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Recent MELCOR and VICTORIA Fission Product Research at the NRC*

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ABSTRACT

The MELCOR and VICTORIA severe accident analysis codes, which were developed at Sandia National Laboratories for the U. S. Nuclear Regulatory Commission, are designed to estimate fission product releases during nuclear reactor accidents in light water reactors. MELCOR is an integrated plant-assessment code that models the key phenomena in adequate detail for risk-assessment purposes. VICTORIA is a more specialized fission-product code that provides detailed modeling of chemical reactions and aerosol processes under the high-temperature conditions encountered in the reactor coolant system during a severe reactor accident. This paper focuses on recent enhancements and assessments of the two codes in the area of fission product chemistry modeling.

Recently, a model for iodine chemistry in aqueous pools in the containment building was incorporated into the MELCOR code. The model calculates dissolution of iodine into the pool and releases of organic and inorganic iodine vapors from the pool into the containment atmosphere. The main purpose of this model is to evaluate the effect of long-term revolatilization of dissolved iodine. Inputs to the model include dose rate in the pool, the amount of chloride-containing polymer, such as Hypalon, and the amount of buffering agents in the containment. Model predictions are compared against the Radioiodine Test Facility (RTF) experiments conducted by Atomic Energy of Canada Limited (AECL), specifically International Standard Problem 41.

Improvements to VICTORIA's chemical reactions models were implemented as a result of recommendations from a peer review of VICTORIA that was completed last year. Specifically, an option is now included to model aerosols and deposited fission products as three condensed phases in addition to the original option of a single condensed phase. The three-condensed-phase model results in somewhat higher predicted fission product volatilities than does the single-condensed-phase model. Modeling of UO_2 thermochemistry was also improved, and results in better prediction of vaporization of uranium from fuel, which can react with released fission products to affect their volatility. This model also improves the prediction of fission product release rates from fuel.

Finally, recent comparisons of MELCOR and VICTORIA with International Standard Problem 40 (STORM) data are presented. These comparisons focus on predicted thermophoretic deposition, which is the dominant deposition mechanism. Sensitivity studies were performed with the codes to examine experimental and modeling uncertainties.

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1.0. Introduction

MELCOR [1] and VICTORIA [2] are computational tools that have been developed by Sandia National Laboratories for the U. S. Nuclear Regulatory Commission (USNRC). The two codes are similar in many respects but also have distinct differences. Both codes are intended for severe accident analysis of light water reactors and treat fission product release from fuel and transport through the reactor coolant system (RCS). However, MELCOR provides an integrated analysis while VICTORIA is more detailed but not fully integrated.

MELCOR includes models of thermal hydraulics, melt progression, fission product release from fuel, and fission product transport within the RCS and containment. These models are all fully integrated. VICTORIA, on the other hand, models fission product release and transport in a highly detailed fashion, melt progression in minimal detail, and thermal hydraulics not at all. MELCOR is primarily used to perform integrated analyses of reactor safety issues; VICTORIA is also used to perform analyses of reactor safety issues, but primarily to assess fission product behavior and to benchmark MELCOR.

2.0. Recent MELCOR Development, Testing, and Applications

Much has been accomplished since the release of MELCOR 1.8.4 in July 1997. In the area of model development, an iodine aqueous chemistry model has been developed and implemented. Also, the treatment of control and support structures has been improved. This latter accomplishment paves the way for future improvements in modeling of melt progression. In the area of testing, two International Standard Problems (ISPs) have been used to assess aerosol deposition models and the new aqueous chemistry model. These are described in this section and in Section 4. The primary USNRC application since the release of MELCOR 1.8.4 was to evaluate margin and containment thermal hydraulics for rebaselining with the revised source term [3,4].

The main function of the iodine aqueous chemistry model in MELCOR is to determine the partitioning of iodine within the reactor containment among an aqueous pool, the atmosphere, and surfaces. This partitioning is important because it affects potential fission product releases to the environment. The approach taken in developing this model is to use a relatively mechanistic treatment so that future refinements can easily be made. The model currently treats water radiolysis, atmosphere radiolysis (primarily formation of nitric and hydrochloric acids, which can acidify the aqueous pool), changes in pool pH, effects of buffering agents, mass transfer between pool and atmosphere and between atmosphere and surfaces, and formation of organic iodides. Iodine kinetics in the pool are assumed to be rapid (i.e., iodine species are assumed to be in equilibrium).

