Uncertainty Analyses Using the MELCOR Severe Accident Analysis Code

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Abstract

The MELCOR code is a detailed system level computer code capable of performing integrated self-consistent analyses of severe accident progression in commercial nuclear power plants, supporting level 2 probablilistic risk assessment (PRA) studies. Originally developed as a fast running tool with simplified models for performing probabilistic safety analyses and sensitivity studies, MELCOR now employs largely best estimate models for severe accident phenomena while retaining rich capabilities for performing sensitivity and uncertainty analysis. Extensive user access to fundamental coefficients and parameters of MELCOR underlying physics models combined with the advent of fast and increasingly economical computing power has enabled complex system models like MELCOR to be applied to uncertainty analyses such as those performed using Monte Carlo and Latin Hypercube Sampling (LHS) methods. This paper illustrates two such recent applications of MELCOR 1.8.5 to the uncertainty analysis of hydrogen production and of containment aerosol behavior in severe reactor accidents. The examples illustrated in this paper show both the application of LHS to accommodate computationally intensive accident models and a Monte Carlo analysis involving larger sample size for less computationally intensive analyses to attain better sampling statistics.

Keywords: Severe accidents, light water reactor accidents, MELCOR, melt progression, uncertainty analysis, Monte Carlo Sampling, Latin Hypercube Sampling, risk informed regulation.

1. Introduction

In support of risk-informed regulation the MELCOR code has been used recently in a probabilistic mode, making use of sampling of uncertain code input values in order to produce an estimate of a distribution of code predictions with quantified statistical variances owing to the uncertainties in code input. This approach is being pursued as an alternative to traditional deterministic analyses that are often conservative in nature with uncharacterized safety margins. In the probabilistic approach, best estimate modeling methods are applied together with a quantitative uncertainty analyses in order to provide an objective means of quantifying reasonable and not-overly-conservative safety margins for regulatory decision processes. This paper illustrates two such recent applications of the MELCOR code, one [Gauntt, 2005] using Latin Hypercube Sampling [Helton, 2002; Wyss, 1998] to assess expected variability in in-vessel hydrogen production, and a second application using traditional Monte Carlo sampling [Gauntt, 2004] involving assessment of aerosol fallout behavior in a reactor containment.

The first application was focused on determining an estimate of the amount of hydrogen that might be expected under station blackout conditions in an Ice Condenser plant housing a 4-loop Westinghouse pressurized water reactor (PWR). Because the supporting analyses were particularly time intensive, LHS sampling was employed to gain optimum coverage of parameters using only 40 samples.

The second application made use of a fast running MELCOR model of the AP1000 containment to evaluate aerosol deposition behavior, and for this study simple Monte Carlo sampling was employed involving 150 code realizations. Both analyses used the MELCOR code [Gauntt et al., 2001] as the system model to propagate uncertain parameters and estimate resulting distributions of particular figures of merit. Following sections will provide a brief overview of the MELCOR severe accident analysis code and its application to two different kinds of "level 2" analysis applications, illustrating two different methodologies for applying computationally intensive analysis codes in an efficient manner for uncertainty analyses.

2. MELCOR Severe Accident Analysis Code

MELCOR is a fully integrated, engineering-level computer code whose primary purpose is to model the progression of accidents in light water reactor nuclear power plants. A broad spectrum of severe accident phenomena in both boiling and pressurized water reactors is treated in MELCOR in a unified framework. In addition, MELCOR is also used in the analysis of hazardous material transport in non-nuclear power plant facilities.

The MELCOR code is composed of an executive driver and a number of major modules, or packages, that together model the major systems of a reactor plant and their generally coupled interactions. Reactor plant systems and their response to off-normal or accident conditions include:

- thermal-hydraulic response of the primary reactor coolant system (RCS), the reactor cavity, the containment, and the confinement buildings,
- core uncovering (loss of coolant), fuel heatup, cladding oxidation, fuel degradation (loss of rod geometry), and core material melting and relocation,
- heatup of core support structures and reactor vessel lower head from relocated fuel materials, and the thermal and mechanical loading and failure of the vessel lower head, and transfer of core materials to the reactor vessel cavity,
- core-concrete attack and ensuing aerosol generation,
- in-vessel and ex-vessel hydrogen production, transport, and combustion,
- fission product release (aerosol and vapor), transport, and deposition,
- behavior of radioactive aerosols in the reactor containment building, including scrubbing in water pools, and aerosol mechanics in the containment atmosphere (such as particle agglomeration and gravitational settling), and,
- impact of engineered safety features on thermal-hydraulic and radionuclide behavior.

Figure 1 shows an illustration of the scope of severe accident phenomena treated in MELCOR in an integrated and self consistent calculational framework.

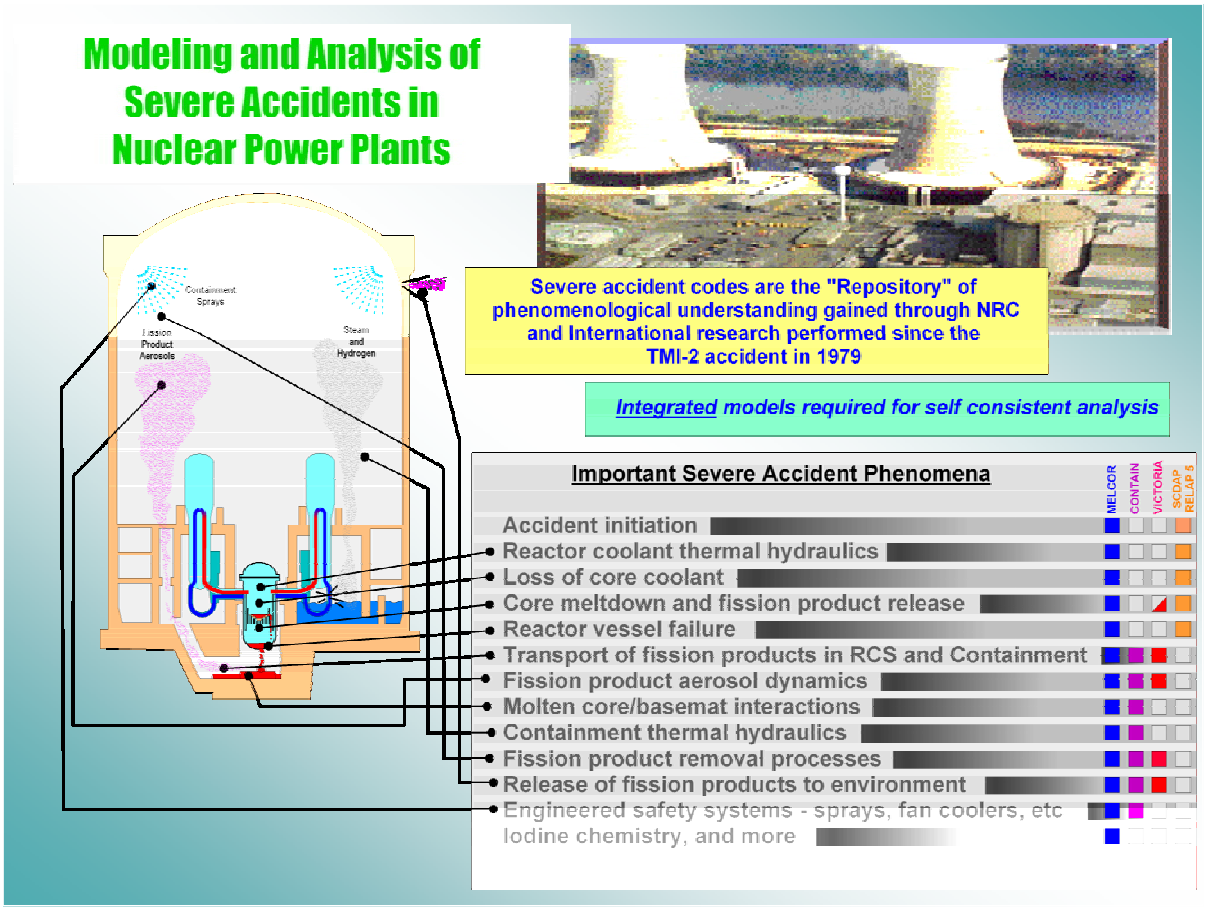

Figure 1 Illustration of the scope of MELCOR severe accident modeling.

3. Sequoyah Hydrogen Uncertainty Analysis

The objective of this first study was to characterize uncertainty in the hydrogen produced from in-vessel processes, predicted using the MELCOR severe accident analysis code for an un-recovered station blackout accident in the Sequoyah Ice Condenser plant. Sources of uncertainty considered were principally physics and modeling uncertainties associated with the melt progression and hydrogen generation models in MELCOR. While this study has emphasized uncertainty in hydrogen production, the methodology can be used to characterize uncertainty in the prediction of other issues, such as fission product source terms.

