeled as part of the core. Based on this, a strong recommendation is made to add the capability in MELCOR to model oxidation of heat structures, as in SCDAP. The other recommendation is that the relocation model in MELCOR may need to be examined closely for its adequacy, since the code predicts severe material relocation and significant blockage in the lowest regions of the bundle, which is contrary to the post irradiation examination of the FLHT-4 and FLHT-5 fuel bundles.

An evaluation of MELCOR improvement has shown that MELCOR 1.8.2 is a more robust code, with significant improvement in its numerical behavior. Based on results from the FLHT-5 analyses, the selection of the most appropriate timestep size appears to be less critical with the new code version. Several new models have been added to MELCOR 1.8.2, that have enhanced MELCOR's modeling capabilities.

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