MELCOR was recently validated against International Standard Problem 41 (ISP-41), which is an iodine pool experiment conducted in the Atomic Energy of Canada, Ltd., (AECL) radioiodine test facility (RTF). The final report for ISP-41 is not yet available. The single test that was performed for this ISP was done in two phases, each with its own pH history. A schematic of the RTF is shown in Figure 1. The main vessel used in the ISP-41 test contained an aqueous iodine pool, an atmosphere, and surfaces on which iodine could deposit. An aqueous recirculation loop was used to keep the pool well mixed and to regulate pool pH. A gas recirculation loop was used to keep the atmosphere well mixed and to monitor H_2 production. An aqueous sampling loop was used to monitor pH and aqueous iodine concentrations. Participants in this ISP were provided with the test configuration, conditions such as temperature and total

iodine content, and pH history. Participants were required to calculate the partitioning of iodine among the pool, atmosphere, and surfaces.

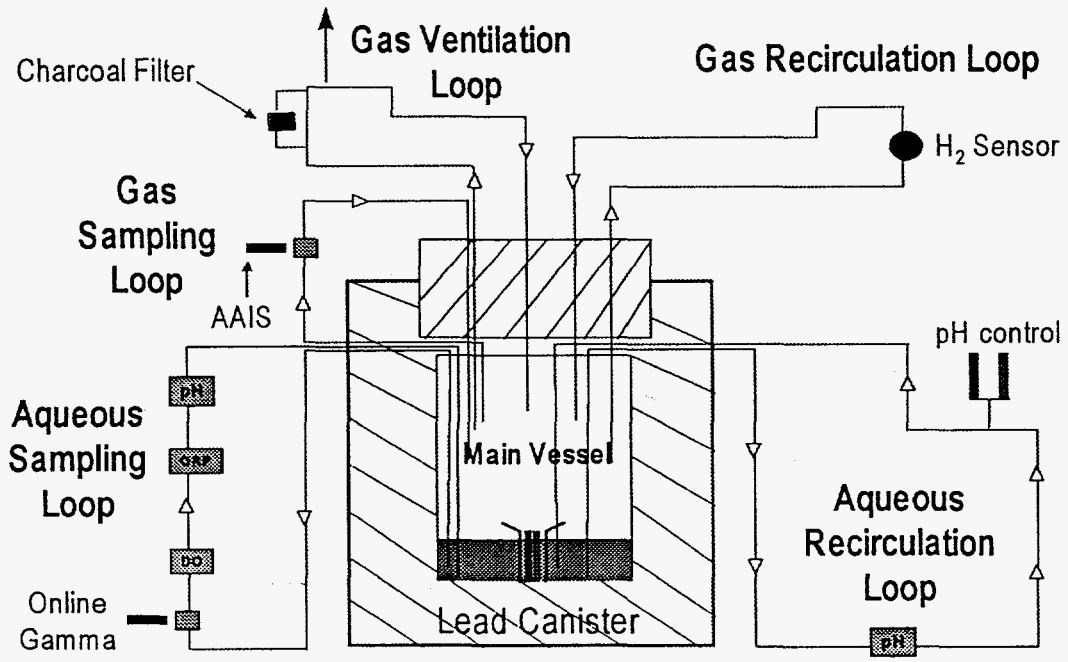

Figure 1. Schematic of the ISP-41 test configuration.

Phases 1 and 2 of ISP-41 were similar, so results for only one of these are shown here. Phase 2 is presented because pH was varied over a wider range and because the pH history is composed of a series of step functions separated by plateaus, as shown in Figure 2. Because of the simple nature of the pH history, the results are somewhat easier to describe than those for Phase 1.

MELCOR predictions for the number of moles of iodine on surfaces and for the concentrations of iodine in the atmosphere and pool are shown in Figures 3 through 5, respectively. A rapid decrease in pool pH results in a sudden increase in the concentration of iodine in the atmosphere because iodine is less soluble in the pool at lower pH, as seen by comparing Figures 2 and 4. This rapid change is an equilibrium chemistry effect. The sudden increase is followed by a gradual decrease in atmospheric iodine concentration. During the gradual decrease, iodine partitions out of the aqueous pool and onto surfaces. The time scale for the gradual decrease is controlled not by chemistry but by mass transfer. At the end of the test the pH is suddenly increased back to the initial value of about 10. This results in a very gradual redistribution of iodine from the surfaces back to the pool. The time scale for this process is also controlled by mass transfer.

Figures 3 through 5 do not show the experimental data, but the MELCOR predictions are within a factor of three of the data. While a factor of three sounds large, it is considered good agreement for this type of model and is as good as other participants in this ISP were able to obtain.

