## A Sensitivity Study Supporting Comparative Analysis of MELCOR and GOTHIC Large Dry Pressurized Water Reactor Containment Models

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# Abstract

The thermal-hydraulic response of large dry pressurized water reactor (PWR) containments under loss-ofcoolant accident (LOCA) conditions - particularly with respect to containment pressure and sump pool temperature - is crucial for risk informed decision making about GSI-191. Texas A&M University (TAMU) has developed models with several computer codes including MELCOR and GOTHIC.

MELCOR is a best-estimate thermal-hydraulics and severe accident code created and actively maintained by Sandia National Laboratories for the Nuclear Regulatory Commission (NRC). GOTHIC is a thermalhydraulics software package meant for design, licensing, and safety calculations for, among other systems, nuclear power plant containments. It was developed and is maintained by Numerical Applications Inc. (Zachry Nuclear Engineering, Inc.) for the Electronic Power Research Institute (EPRI).

The overarching goal of this paper is to investigate differences in best estimate calculations of thermalhydraulic response to a double-end guillotine break (DEGB) LOCA for similar MELCOR and GOTHIC containment models. The code predictions themselves are presented in a separate paper wherein reasonable though unsupported conjectures about code disagreements are made. These hypotheses are examined here via a MELCOR-to-GOTHIC comparative sensitivity study because they stem from either code input restrictions (such as DEGB source mass/enthalpy definition) or code physics/equipment models (e.g. for condensation/films or various engineered safety features). Therefore the "sensitivity" in this context is that of the comparative thermal-hydraulic response to the code inputs or phenomenological models in question. Sensitivity calculations are performed so as to exclude, in turn, the effects on comparative thermal hydraulic response of: containment fan coolers, containment sprays, thermal surface condensation/films, and break source definition. Calculations are also performed with multiple models excluded. Using containment sump pool temperature as an indicator, the most impactful physics in terms of code agreement are those of thermal surfaces (condensation, film phenomena) whereas fan cooler models have a minimal effect. Containment spray exclusion has mixed effects while break source definition and/or break effluent flashing models lead to disagreement.

Keywords: MELCOR, GOTHIC, comparison, sensitivity

### 1. Introduction

Computational and experimental activities are currently focusing on the resolution of Generic Safety Issue (GSI) 191. System codes have been extensively used to perform thermal-hydraulic calculation of the reactor and containment response under specific accident scenarios to support the ongoing research. A set of computations performed with MELCOR and GOTHIC have been selected and presented in this paper. Using both codes, models of a typical large dry PWR containment were developed. These models were used to predict the containment thermal-hydraulic response under postulated DEGB conditions with particular emphasis on obtaining a time profile of the sump pool temperature. Because sump pool temperature has an impact on sump pool chemistry, residual heat removal during recirculation cooling, and sump screen pressure drop, information about the sump pool temperature response is vital to industry decision-making for GSI-191.

A separate paper [1] documents MELCOR and GOTHIC "best-estimate" calculations of containment thermal hydraulic response in terms of steam/air atmosphere pressure and sump pool temperature. The reader is referred to that paper for a description of the MELCOR and GOTHIC containment models. For simulation of a DEGB LOCA, certain aspects of the code calculations agree. However, there is a significant discrepancy in prediction of sump pool temperature between ESF actuation and sump switchover. This disagreement is the main focus of the present study, though other disagreements related to 1) the blowdown phase of the transient, and 2) the response to sump switchover are also addressed. Conjectures based on qualitative arguments were made in the complementing paper as to which code characteristics are causes of the discrepancies:

- Input restrictions on break source specification
- Break source flashing models
- Thermal surface physics models (condensation heat/mass transfer, film drainage, pool heat transfer)
- Engineered Safety Feature (ESF) models (fan cooler correlations, mathematical treatment of spray droplets)

For each member of the list above, an overview of its treatment in MELCOR and GOTHIC is given below to establish a better understanding. Sensitivity calculations documented below further point out which of the code differences is most impactful as a contributor to MELCOR/GOTHIC disagreement.