Hydrogen is produced in a severe accident in the reactor core when loss of water results in sufficiently high Zircaloy cladding temperatures that an exothermic Zr-steam oxidation reaction occurs, producing heat and hydrogen gas. The heat produced from the oxidation escalates the reaction rate producing a thermal runaway. The heat from Zr oxidation can be the principal heating term that drives the initial fuel failure and melting in an unrecovered accident. Hydrogen can also be produced after vessel failure by interaction between molten core materials and the concrete basemat, again driven by metal-water oxidation; however, in this case the source of metal includes that contained in the core materials and the concrete reinforcing steel, and the source of water is from the concrete ablation and dehydration. Once in the containment building, hydrogen buildup is of concern owing to the potential for deflagrations or explosions that might compromise the integrity of the containment building. Hydrogen control can be exercised by use of igniters whose purpose is to burn the hydrogen before high concentrations can be accumulated. The uncertainty characterization of hydrogen generation in a

station blackout accident can be used to perform assessments of igniter and recirculation fan efficacy in ice condenser plants and to assess the advisability of providing backup power to igniters under short term station blackout (STSBO) conditions.

In this study, the analyses are carried out using the MELCOR code, version 1.8.5 [Gauntt 2001]. This includes coupled analysis of initiating RCS thermal hydraulics, coolant loss, heating of core fuel and cladding, initiation of cladding oxidation and hydrogen production, core melting and relocation, RCS heatup and failure, fission product release and transport, and thermal hydraulic response of the containment.

The basic approach of this methodology is to 1) identify the MELCOR input parameters, sensitivity coefficients, and modeling options that describe or influence the predicted quantity of interest (hydrogen generation), 2) prescribe likelihood descriptions of the potential range of these parameters, and 3) evaluate the code predictions using a number of random combinations of parameter inputs sampled from the likelihood distributions. This method of characterizing uncertainty in reactor accident progression is quite similar to the method used by Khatib-Rahbar [Khatib-Rahbar, 1989] where an ensemble of computer codes known as the Source Term Code Package (STCP) was used. Our approach represents an improvement to the STCP-based method in that greater consistency in physics integration is offered by the modern MELCOR code system. In order to limit the number of "realizations" (code calculations) needed to characterize the full range of uncertainty, the Latin Hypercube Sampling method [Wyss, 1998] (LHS) is used to sample the input parameter distributions. Alternatively, simple Monte Carlo sampling can also be used. Later in this paper we compare the results of this study with the expert elicitation process for characterizing uncertainty used in the NUREG-1150 project [Harper, 1990].

In this study, we have focused primarily on the characterization of knowledge-based uncertainties affecting hydrogen generation for a specific accident scenario, STSBO, for the Sequoyah Ice Condenser plant. Knowledge-based uncertainty refers to uncertainties in the modeling of the physical processes affecting hydrogen generation as opposed to uncertainties in the accident boundary conditions, such as STSBO sequence variations for example.

3.1. MELCOR Model of Sequoyah Ice Condenser Plant

The MELCOR model of the Sequoyah plant is comprised of a 4-loop Westinghouse nuclear steam system (3411MWth) housed in an ice condenser type containment system. Details on the plant are taken from the Sequoyah Final Safety Analysis Report-1974. The MELCOR code does not contain any predefined models of reactors or containments. Such models are assembled using primitive elements in MELCOR which include heat structures, control volumes and flow paths. MELCOR includes special core components such as fuel, cladding and control materials and containment specific features such as sprays, fan coolers and ice beds. User-programmable control functions provide active dynamic specification of plant behavior such as opening of valves and failure of RCS components. Using these primitive components, quite detailed and dynamic models of reactor systems can be developed. Figure 2 shows the MELCOR thermal hydraulic nodalization of the core region of the reactor vessel. The core model uses 5 radial rings and 4 axial levels in the core region with additional thermal hydraulic volumes in the lower and upper plenum. The thermal hydraulic volumes are connected by flow paths that prescribe the flow resistances as affected by fuel assemblies, degraded core geometry and open flow regions. The nodalization allows for simulation of two-dimensional flow.

Figure 3 similarly shows the thermal hydraulics nodalization of the balance of the RCS. In this model three steam generators are lumped into one equivalent generator and the remaining steam generator on the pressurizer loop is modeled individually. In addition, the hot legs of each generator are nodalized

to allow for prediction of counter current natural circulation flow when the loops become voided of water. This involves a recirculation loop between the vessel upper plenum and the steam generator, where the hot leg carries an outgoing “hot” flow in the upper half of the pipe and a cooler flow returning to the vessel in the lower half of the hot leg. This circulation pattern occurs when cooler steam in the steam generator exit plenum below the tube sheet seeks a buoyancy driven return path to the entrance plenum by reversing flow directions. In this situation about half the steam generator tubes on the normally up-flow side are actually in down flow, returning cooler steam to the inlet plenum. This phenomena affects heatup of the hot leg and steam generator tubes and can influence where RCS failure and system depressurization might first occur.

Finally, Figure 4 shows the thermal hydraulic nodalization used in the containment building housing the ice beds. The RCS nodalization resides within the containment nodalization and the two are connected via flow paths representing relief valves, leaking pump seals, and potential RCS failure locations such as the vessel lower head and the RCS hot leg. The RCS failure locations open flow paths from the RCS to the containment whenever component failure criteria are met. Larsen-Miller (LM) type failure criteria are used to determine failure of the lower head and RCS hot leg. In the lower head the LM model uses a one dimensional treatment considering the thermal gradient through the head wall [Gauntt et al., 2001, COR Reference Manual, pg.103], whereas, for the hot leg, a similar zero dimension model is applied using the single lumped wall temperature. It is often observed that these components can fail suddenly whenever transient primary system pressurizations occur such as might be accompanied by relocation of degrading core materials into a water-filled lower vessel plenum. Pump seals are modeled to leak initially at 25 gallons per minute due to loss of back pressure during station blackout, and to later degrade to 250 gallons per minute when high steam temperatures in the RCS are judged to degrade the elastomer seals in the pumps.

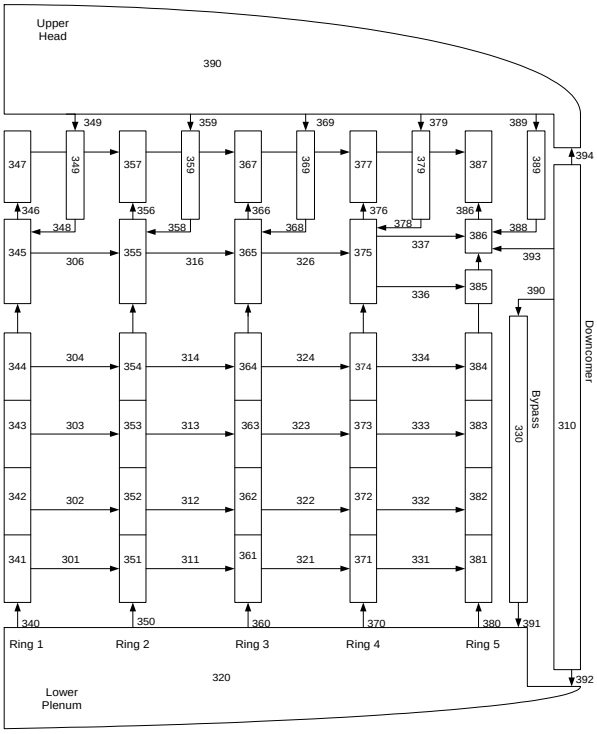

Figure 2 Thermal hydraulic nodalization of the reactor core and vessel.

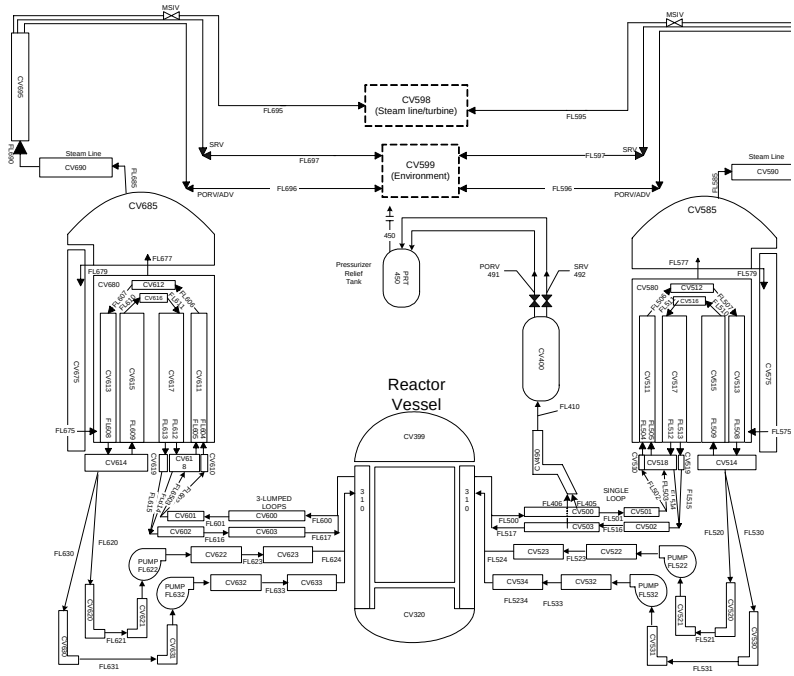

Figure 3 Thermal hydraulic nodalization of the reactor coolant system with ability to model counter-current natural circulation.