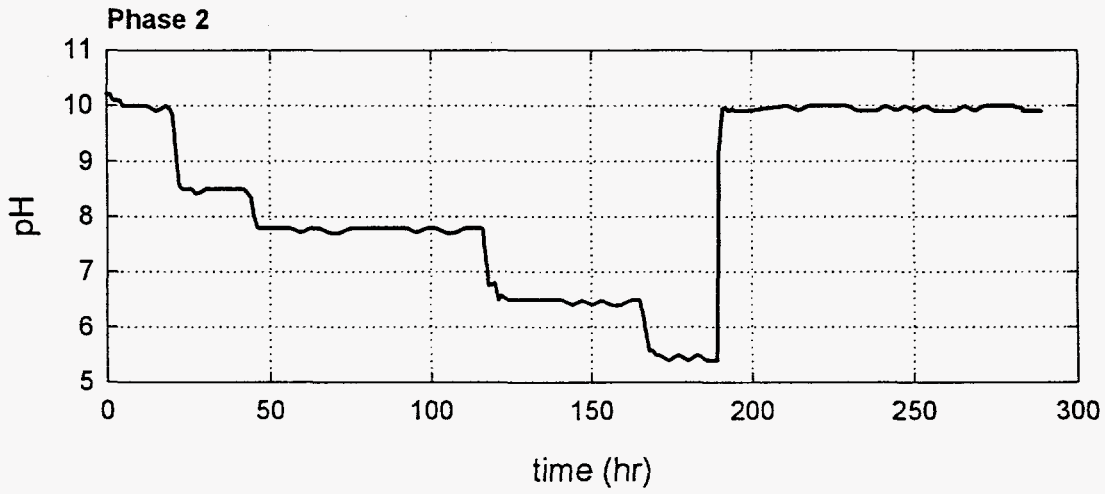

Figure 2. pH history for Phase 2 of the ISP-41 test.

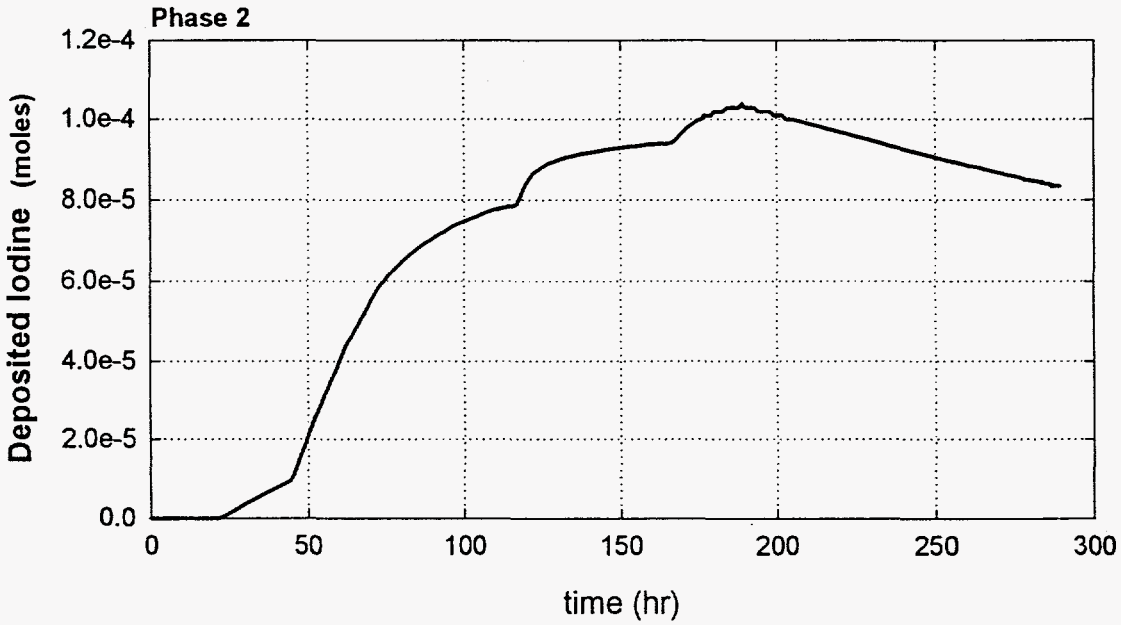

Figure 3. MELCOR-predicted moles of iodine on surfaces for Phase 2 of the ISP-41 test.