### 2. Exposition of Important MELCOR Phenomenological Models

In MELCOR, the break source enthalpy is described as either an integral, rate, rate per mass, or rate per volume. Enthalpy rate [e.g. J/s] is specified in MELCOR and is linked to a break mass flow rate via tabular input. The lower compartment control volume (CV), initially at atmospheric pressure, is assigned the break mass/enthalpy source. Due to the high source enthalpy, the low CV pressure, and other source characteristics, MELCOR predicts the highly-pressurized, subcooled water becomes superheated and consequently flashes to a mixture of vapor (steam), fog (small water droplets in the CV atmosphere), and liquid. There is little detail in the MELCOR manuals as to the internal calculations for liquid/vapor split fraction upon flashing. The point is simply made that source liquid water which would be superheated at the current CV pressure is brought to equilibrium at that CV pressure. The source information and the pressure of the receiving CV are used to define an average enthalpy and thereby obtain a liquid/vapor split fraction [2]. Given the lack of mathematical detail, it may be difficult to ascertain the substantive difference between MELCOR and GOTHIC in terms of flashing treatment.

For MELCOR heat structures (HS) of plane wall geometry, the one-dimensional conduction heat transfer equation and its numerical solution is not expected to differ from those in GOTHIC to a great extent. However, MELCOR calculations of transfer processes between CV contents and thermal surfaces should be reviewed, at least in general terms, for comparison to GOTHIC. Concerning atmosphere/structure heat transfer, the MELCOR approach is to compute a Nusselt (Nu) number by correlation. Two general Nu correlations depending on the Rayleigh (Ra), Reynolds (Re), Prandtl (Pr), and Grashof (Gr) numbers are used to calculate natural and forced convection [2]:

$Nu_{natural} = CRa^m + D$	(1)
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$$Nu_{forced} = CRe^m Pr^n + D \tag{2}$$

The constants (C, D) and exponents (m, n) appearing in Equations 1 and 2 are functions of the type of flow (internal vs. external), surface geometry, and flow regime (laminar vs. turbulent). To decide whether laminar or turbulent natural, forced, or mixed convection exists, MELCOR weighs the relative magnitudes of appropriate dimensionless groups. The same approach is followed for pool/structure heat transfer, though different sets of constants and exponents exist for use in Equations 1 and 2. At any given time, structure surface heat transfer can occur to either the pool or the atmosphere or both, the deciding parameters being the critical pool fractions. These user-defined quantities govern the CV pool volume fractions above which and/or below which heat transfer proceeds between a structure surface and only the pool, only the atmosphere, or both.

Steam condensation mass transfer from a CV atmosphere to structural surfaces is crucial to containment response since it strongly influences containment pressure. Mass transfer results in condensate films on thermal surfaces and subsequent heat transfer must occur within and across a flowing film. At the same time, noncondensible gas accumulation near the film surface can inhibit further condensation. Condensate films can drain across a network of structures, affecting heat transfer along the way. The above effects must all simultaneously factor into the analysis. MELCOR predicts steam condensation to occur on a thermal surface when its temperature is below the dew point of an interfacing CV atmosphere. When a condensate film appears, extra terms are added to the finite difference equation of the thermal surface. After condensation begins, MELCOR imposes diffusion rate limits on steam condensation at a surface if, in the interfacing CV atmosphere, the ratio of steam partial pressure to total pressure falls below a critical value. The problem of condensation mass transfer reduces to prediction of a diffusion mass transfer coefficient via heat and mass transfer analogy (and hence the code prediction of Nu). Diffusion rate limitation, heat transfer, and flowing film effects factor in to the prescription for mass transfer coefficient that characterizes atmosphere/structure mass transfer.

Mass transfer between a structural surface and a CV pool is crucial to containment response since it strongly influences sump pool temperature. Based on a condensate film mass balance, maximum allowable film thickness, and film Reynolds number, the amount of condensate drainage to an interfacing pool across a time-step is deduced. Liquid water in a film on a surface drains at a temperature determined by an average enthalpy. This average is a function of saturated liquid enthalpies evaluated at the film/structure interface and the film/atmosphere interface.