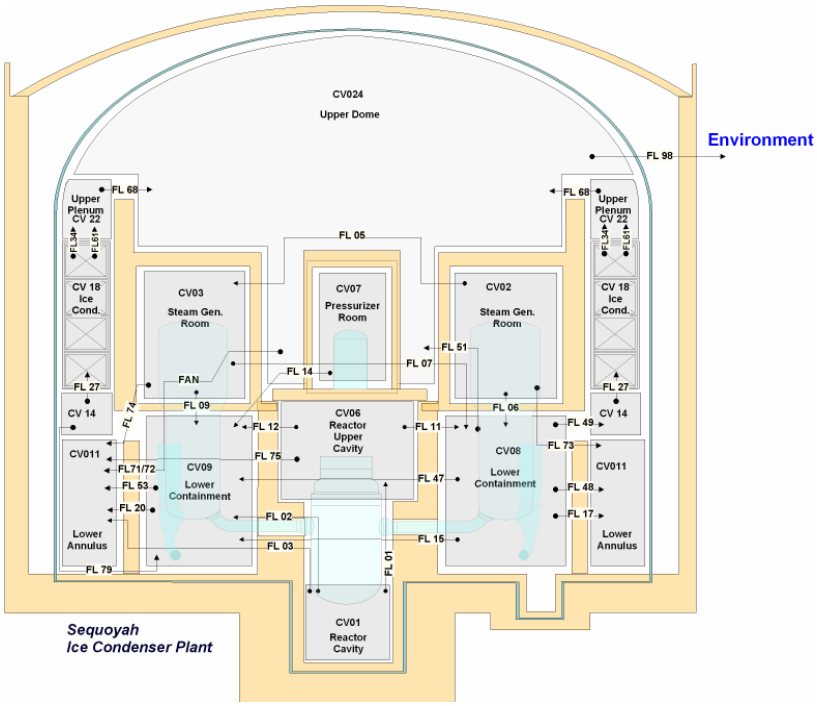

Figure 4: Thermal hydraulic nodalization of the ice condenser containment.

3.2. Sampling Strategy in Hydrogen Uncertainty Study

The MELCOR analysis of in-vessel hydrogen generation required use of all major MELCOR physics packages and a detailed RCS nodalization in order to produce the best estimate predictions desired in this study. For this reason, the computer execution time was on the order of days for each analysis

performed. In order to minimize the total computer execution time required in performing an uncertainty analysis, LHS sampling involving 40 separate calculations sampling 11 independent uncertainty parameters was used in this study. To minimize the total clock time to perform the 40 analyses, a large cluster of processors on the Sandia Laboratories QT system was used to perform all 40 analyses simultaneously. Until recently, adequately fast and inexpensive massive computing resources such those used in this study have not generally been available. This example provides an illustration of a strategy to perform computationally intensive uncertainty analyses, namely by using massive parallel computing resources run in serial manner and by employing LHS sampling to optimize parameter coverage with minimum sampling.

3.3. Sources of Uncertainty in the prediction of hydrogen

The MELCOR code allows considerable user control over the physical models in use, including user over-ride of particular constants used in the engineering correlations for heat transfer, fluid flow, fuel degradation modeling and cladding oxidation for example. This feature of the code architecture was included specifically to facilitate sensitivity analysis. In this study, a collection of input parameters and model parameters known (or reasoned) to affect hydrogen generation during a severe accident are identified, and their uncertainty is characterized using a user specified cumulative distribution. In general, these parameters were selected based on prior experience with running MELCOR in the analysis of experiments where hydrogen generation is a principal experimental objective such as the Phebus FPT-1 experiment [Clement and Haste, 2003], first hand knowledge of the physics models in the MELCOR code, and on insights gained from prior full plant analyses focusing on hydrogen generation. Following is a discussion of one such uncertain parameter, the molten Zircaloy breakout temperature.

In the MELCOR model for Zr oxidation, the exothermic reaction with steam produces chemical heating of the fuel rod cladding significantly above that resulting from decay heat in the fuel. This heating will quickly result in melting of the unoxidized metal cladding; however, the molten clad is also known to be retained for a time under an outer robust ZrO_2 shell. The temperature at which the molten oxidizing metal is released from the retaining shell is known to be a dominant factor in the amount of hydrogen that is ultimately produced, since the local oxidation reaction effectively ceases when the oxidizing melt relocates to a cooler region. Experimental evidence suggests that this release temperature is in the range of 2400K, a few hundred degrees above the Zr melting point. Figure 5 provides a distribution of likely values for this parameter which bounds the melt release temperature between the melting point and about 2550K, since no relocation can occur below the Zr melting point at ~2200K, and since the entire fuel rod is known to collapse by about 2550K. The shape of the distribution was selected to represent our views about how this failure temperature is distributed. In this case a symmetric normal-like distribution was used.

Figure 5 shows both the underlying assumed uncertainty distribution as well as the 40 sampled values used in the collection of MELCOR runs for the uncertain parameter "Zr Melt Breakout Temperature." This parameter controls the local release of molten Zr confined beneath an outer ZrO_2 shell and is a key parameter affecting the total amount of Zr oxidized locally and thus the total amount of hydrogen produced. A low melt release temperature will terminate local oxidation by releasing the molten oxidizing metal to relocate to colder regions of the core, whereas a high melt release temperature will prolong oxidation by retaining the oxidizing melt in high temperature regions. The cumulative distribution shown expresses the belief that it is 0% likely that the melt release temperature lies below 2200K, 50% likely to lie below the value of 2400K and 100% likely to lie below 2550K. Similar uncertainty distributions are defined for the other uncertain parameters considered in this study. They are described in less detail below.

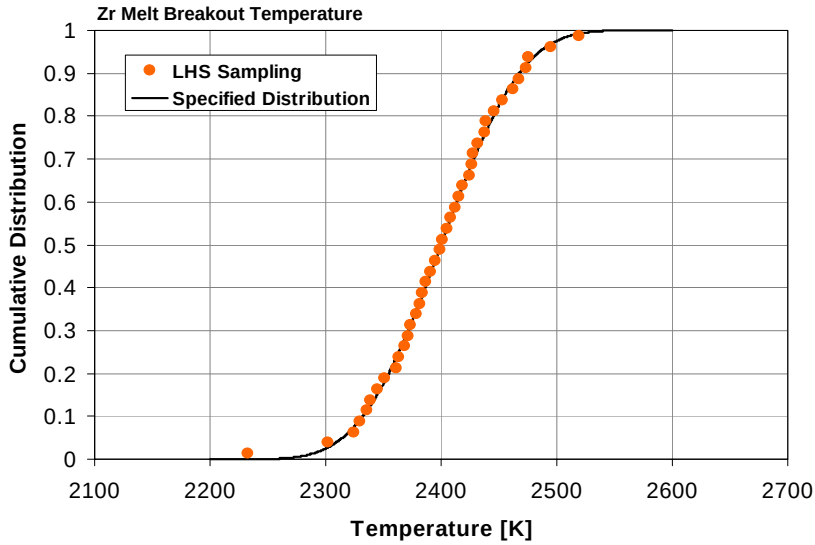

Figure 5 Uncertainty in value of Zircaloy melt breakout temperature used in MELCOR core degradation modeling.

In addition to the Zr melt release temperature, several other model parameters were considered in this study. These parameters were selected based on significant prior experience with MELCOR, and insights from experimental studies and from numerous full plant analyses. They are summarized in Table 1 below. These parameters were each sampled randomly using the LHS technique, a method similar to Monte Carlo sampling, which selects N values randomly from N equally spaced (equally probable) intervals of the cumulative distribution, thereby ensuring good sampling of the distribution tails with minimum numbers of samples. Forty samples of each parameter were taken by this method and used to form 40 separate MELCOR analyses of the STSBO accident in Sequoyah. The results of the 40 MELCOR analyses constitute samples of the true distribution of hydrogen production given the uncertainties expressed in the following table.

Table 1: Summary of MELCOR modeling parameters considered in this study to affect hydrogen generation. MELCOR parameter names are indicated in parenthesis in column 1. Complete rationale for parameter selection are provided in a report provided to the United States Nuclear Regulatory Commission (USNRC) titled "An Uncertainty Analysis of the Hydrogen Source Term for a Station Blackout Accident in Sequoyah using MELCOR 1.8.5" (draft letter report Oct 2003).