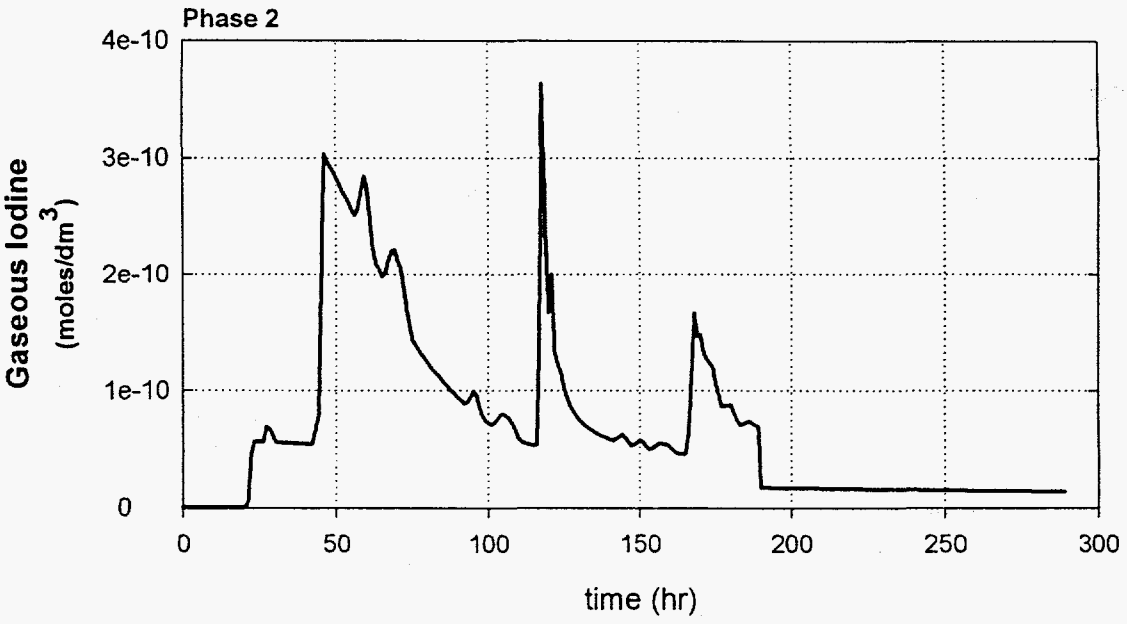

Figure 4. MELCOR-predicted gaseous iodine concentration for Phase 2 of the ISP-41 test.

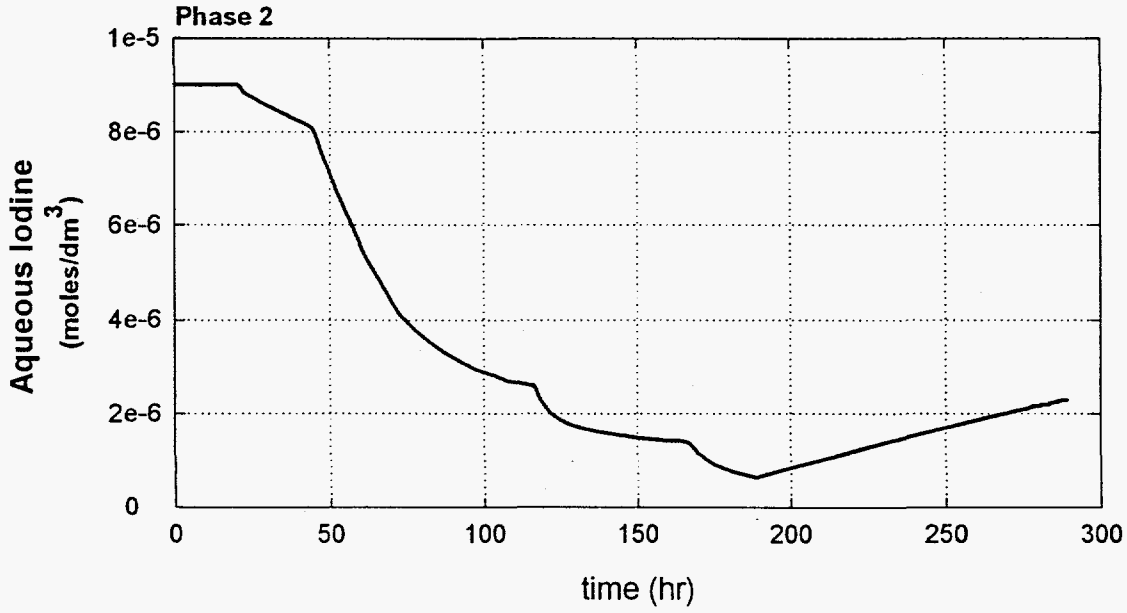

Figure 5. MELCOR-predicted aqueous iodine concentration for Phase 2 of the ISP-41 test.

3.0. Recent Improvements in VICTORIA

A peer review of the VICTORIA code was completed in 1997 [5]. Recommendations from the peer review committee were categorized as findings and high-, medium-, and low-priority concerns. To date, all of the findings and high-priority concerns have been addressed. Plans are to address the medium-priority concerns during 1999.