Fan coolers in MELCOR are modeled with a relatively simple empirical correlation that yields total heat transfer coefficient as the sum of a convective component (sensible heat transfer) and a condensation component (latent heat transfer). Rated, i.e. nominal, fan cooler conditions are supplied in user input and a total, effective cooler heat transfer surface area is deduced. This area is used in the empirical equations to predict fan cooler performance (heat transfer coefficients) as a function of steam mole fraction. Spray droplets are introduced into a host CV at some elevation and with some volumetric flow rate, temperature, and size distribution. Droplets are strictly spherical and are assumed to fall vertically, isothermally, and at a terminal velocity through the host CV. In the case of a single, mono-disperse droplet distribution, three differential equations for mass transfer, heat transfer, and fall velocity are integrated over the droplet fall height. The results are scaled according to the total droplet population. Droplets that reach the bottom of their host CV can either enter the host CV pool or continue falling through atmospheres of other CVs. MELCOR apportions droplets to other CVs according to user instructions.

#### 3. Exposition of Important GOTHIC Phenomenological Models

In GOTHIC, the break source enthalpy is described as a specific enthalpy. Thus the enthalpy rate is obtained upon multiplication of the specific enthalpy by the mass flow rate. The lower compartment CV, initially at atmospheric pressure, is connected to a flow boundary condition that represents the break

mass/enthalpy source. GOTHIC predicts flashing by first fixing a saturation pressure  $P_s$  (in this case, the lower compartment CV pressure) and then computing a steam quality (*x*) for the flashed mixture (liquid/steam) as [3]:

$$x = \frac{h - h_f(P_s)}{h_{fg}(P_s)} \tag{3}$$

Note the subscripts f and g represent liquid and vapor, respectively. A liquid volume fraction for the flashed steam/liquid mixture is calculated from this quality, thus the amounts of steam and liquid entering the simulation domain from the source are determined.

For GOTHIC thermal conductors (TC) of the internal type and of plane wall geometry, the conduction heat transfer equation and its numerical solution do not differ from MELCOR to a great extent. However, GOTHIC calculations of transfer processes between CV contents and thermal surfaces should be reviewed, at least in general terms, for comparison to MELCOR. Concerning atmosphere/structure heat transfer, the GOTHIC approach is to compute heat transfer coefficients by correlation based on dimensionless quantities that characterize natural and forced convection. The user chooses definitions for terms appearing in the heat rate equation [3]:

$$Q_{w,v} = \lambda_{w,v} A_{cn} H_{conv,v} \Delta T_{conv,v}$$
(4)

The heat transfer coefficient  $H_{conv,v}$  is calculated from user choices for type of convection (natural vs. forced, pipe flow vs. external) and surface geometry. From there, the maximum coefficient value as determined from three expressions (laminar, turbulent, minimum based on fluid conduction) is chosen. The factor  $\lambda_{w,v}$  is fixed by user options for splitting surface heat transfer between pool and atmosphere of an interfacing CV. It is computed with user-defined minimum/maximum CV liquid volume fractions. The surface area  $A_{cn}$  follows from TC input. The pool/structure heat transfer is treated analogously, and in fact the very same heat transfer coefficient correlations are applied whether the TC surface interfaces with pool or atmosphere.

There are several "condensation options" available in GOTHIC for purposes of modeling condensation mass transfer from a CV atmosphere to a TC surface. Each of these options constitutes a different route to determining a heat transfer coefficient that may be used to compute condensation heat and mass transfer rates [3]:

$$Q_{cond} = \lambda_{w,v} A_{cn} H_{cond} \Delta T_{cond}$$
<sup>(5)</sup>

$$\Gamma_{w}^{cond} = \frac{Q_{cond}}{h_{vs} - h_f(P_{vs})} \tag{6}$$

In addition to selecting an empirical correlation for  $H_{cond}$ , a characteristic  $\Delta T_{cond}$  must be chosen as well. Note the subscript vs stands for "vapor/steam", i.e.  $h_{vs}$  is steam enthalpy and  $P_{vs}$  is steam partial pressure.

Mass transfer between a structural surface and a CV pool is crucial to containment response since it strongly influences sump pool temperature. For certain condensation options, the GOTHIC formulation includes thermal conductor mass and energy source terms (for liquid and vapor phases) in the lumped parameter CV governing equations. These source terms make use of the condensation mass transfer rate as written above in Equation 6. The energy source term to a CV liquid phase consists of the condensation rate multiplied by the saturated liquid enthalpy at steam partial pressure. When the diffusion layer model is active, the treatment is slightly different.