MELCOR Parameter	Description	Range Investigated
Zr-Steam Oxidation Parameters	Parameters in parabolic rate equation describing oxidation rate as a function of temperature and oxide shell thickness	Parameters selected to range between values for Urbanic-Heidrick and Lemmon.
Zr melt breakout temperature (SC1131)	Temperature at which molten cladding is released from retaining oxide shell (Figure 3)	2100K to 2550K using a normal-like distribution – median value of 2400K. Lower limit based on Zr melt temperature; upper bound based on likely rod collapse temperature.
Fuel rod collapse temperature (SC1132)	Temperature at which fuel rod collapses from rod-like geometry to a	2400K to 2800K with a normal-like distribution – median value of 2550K (note: rod collapse also

	rubble form	results in molten Zr release). Lower bound based on experimental insight; upper bound based on UO_2/ZrO_2 eutectic melt.
Fractional local dissolution of UO_2 in molten Zr (COR0007)	The fractional amount of UO_2 that is assumed to be dissolved in the molten cladding at time of cladding melt relocation	Range between 0 and 50% with a median value of 20%. Distribution biased slightly above the median value. Values based on U-Zr-O ternary phase diagram and engineering judgment.
Melt relocation heat transfer coefficient (COR0005)	Heat transfer coefficient for use in calculating freezing and blockage behavior for relocating molten core materials	2000 to 22000 watt/m^{2}K with a median of about 8000 and distribution biased above the median value. Considers unique aspects of MELCOR freezing model and observations from experiments.
Particulate debris characteristic size following core collapse (CORijj04)	Characteristic debris size in core region affecting subsequent heat transfer and oxidation surface areas	2mm to 5cm log-normal like distribution with median size near 1 cm representing pellet fragments to sintered agglomerates larger than a pellet. Range based on observations from irradiated fuel examinations and consideration of melt/debris agglomeration.
Particulate debris characteristic size following relocation to lower plenum (CORijj04)	Characteristic debris size in lower plenum affecting subsequent heat transfer and oxidation surface areas	1cm to 6cm log-normal like distribution with median or 2.5cm representing sintered fragments larger than a fuel pellet
Falling debris quenching parameters (COR00012)	Heat transfer coefficient for fuel debris falling through water filled lower plenum	Range between 125 and 400 watt/m^{2}K based on consideration of FARO experimental data and tendency for debris to fragment
Porosity of fuel debris beds (PORDP)	The porosity of debris affecting heat transfer and surface areas	Range between 0.1 and 0.5 with median value of 0.38; lower values represent debris densification by fusing and sintering; porosity above 50% not considered stable
Thermal radiation exchange parameters (FCELA and FCELR)	Parameters affecting inter-cell radiation incorporating view factor and spatial information	Range between 0.02 and 0.18 with a media value near 0.1
Ex-vessel debris/water heat transfer parameters	Enhancements to planar geometry conduction heat transfer to account for overlying water intrusion into cracks and fissures – affects molten core concrete interaction	Heat transfer enhancement ranging between 5 and 100 with median value of 35. Corrects simplified modeling of ex-vessel debris cooling in MELCOR.

In this study, correlation between parameters was not considered in the sampling process and all parameters were treated as independent. This could have the effect of narrowing resultant distributions by failing to adequately account for cases where correlations of parameters reinforce the calculated figure of merit. Correlation of two parameters in particular was evaluated, the Zr melt breakout temperature and the fuel rod collapse temperature and deemed to be self-correcting. If the sampled melt breakout temperature was higher than the sampled fuel rod collapse temperature, a clearly unphysical situation, the MELCOR physics treatment would preside, causing Zr-melt release to occur at the time that the fuel rod collapse was predicted to occur, thereby avoiding an unphysical prescription.

3.4. Results of the hydrogen uncertainty analyses

The results of all 40 analyses performed in the LHS sampling of the uncertain code parameters is shown in Figure 6. The produced hydrogen can be characterized as that hydrogen produced during the early in-vessel degradation period before RCS failure and the late in-vessel degradation period following RCS failure. The hydrogen produced during the early in-vessel degradation period ranged between 360 kg and 510 kg, and the late in-vessel degradation period brought this total to between 450 kg and 710 kg.

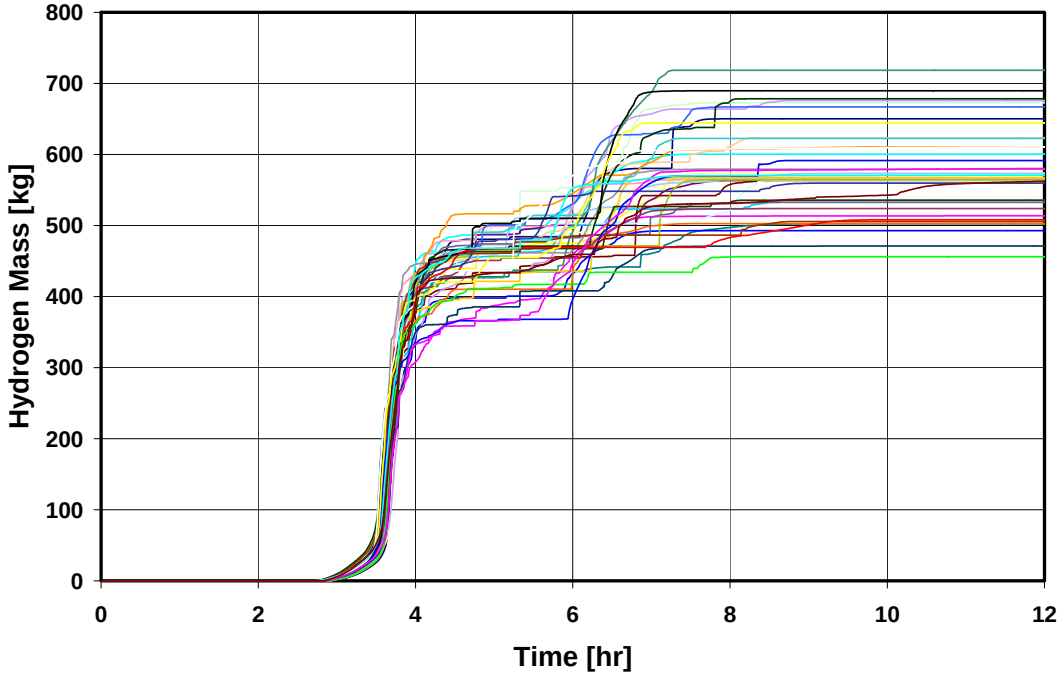

Figure 6 In-vessel hydrogen generation in short term station blackout in Sequoyah for all cases in study.

Samples of the distribution of hydrogen produced at 4, 5 and 8 hours are shown in Figure 7 plotted as fraction of core Zr oxidized. These distributions were obtained by placing the observed values for all cases in rank order and plotting the results as a cumulative distribution. At 4 hours, the median value of hydrogen produced is about 395 kg with 5th and 95th percentile values of 332 kg and 433 kg respectively. By 5 hours, the end of the early in-vessel degradation phase, the median, 5th and 95th percentile estimates are 462, 366 and 503 kg respectively, and by the end of the late in-vessel degradation period at 8 hours these values have increased to 566, 471 and 674 kg respectively. In order to facilitate comparison to NUREG-1150 expert elicitation results, the predicted hydrogen produced is expressed in terms of fraction of Zr content in the core that is oxidized. The distribution observed at 8 hours for the late in-vessel hydrogen is broader than the distributions observed during the early in-vessel period and appears to be slightly bi-modal.

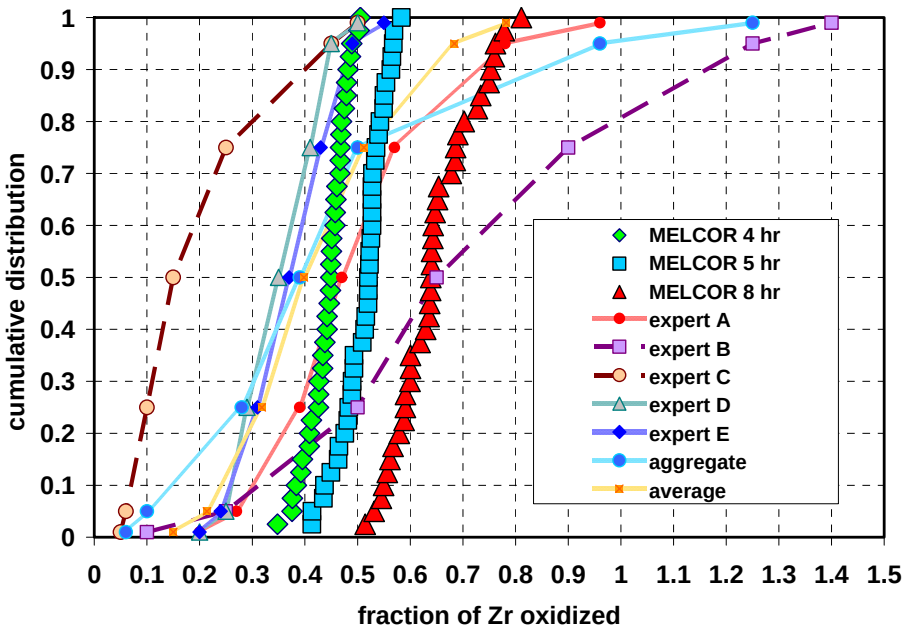

Figure 7 Sampled hydrogen distributions for Sequoyah uncertainty study for 4 hours and 5 hours (early in vessel), and 8 hours (late in vessel following RCS failure), expressed in terms of fraction of Zr inventory oxidized. Uncertainty distributions are compared to NUREG-1150 expert elicitations on in-vessel hydrogen generation, also expressed as fraction of Zr oxidized – fractions greater than 1.0 include steam oxidation of in-vessel stainless steel.