A new code version, VICTORIA 2.0 [1], has resulted from implementation of the peer review findings and high-priority concerns, as well as improvements that had been made prior to the peer review. The improvements are in two major areas: chemistry and user friendliness. Chemistry improvements include an option to treat three condensed phases as opposed to a single condensed phase and an improved treatment of fuel thermochemistry, which incorporates Blackburn's analysis of the thermochemistry of $UO_{2\pm x}$. Implementation of this latter model modifies predictions of releases of fission products from fuel and especially predictions of uranium release from fuel. At this point, Blackburn's model is implemented only for UO_{2+x}, where x is greater than 0. Improvements in user friendliness include warnings when thermal-hydraulic inputs have been chosen in an inconsistent manner and when the time-step size is larger than the Courant limit.

Other improvements in VICTORIA 2.0 include a treatment of fission product release from rubble beds based on the Booth approach, chemisorption models for HI and I_2, a simple model for chemical kinetics at low temperatures, a model for aerosol deposition in a vena contracta, simplified input of bulk gas flow rates, and a method for representing a domain (mathematical representation of a physical region) as coupled subdomains. That last improvement is especially useful for complex geometries and for sensitivity studies.

4.0. Comparisons of MELCOR and VICTORIA with ISP-40 Deposition Data

International Standard Problem 40 (ISP-40) was performed at the STORM facility in Ispra, Italy. This ISP test consisted of two phases: In the first, aerosols were deposited in a 5-m test section; in the second, part of the aerosols were mechanically resuspended. The ISP-40 test configuration is shown schematically in Figure 6. Aerosols and vapors were injected into a large chamber upstream of the test section. Flow through the test section was from left to right. Aerosol size distributions were measured upstream and downstream of the test section through sampling ports not shown in the schematic.

Conditions during the deposition phase of the ISP-40 test were nearly steady state. The test configuration, surface and gas temperatures, and mass injection rates were provided to participants of the ISP. Participants were required to calculate the final deposition profile for comparison with estimated data. Data for the deposition phase of the test were only estimated because direct measurement would have precluded conduct of the second phase of the test in which the deposited aerosols were mechanically resuspended. Greater confidence should be placed on the overall quantity of aerosol that deposited (which was determined by mass balance) than on the deposition profile (which was estimated using results from previous tests).

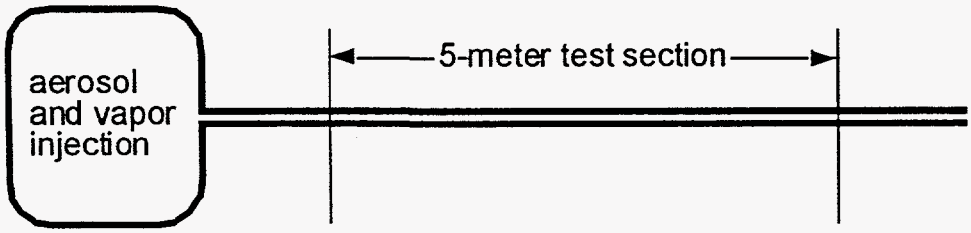

Figure 6. Schematic of the ISP-40 test configuration.

4.1. Modeling Considerations

Several considerations are central to modeling of aerosol deposition during an ISP-40 test. First, it is important to represent the aerosol size distribution well; this had a geometric mean of 0.43 μ and a standard deviation of 1.7. Furthermore, because only a small fraction of the aerosols deposit as they pass through the test section and agglomeration is relatively unimportant, the size distribution is nearly the same at the entrance and exit.

The second consideration is the appropriate calculation of the Reynolds number in each computational node. Many codes, including MELCOR and VICTORIA, compute the Reynolds number based on an average of inflow and outflow velocities for a node. If vapors are injected into the first computational node as a source, then the inflow velocity is zero and the Reynolds number in the first node is calculated to be one-half of the correct value. There are several ways to overcome this problem; the best is usually to create a dummy upstream node. If the Reynolds number is calculated incorrectly in the first node, then the predicted deposition profile will exhibit an unphysical depression at the upstream end of the test section.

All participants in ISP-40 determined that thermophoresis was the dominant deposition mechanism during the deposition phase of the test. This implies that the differences between gas and surface temperatures strongly influence predictions of the deposition profile. ISP-40 participants were provided with surface temperature data that were measured with thermocouples and gas temperature data that were calculated using a heat-transfer correlation. Some codes, like VICTORIA, were able to use the supplied data for surface and gas temperatures directly; other codes, like MELCOR, calculated their own gas temperatures given the surface temperatures. To match the ISP-supplied gas temperature profile, some participants modified the heat-transfer correlation used in MELCOR. However, modifying this correlation also modifies the calculated gas temperature gradient near the surface, which directly influences thermophoresis in the MELCOR treatment. This point is discussed further in the next subsection.

Finally, some codes, such as MELCOR, calculate the deposition and agglomeration integrals only at a few points in temperature and pressure, then interpolate to get values at intermediate temperatures and

pressures. MELCOR calculates these integrals at four points representing two pressures and two temperatures. By default, the temperatures are 273 and 2000 K and the pressures are 1 and 200 bar. These broad ranges are appropriate for severe accidents but are not generally appropriate for small-scale tests like ISP-40. This point is also discussed further in the next subsection.

4.2. MELCOR Analyses

Three MELCOR calculations were performed, which represent a base case and two sensitivity cases. The first, or base, case was to specify the gas injection temperature according to the ISP recommended value but to let MELCOR calculate the gas temperature profile according to the default internal correlation for heat transfer. Adjusting the default heat-transfer correlation to better match the ISP-provided gas temperature profile was considered, but this idea was rejected because of the direct impact on thermophoretic deposition. Figure 7 compares the ISP-provided and the MELCOR-calculated gas temperature profiles. Because the MELCOR-calculated profile was somewhat lower than the ISP-provided profile, a second case was run with an inlet temperature that was 12 K higher than the recommended value. This resulted in about a 10% increase in the difference between gas and surface temperatures at the inlet. The MELCOR-calculated temperature profile for Case 2 is also shown in Figure 7. Case 3 was run with the same inlet temperature as Case 2, but used a narrower range of temperatures and pressures for calculating the agglomeration and deposition integrals: 550 and 650 K for temperature and 1 and 1.5 bar for pressure.

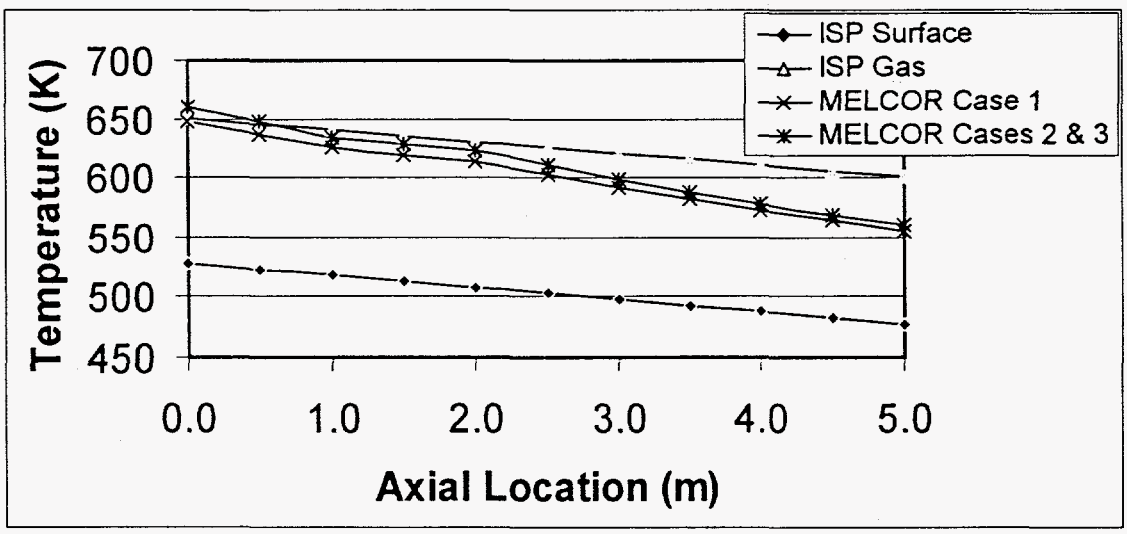

Figure 7. ISP-provided surface and gas temperature data MELCOR-predicted gas temperatures for Case 1 and for Cases 2 and 3.

Figure 8 shows the ISP-estimated and MELCOR-predicted deposition profiles for the three cases. For all cases, the MELCOR predictions are in very good agreement with the estimated data. The higher gas inlet temperature used in Case 2 than in Case 1 results in a modest improvement in agreement with the data. The agreement between Case 3, which used a narrower range of temperatures and pressures for calculation of the agglomeration and deposition integrals, and the estimated data is excellent.

Predicted total masses deposited in the test section for Cases 1, 2, and 3 were 127, 137, and 163 g, respectively. The measured total deposition was 162 g. This level of agreement between predictions and data is much better than that achieved by the ISP-40 participants [7] and was achieved without any attempt to tune the standard correlations used in MELCOR. In fact, it appears that the MELCOR-calculated gas temperature profile may be a better representation of actual conditions than the one provided to the ISP participants. This point is discussed further in the next subsection.