Also shown in Figure 7 for comparison are the estimated distributions for a similar generic PWR accident scenario rendered by the expert elicitation process used extensively in the preparation of the NUREG-1150 report [Harper, 1990]. Notable is the fact that in this study, the MELCOR-predicted median value for Zr-oxidation generally exceeded the values estimated by the NUREG-1150 experts, with the exception of Expert B, and that the current study produces this larger median estimation with greater certainty (i.e. a narrower distribution about the median). In retrospect, those NUREG-1150 expert views expressing significant likelihoods for Zr oxidation fractions below 0.3 for an un-recovered core melt accident seem naively optimistic based on the significant knowledge gained since the NUREG-1150 study from experimental research such as the Phebus program [Clement, 2003]. In general, the cumulative knowledge invested into integral codes such as MELCOR would be expected to lead to greater certainty in predictions, and is offered here as the principal reason for narrower distributions for hydrogen predictions in comparison with the expert elicitation process used in NUREG-1150.

In addition to characterizing the distribution of predicted hydrogen in this study, regression analyses were also performed in order to identify which of the uncertain input parameters were most responsible for the observed variances. In general, regression coefficient r-squared values were not particularly large, with the two most significant parameters determined to be the Zr-melt breakout temperature and the particulate debris hydraulic diameter, shown plotted in Figure 8 and Figure 9. These results were produced by performing linear regression on the predicted hydrogen for each case after sorting the results in rank order of the uncertain parameter varied. The ranking of these parameters in particular over others was not unexpected; however, larger regression coefficients were initially anticipated. The fairly low values for the regression coefficients may be explained by both the

relatively small sample size of 40 realizations and due to the neglect of correlation among the sampled parameters, as observed by Helton, et al. [Helton, 2002].

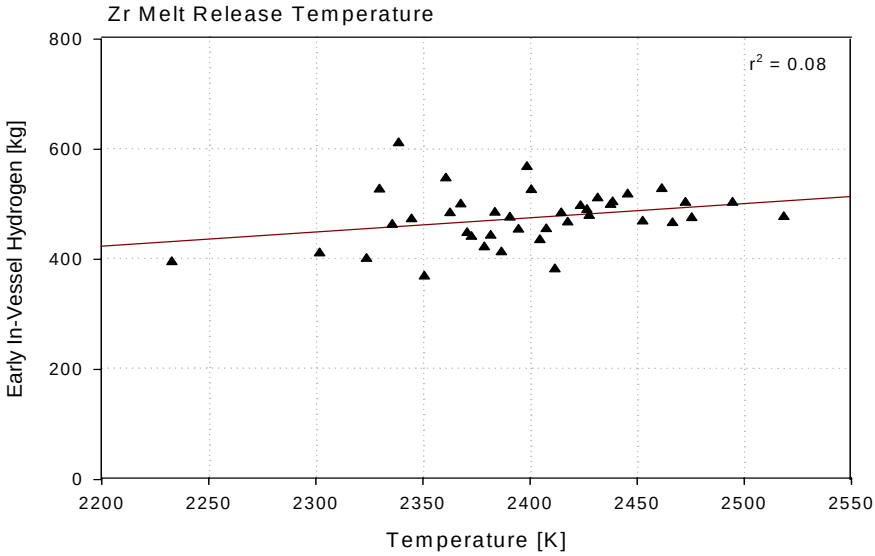

Figure 8 Scatter plot of hydrogen predicted plotted as against the temperature for molten zircaloy breakout from the outer cladding oxide shell.

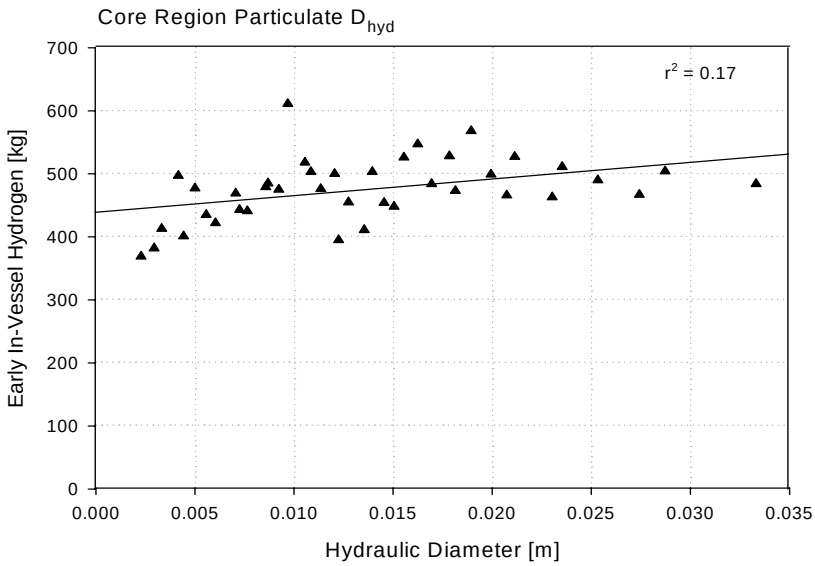

Figure 9 Scatter plot of hydrogen predicted plotted as against the assumed core region particulate debris size..

4. AP1000 Containment Aerosol Depletion Study

The next example illustrates the use of MELCOR in a non-standard way to produce a fast running model suitable for performing large numbers of calculations in a short time by means of simple Monte Carlo sampling. The method illustrated amounts to running MELCOR once to produce high fidelity containment thermal hydraulic boundary conditions from the RCS behavior, and then using the results

of the detailed T-H analysis to drive a sampling of different containment analyses. This is possible because of the minimal T-H coupling and feedback between the containment and the RCS. The method makes use of special edit features of the MELCOR code and permits simplified analyses to be performed using self consistent high fidelity boundary conditions without the numerical overhead normally required by the RCS analysis portion of a full plant analysis.

4.1. Aerosol Settling and Depletion Processes in Containment

The objective of the AP1000 containment aerosol analysis was to provide an estimate of the range of behaviors reasonably expected of aerosol natural depletion processes given modeling and physics uncertainties associated with the aerosol fallout and deposition mechanisms. In particular, it was desired to characterize the time constant for aerosol depletion (fallout and deposition) as implied by the first order equation:

$$\frac{dm}{dt} = \dot{S} - \lambda \cdot m \quad , \qquad [1]$$

where m is the instantaneous mass of airborne containment aerosol, S is the source rate of aerosols entering the containment from the RCS and λ is the time constant for aerosol depletion usually characterized in hr^{-1}.

The rate equation thus described can be solved for λ as follows (Eq [2]) to produce an "instantaneous" value for the decontamination coefficient. This expression of the decontamination coefficient can be applied over the entire duration of the source-depletion time period.

$$\lambda = \frac{1}{m} \cdot \left(\dot{S} - \frac{dm}{dt} \right) \qquad [2]$$

In this study, the MELCOR code is used to model the aerosol depletion process in the AP1000 containment, and thereby to determine the overall instantaneous value of λ as a function of time in the analysis using Eq. [2] and MELCOR-calculated airborne mass. Aerosol behavior in MELCOR is calculated using the sectional method developed by Gelbard [Gelbard, 1982] as described in the MELCOR 1.8.5 Reference Manuals. In this treatment the aerosol size distribution is described by discretizing the airborne mass into size bins between 0.1 μm and 50 μm, typically using 10 equal logarithmic size sections. Agglomeration of smaller aerosol particles to form larger particles is calculated, and deposition velocities are calculated for each section, including effects of thermophoresis, diffusiophoresis, and gravitational settling.

This study focused on determining the expected distribution of possible values for the decontamination coefficient, λ, for a medium break LOCA involving the direct vessel injection (DVI) line (accident sequence 3BE). The LOCA conditions establish thermal hydraulic boundary conditions for the containment environment, driven by the RCS blowdown and subsequent safety system responses such as RWST tank draining, vessel injections, and cavity flooding. These events affect containment aerosol behavior by influencing relative humidity and steam condensation rates. Additionally, it was desired to assume an idealized aerosol source term introduced to the containment. These sources and boundary conditions are described in the following sections.

4.2. Radioactive Aerosol Source Term to the Containment

It was desired in this study to make use of the so-called Alternative Source Term (AST) as specified in the NUREG-1465 report [Soffer, 1995] on the subject. The NUREG-1465 "AST" is a stylized source

term approved by the USNRC for use in certain regulatory applications as an alternative to the more conservative source term described in TID-14844 [DiNunno, 1962]. The NUREG-1465 source term prescribes fission product releases to the containment in terms or release fractions and durations for 8 volatility classes (Noble Gas, Halogens, Alkali Metals, Tellurium Group, Barium/Strontium, Noble Metals, Cerium Group, and Lanthanides). The release fractions are further defined in terms of major accident progression stages including the Gap Release Phase (release of cladding gap inventory), Early In-Vessel Phase (initial release from fuel in core), Ex-Vessel Phase (core-concrete interaction releases) and Late In-Vessel Phase (late fuel release and revaporization from the RCS). This focus of this study was limited to the Gap Release and Early In-Vessel release phases. The NUREG-1465 source term, as described above was used as the source of radioactive aerosols to the AP-1000 containment building, appropriately offset in time to correspond to the RCS thermal hydraulic temporal progression.