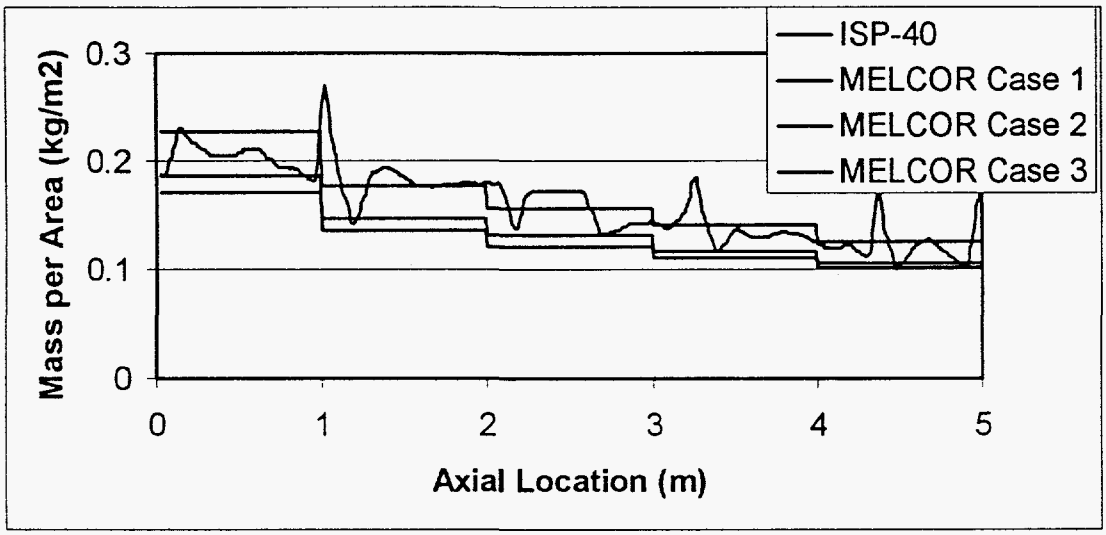

Figure 8. ISP-estimated deposition data and MELCOR-predicted deposition profiles for the three cases.

4.3. VICTORIA Analyses

Two VICTORIA cases are described. Other cases were run to demonstrate that predicted results were relatively independent of the number of nodes and of time-step size. It was determined that 5 nodes (plus an upstream dummy node) and a time step of 0.025 s were sufficient to give good predictions. With these choices, VICTORIA ran at approximately real time. (VICTORIA and MELCOR run times were similar.) The two cases, Cases 1 and 2, were performed with the ISP-supplied and the MELCOR-predicted gas temperature profiles, respectively. As with the three MELCOR cases, the ISP-provided surface temperature data were used. Thus, the surface and gas temperatures used in VICTORIA are the ones shown in Figure 7.

Figure 9 shows the VICTORIA-predicted deposition profiles for the two cases. The equation used to represent thermophoretic deposition in VICTORIA is the same as the one used in MELCOR, namely the Brock equation [8]. However, VICTORIA uses as defaults the coefficients recommended by Talbot et al. [9], while MELCOR uses coefficients similar to the original ones recommended by Brock. As seen by comparing Case 3 in Figure 8 and Case 2 in Figure 9, predicted thermophoretic deposition is greater using the Talbot et al. coefficients than using the Brock coefficients. The same trend is observed for other participants in the ISP who used the Talbot et al. coefficients in their analysis.

Many experts in aerosol science regard the Brock equation with the coefficients proposed by Talbot et al. as the best model available for thermophoretic deposition. It should not be argued based on this single comparison that the Talbot coefficients should be discarded in favor of the original coefficients proposed by Brock, because the preponderance of evidence goes the other way.

A second point to note from Figure 9 is that using the ISP-provided gas temperature profile (Case 1) results in nearly a flat deposition profile, which is because the temperature difference between the gas and the wall is nearly uniform. This result is not in agreement with the estimated trend, where mass per surface area decreases approximately linearly from inlet to outlet of the 5-m test section. The trend using the MELCOR-predicted temperature profile (Case 2) is in much better agreement with the estimated trend than that obtained using the ISP-provided profile. This indicates that the heat-transfer correlation in MELCOR is a better approximation than the one used in the ISP. This may explain, at least in part, why the deposition profiles predicted by ISP participants did not match the trend of the estimated data.