The NUREG-1465 source term was mapped to the MELCOR fission product class structure and used as the source term to the AP1000 containment as shown in Table 2. In the 3BE calculations analyzed in this study, the start of the in-vessel release was initiated 2.1 hours based on comparisons with the start of in-vessel release in the full 3BE analysis. The gap release was initiated 30 minutes prior to this time.

Table 2 NUREG-1465 Source Term Used in AP-1000 3BE Analyses

MELCOR Class	Representative Fission Product	Core Inventory [kg]	Gap fraction [30 minutes]	In-Vessel Release Fraction [1.3 hrs]
1	Xe	342.27	0.05	0.95
2	CsOH	174.20	0.05	0.25
3	Ba	150.10	0	0.02
4	I	0.74	0.05	0.35
5	Te	30.02	0	0.05
6	Ru	211.20	0	0.0025
7	Mo	249.10	0	0.0025
8	Ce	439.50	0	0.0005
9	La	407.70	0	0.0002
10	UO_2	82560.00	0	0
11	Cd	1.00	0	0.05
12	Sn	5.66	0	0.05
16	CsI	28.67	0.05	0.25

4.3. Thermal Hydraulic Boundary Conditions for the Containment

The thermal hydraulic boundary conditions for the containment analysis were determined by running detailed best estimate MELCOR and MAAP analyses of the DVI-line break accident. The full analysis of the accident progression within the vessel, RCS, and the containment using MELCOR 1.8.5 required about a day of computer execution time on a 2 GHz class Windows personal computer. Owing to the relatively long execution time required to produce a single analysis of the full plant response, it was decided to decouple the numerically burdensome vessel/RCS analysis from the containment analysis since the vessel/RCS analysis proceeds relatively unaffected by conditions in the containment. Capabilities exist with the MELCOR code (and MAAP) to produce files describing the source rate and enthalpy of hydrodynamic materials (steam, water, hydrogen) that enter the containment from the vessel and RCS which can subsequently be used as “playback” sources to a

simplified MELCOR model for the containment systems alone. Shown in Figure 10 are the steam sources recorded from a high fidelity RCS calculation used to drive the simplified containment-only model. In addition to steam sources, hydrogen mass and energy sources representing the enthalpy of the hydrodynamic materials, decay energy of transported fission products and heat conducted through the vessel lower head to cavity water were also sourced in the containment model. The advantage of such an approach is that the simplified model using pre-recorded thermal hydraulic sources will execute in about ten minutes, whereas the fully coupled analysis requires on the order of a day. This presents an obvious advantage for conducting Monte Carlo uncertainty analyses where on the order of 150 or more separate analyses are desired.

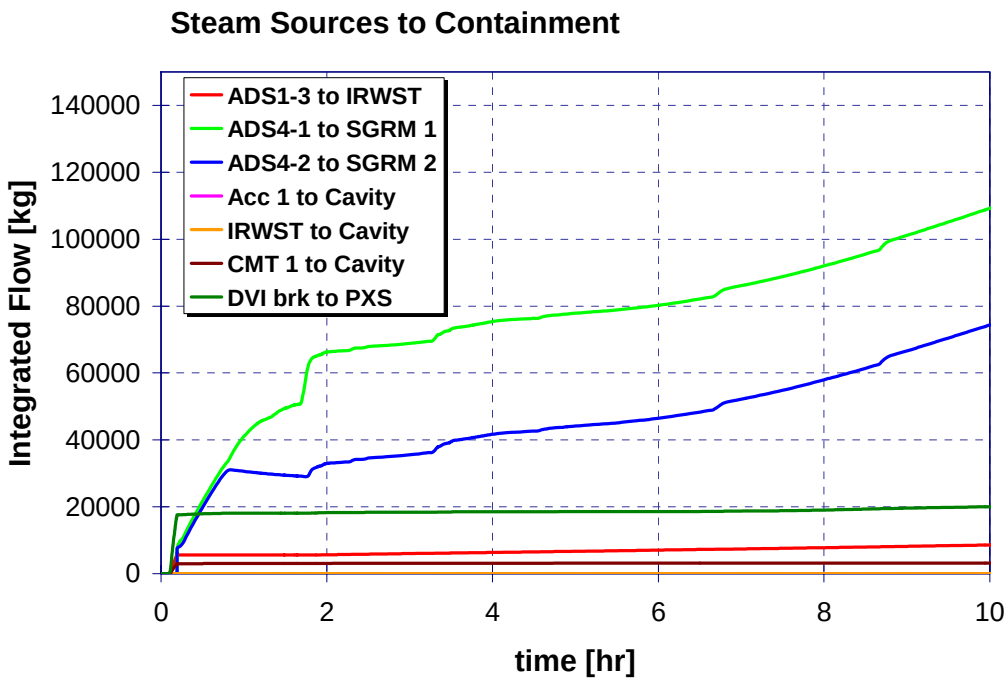

Figure 10 Steam sources into AP1000 containment from high fidelity RCS analysis.

4.4. Statistical Characterizations

The sampled results for the decontamination coefficient calculated for the AP1000 containment were characterized using order statistic methods as described in the statistics text by Hogg and Craig [Hogg, 1970] and summarized by Powers [Powers, 1993] which begins with placing the sampled values for λ in rank order, as suggested by the following hypothetical illustration involving 100 observations of a parameter Z (i.e. λ).

1%	2%	3%	4%		100%
Z_1 ,	Z_2 ,	Z_3 ,	Z_4 ,	……..	Z_{100}

Placing the observations in rank order immediately produces an estimate of the underlying cumulative distribution function (CDF) since (in this illustration) 1% of the observations of Z lie below or equal to Z_1, 50% below or equal to Z_{50}, and so on. However the non-parametric order statistics treatment

allows one to establish confidence bounds on the underlying distribution for Z without making any assumptions about the nature of the distribution. Following the description in Hogg and Craig, it can be shown that the probability that the kth ranked observation of Z within a population of n observations lies below the ξ percentile of the CDF with confidence "p" is described by the following equation, where p is the desired confidence level.

$$\Pr(Z_k < \xi_p) = \sum_{i=k}^{n} \frac{n!}{i!(n-i)!} \cdot p^i (1-p)^{n-i} \qquad [3]$$

Furthermore, the probability that the ξ_p percentile of the CDF lies between the i-th and j-th sampled value is expressed by the following expression, where again "p" is the confidence level.

$$\Pr(Z_i < \xi_p < Z_j) = \Pr(Z_i < \xi_p) - \Pr(Z_j < \xi_p) \qquad [4]$$

These expressions can be used to produce estimates of the confidence intervals for each percentile of the sampled CDF, where "p" is the confidence level. This method was used in the AP-1000 study to produce confidence intervals for the distribution of sampled values for the decontamination coefficient, λ, as shown later in this paper.

4.5. Uncertain Parameters in Aerosol Depletion Rate Analysis

Without going into a detailed discussion of the aerosol deposition processes in the containment environment, the following aerosol physics modeling parameters accessible in MELCOR were treated as uncertain, where distributions were estimated describing the range of uncertainty for each parameter, as summarized in the following table. These parameters affect gravitational settling, thermophoresis, diffusiophoresis, particle agglomeration, and diffusive deposition processes, as described in the MELCOR 1.8.5 Reference Manuals.

Table 1 Summary of uncertain parameters and the distributions used to characterize them.

Parameter	Bounds	Distribution
Non-radioactive structural aerosol mass	50 – 300 kg	uniform
Aerosol mass mean diameter	1 – 4 μm	uniform
Aerosol GSD for log normal distribution	1.2 - 3	uniform
Aerosol shape factors for diffusive, thermophoretic and gravitational settling deposition velocities	1 – 5	Beta (p=1,q=3)
Particle slip factor in Cunningham slip correction	1.2 – 1.3	Beta (p=4, q=4)
Particle-particle agglomeration sticking probability	0.5 – 1.0	Beta biased to 1 (p=2.5, q=1)
Boundary layer thickness for diffusion deposition	5 - 20 μm	uniform
Factor in Thermal Accommodation Coeff.	2.2 – 2.5	uniform
Gas/particle thermal conductivity ratio in thermophoresis deposition velocity	0.006 – 0.06	log uniform
Turbulent energy dissipation in agglomeration coefficients	0.00075 – 0.00125	uniform
Aerosol particle effective material density	1000 – 5000 kg/m^3	Beta biased to 2000 (p=1.5, q=2.5)
Heat/Mass Transfer multiplier for steam condensation in containment	0.75 – 1.25	Beta (p=1.5, q=1.5)

These parameters were sampled using simple Monte Carlo sampling and used to produce 150 estimates of the decontamination coefficient as a function of time, using the thermal hydraulic boundary conditions in the AP1000 containment for the 3BE accident as described in Section 4.3 and the NUREG-1465 aerosol source term described in Section 4.2. The airborne Cs mass as a function of time for each of the sampled cases is shown in Figure 11 plotted on a log-y axis. The slope of the depletion curve indicates the value of the decontamination coefficient, and the coefficients can be seen to range between 0.3 hr^{-1} and 3 hr^{-1} throughout the aerosol depletion period.

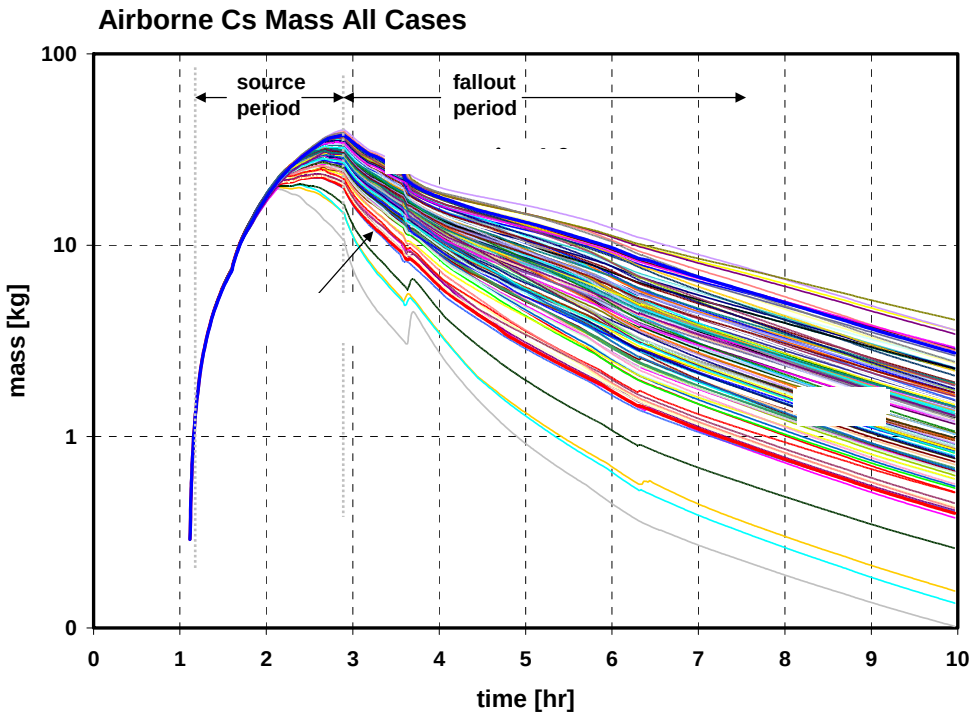

Figure 11 Airborne Cs mass for all runs showing time dependent depletion rate.

At selected points in time the samples of the decontamination coefficient were characterized using the order statistic methods described in Section 4.4 to produce estimates of the distribution of values and the 95% confidence intervals for each percentile of the distributions. Several of these are illustrated in Figures 12 through 14 below. As can be seen, the spread in the distribution varies in time, generally becoming narrower in time as the suspended aerosol mass diminishes and only the smaller particles in the aerosol size distribution remain airborne. This characterization of the expected variance in decontamination coefficient for this accident sequence was compared to separate deterministic analyses produced by the MAAP code, as shown in Figure 15. As seen in Figure 15, the deterministic MAAP-predicted estimates for the decontamination coefficient lie generally within the 95% confidence intervals for 5th and 95th percentile of the MELCOR-predicted CDF's for λ, thereby generally substantiating the MAAP estimates.

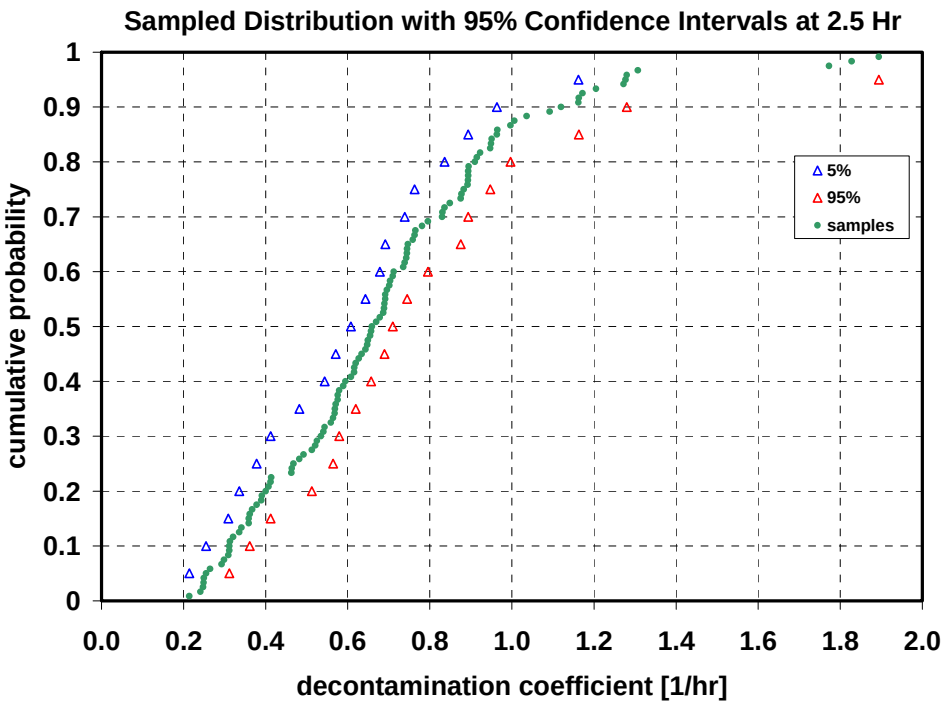

Figure 12 Distribution of decontamination coefficients determined at 2.5 hrs.

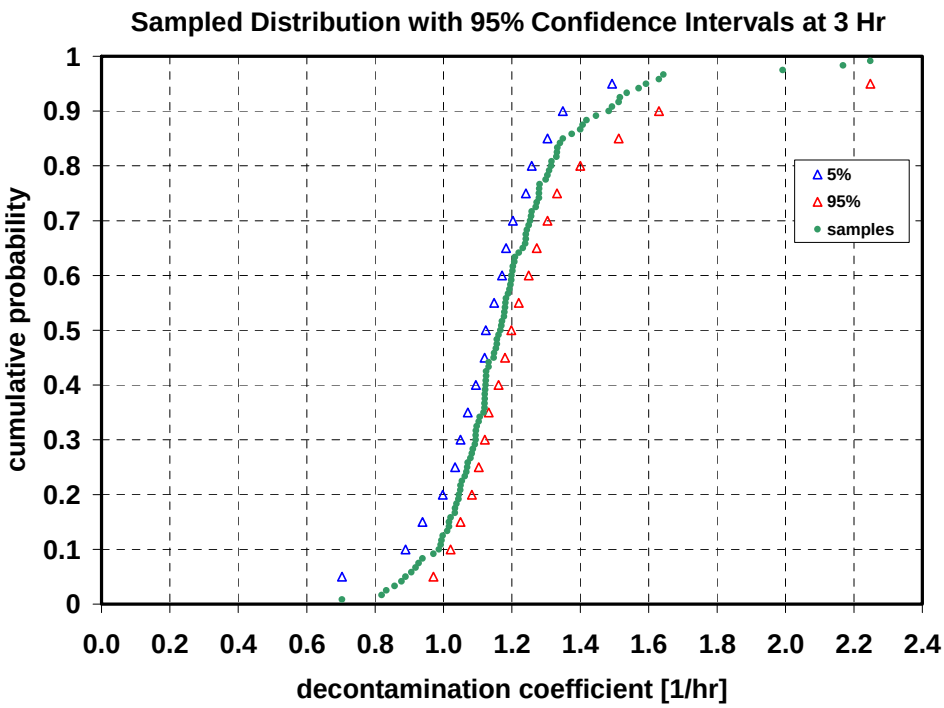

Figure 13 Distribution of decontamination coefficients determined at 3 hrs.

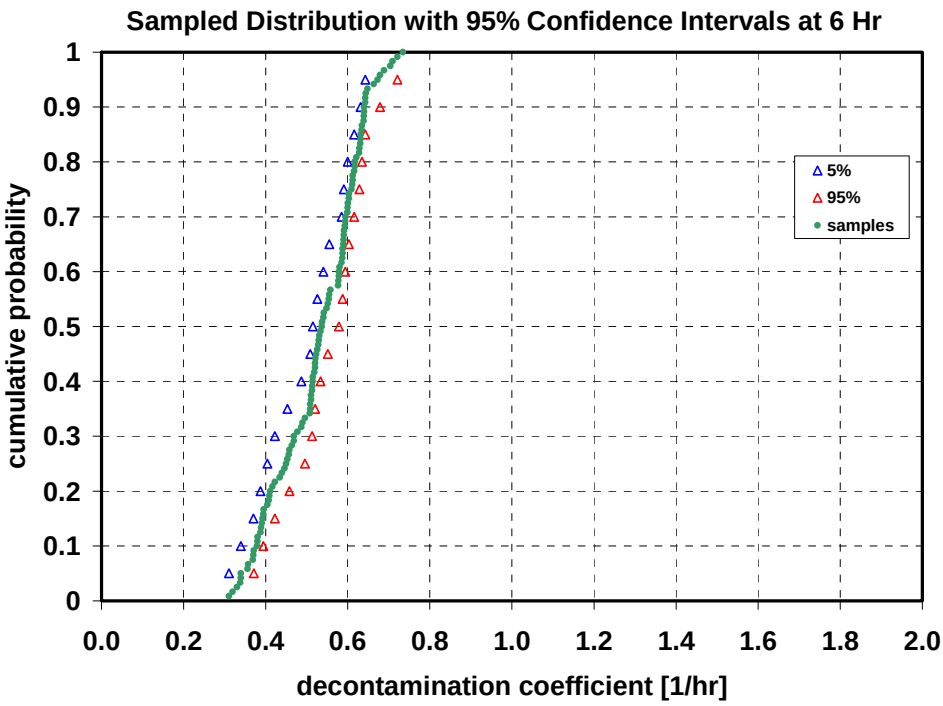

Figure 14 Distribution of decontamination coefficients determined at 6 hrs.