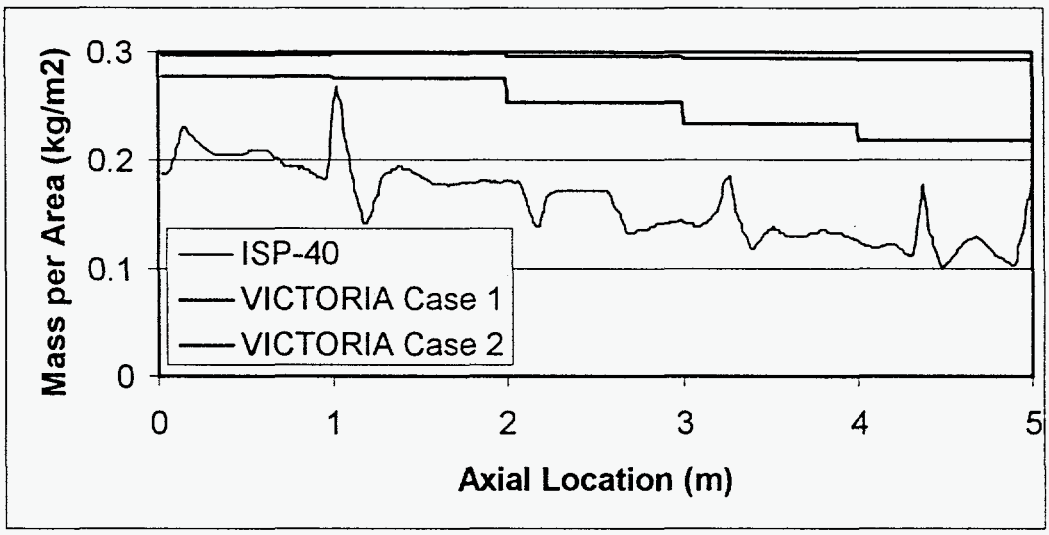

Figure 9. ISP-estimated deposition data and VICTORIA-predicted deposition profiles for the two cases.

The total deposited masses predicted by VICTORIA for Cases 1 and 2 were 293 and 249 g, respectively. These are both significantly higher than the measured value of 162 g, but are consistent with other codes using the Brock/Talbot correlation. Futhermore, this level of agreement is considered by the authors to be acceptable.

5.0. Status and Future Directions

Development and application of both MELCOR and VICTORIA are continuing. Some of the ongoing and future activities are described in this section.

5.1. Status of MELCOR and VICTORIA

MELCOR model development continues in several areas, including reflood/quenching phenomena, core degradation modeling improvements, and iodine chemistry modeling. Currently, a comprehensive test matrix is being developed. The test matrix will include experimental data and International Standard Problems on core degradation, fission product release and transport, and containment phenomena. The matrix will also include plant applications. Future activities will include a strong emphasis on assessment analyses.

Peer review findings and high-priority concerns have been addressed. The modified code version, VICTORIA 2.0, has been tested and is scheduled to be released, along with supporting documentation, by the end of 1998. Medium-priority concerns from the peer review will be addressed during 1999. Ongoing work with the VICTORIA code includes further applications to plant sequences, analyses of Phebus tests, and benchmarking of MELCOR. Experience with the VICTORIA code will be used as a basis for recommendations on improvements to the MELCOR code.

5.2. Future Directions for MELCOR and VICTORIA

There are several specific areas slated for model development for the MELCOR code: (1) improved modeling of failure of support structures, (2) improved geometrical representation of boiling water reactor (BWR) flow channels, (3) implementation of a BWR core spray model, (4) implementation of a core reflood model, (5) implementation of a passive autocatalytic recombiner model, (6) expanded control function capability, (7) upgrades in core degradation modeling, and (8) improved modeling of in-vessel/ RCS natural circulation phenomena.

Further work in the area of testing and assessment of MELCOR is also planned. This work will investigate accumulator water injection during a Surry 6-inch cold leg break sequence, evaluate natural circulation in the core for a Surry TMLB' sequence, and develop a comprehensive test matrix.

Future development of the VICTORIA code is being guided by recommendations made during the peer review [5]. The next phase of development will focus on the medium-priority concerns, which include the following: (1) revise the interpolation scheme for Gibbs free energy data; (2) add a treatment for hypostoichiometric fuel, i.e., for UO_{2-x}; (3) add carbon species to the thermochemical database so that boron control blades and rods can be modeled; (4) investigate the effects of porous media parameters that are used in modeling fission product release from fuel; and (5) modify the XMGR5 code to interface with VICTORIA graphics data to provide simplified postprocessing.

Several applications are planned for the VICTORIA code. These include evaluating the sensitivity of off-site releases to the level of detail of the chemistry modeling, benchmarking MELCOR, recommending improvements for the MELCOR code based on insights gained with VICTORIA, and analyzing some of the Phebus FPT series tests.

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