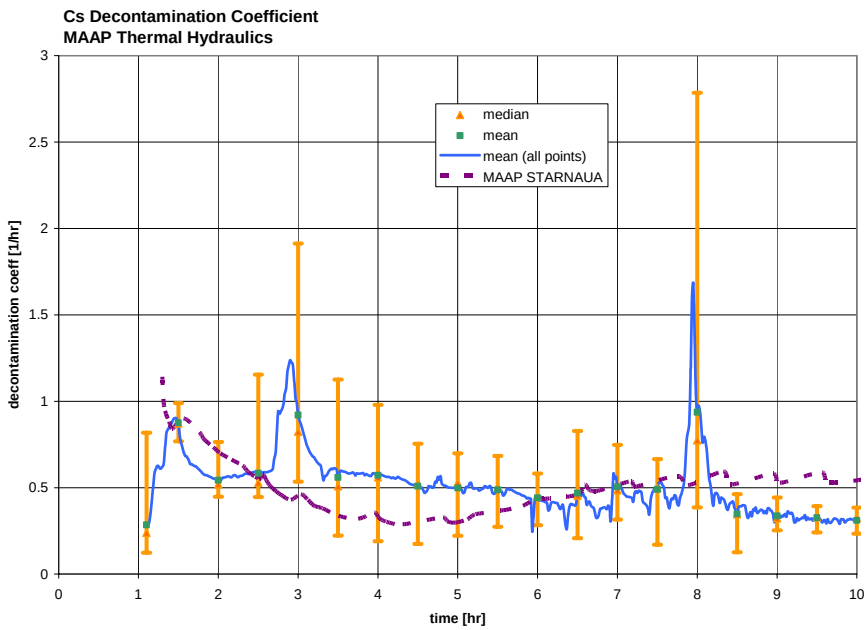

Figure 15 Decontamination coefficient for airborne mass using MAAP-generated thermal-hydraulics, showing 5% and 95% estimates with 95% confidence, the mean and the median for the sampled distribution.

Finally, variance analysis using a regression method was used to rank the uncertain parameters in terms of those most responsible for the observed variation in the decontamination coefficient. This is measured in terms of an r-squared value equivalent to a linear regression on the decontamination coefficient when considered a function of each uncertain parameter independently. These results are shown in Figure 16 and indicate that the most important uncertain parameters generally are the assumed mean particle size, the particle shape factor and the total mass of initially suspended aerosol.

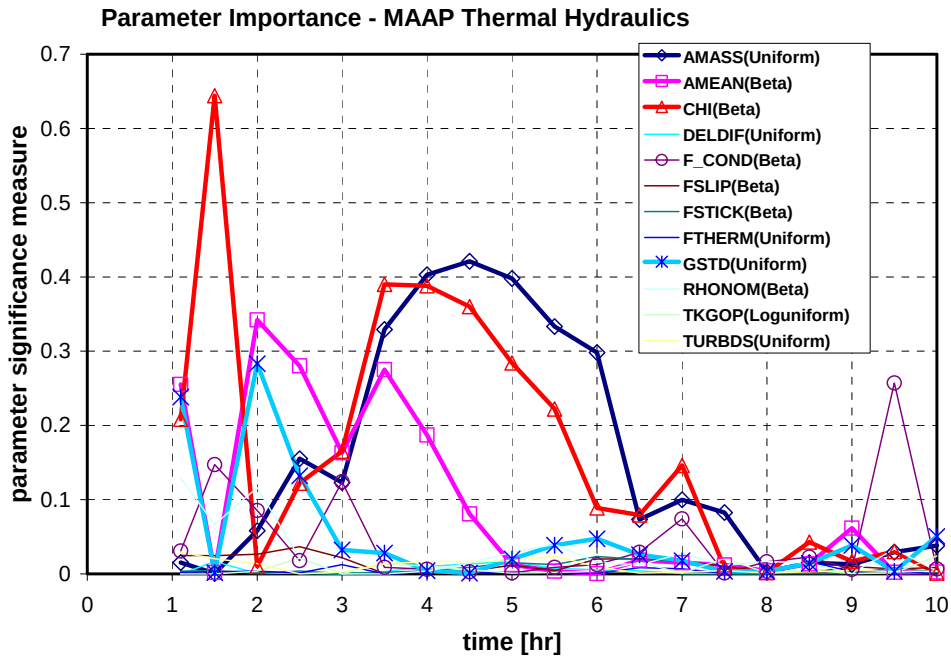

Figure 16 Variance analysis on uncertain parameters on their influence on the decontamination coefficient for the cases using MAAP thermal-hydraulics.

5. Summary and Conclusions

This paper has presented two applications of classic uncertainty analysis using sampling methodologies with the MELCOR severe accident analysis code. One application illustrates the use of LHS sampling with a time intensive analysis of hydrogen production in station blackout accidents in Ice Condenser nuclear power plants. Because each analysis (or sample) required several days to execute on a moderately fast processor (700MHz), the LHS sampling methodology permitted broad coverage of the uncertain input parameters with a minimal number of samples. Even so, the 40 analyses were only feasible by the availability of a large multi-processor computing cluster which allowed all 40 realizations to be executed simultaneously. The second application illustrates an alternative means of producing a fast running equivalent analysis of an otherwise similarly computationally intensive calculation of a medium break LOCA accident in the AP1000 plant, where simple Monte Carlo sampling methods were used. The MELCOR model simplification technique used in this study reduced the run time of a single accident analysis from days, using the complete detailed MELCOR plant model, to about 10 minutes, using a simplified containment-only model that employed a playback of the computationally intensive reactor coolant system thermal hydraulics

portion of the full analysis. In this case the uncertainty study was accomplished overnight using a fast dual Pentium Windows PC.

Both analyses illustrated in this paper produced estimates of the expected distribution of a parameter of interest based on known uncertainty in key model parameters known to dominate the predicted quantity of interest. In the first example, the parameter of interest was hydrogen production as a function of time in a station blackout accident, and in the second case, the parameter of interest was the time dependent time constant for depletion of airborne radioactive aerosol in the AP1000 containment for a medium break LOCA accident. In the hydrogen analysis, the results are compared with the expert elicitation method used in the NUREG-1150 study, which produced significantly broader distributions for estimated hydrogen production.

In the aerosol depletion analysis for AP1000, confidence intervals are computed using order statistics methods to characterize our certainty in the estimated distribution for the depletion time constant. The 95% confidence intervals for the 5th and 95th percentiles of the estimated distribution were used to evaluate a deterministic MAAP prediction of the same accident. The uncertainty assessment concluded that the MAAP analyses lied within expected limits predicted by the MELCOR code.

Both analysis methods benefited significantly from only recently available advanced computing resources that have up to now made such complex uncertainty analyses effectively too burdensome to carry out efficiently. Importantly, these demonstrations illustrate the deficiency of simple deterministic analyses that produce only a single estimate of an accident progression. Uncertainty methods such as this are superior to *sensitivity analyses* which explore a range of possible outcomes with no quantitative prediction of likelihood. These methods are also superior to *bounding analyses* which can produce conservative bounding predictions but offer no quantification of safety margins (possibly unnecessarily excessive margins) between what is *likely* and what is *bounding*. Uncertainty quantification permits assessment of the safety margins between what is likely or expected and what may occur with decreased likelihood, and as such, is a valuable tool in applying risk-informed regulation to the nuclear industry. Analysis of variance, also demonstrated in these studies, provides insights into *which* uncertain parameters are *most* responsible for the observed (calculated) variations in the predicted parameter of interest. This can be used to identify areas where additional research may best be applied to further reduce the residual uncertainties of the predictions, and thereby better apply limited research resources.

The uncertainty analysis methods demonstrated by these studies are much preferable to deterministic methods employing conservative selection of code parameters since realistic estimates of median and variance estimates provide more complete characterization of risks than conservative point value estimates. This methodology provides a powerful alternative to simple deterministic analyses and sensitivity studies for use in a risk-informed regulatory environment.

6. Acknowledgements

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