Fan coolers in GOTHIC can be treated with a variety of code components depending on modeling goals. Cooler and fan components in addition to a detailed heat exchanger component are available. In the present study, a volumetric (indicating volume-to-volume) fan is used along with tabular plant data expressing the fan cooler heat removal rate as a function of saturation temperature (at the pressure of the fan cooler suction CV). As with the break source, spray droplets must enter the simulation via a flow boundary condition across a flow path. A spray nozzle component is placed on the entrance flow path and effectively transforms the liquid flow into a droplet flow of some specified size distribution. Droplets then enter a CV droplet field, which behaves as a flow phase unto itself much like the vapor and continuous liquid phases. Governing equations are solved to predict droplet behavior in each droplet field. Droplets move between CVs through flow paths and can interact with thermal surfaces as well as other phases, e.g. other drop fields, the vapor phase, and the liquid phase. The user has no responsibilities beyond specifying initial droplet conditions and configuring an appropriate number of droplet fields.

#### 4. Comparative Assessment of Code Phenomenological Models

Considering first the break source, previous discussions establish that both the break enthalpy and break effluent flashing are treated differently in MELCOR and GOTHIC. The fact that MELCOR works with enthalpy rate whereas GOTHIC works with specific enthalpy should not lead to appreciable differences in code predictions. However, flashing treatment directly impacts the relative proportion of steam and liquid evolved from the source. Hence, it has direct implications for containment pressurization and sump pool temperature. It is difficult to describe exactly how the two codes differ in this respect. From the flashing model descriptions in MELCOR and GOTHIC code manuals, one can identify a similarity in that both codes use downstream CV saturation conditions to compute the liquid/steam partition after flashing. Within the downstream CV, both codes mathematically treat the break as an external source in the governing equations, and hence the process of equilibration is modeled similarly. However, the liquid/steam split as predicted by MELCOR (using an average enthalpy) may not equal that of GOTHIC (using Equation 3). To ascertain break source effects on comparative containment response, a sensitivity calculation is performed wherein all thermal surfaces and engineered safety features are excluded. Any disagreement that persists can be attributed with confidence to source/flashing treatment.

Considering next the thermal surface effects, there are similarities in how MELCOR and GOTHIC compute atmosphere/structure and pool/structure heat transfer. Both codes use Nusselt number and/or heat transfer coefficient correlations that look alike and, in some cases of plane wall geometry, are identical in terms of constants and exponents. MELCOR allows for a transition between laminar and turbulent flow. The Nusselt number in this transition regime is computed by linear interpolation (e.g. using Reynolds number for forced convection) between the laminar and turbulent results. It is clear that both codes account for condensate film effects in convection and 1-D structural conduction heat transfer calculations, but the methods are not identical. Condensation mass transfer modeling in GOTHIC and MELCOR are not identical but bear some similarities. For example, MELCOR employs a film tracking model whereas GOTHIC opts for more mechanistic approaches but both codes can apply various diffusion layer models to thermal surfaces.

Both kinds of ESFs are modeled differently in the two codes. MELCOR employs an empirical correlation for convection and condensation heat transfer coefficients to characterize fan coolers. By modeling choices in this case, GOTHIC uses tabular functions expressing fan cooler heat removal rate as a function of containment saturation temperature. Note that GOTHIC is capable of much more detailed fan cooler modeling but such options were not pursued in this study. For spray droplets, MELCOR employs a specialized mathematical model with assumptions that necessarily exclude certain physics. Also, the user defines some aspects of droplet behavior beyond just initial conditions. GOTHIC uses the same generalized field equations as for continuous liquid and vapor to treat droplets. The user specifies

flow boundary conditions and initializes droplet fields so that their behavior is governed by conservation equation solutions. Hence there are definite differences in ESF treatment between the two codes.

#### 5. Sensitivity Study Results

At this point, code differences with respect to break source, thermal surface effects, and engineered safety features have been established. To ascertain the quantitative impact of code differences on the comparative containment response, a series of sensitivity calculations are performed. In each calculation, some phenomenological aspect is strategically excluded from the MELCOR and GOTHIC DEGB LOCA calculations in an attempt to resolve the separate effect of that aspect. Sensitivity calculations include:

- 1. A case excluding fan coolers only
- 2. A case excluding sprays only
- 3. A case excluding all ESFs (coolers and sprays)
- 4. A case excluding thermal surfaces only
- 5. A case excluding thermal surfaces and all ESFs (coolers and sprays)

Each calculation results in predictions from each code for containment pressure and sump pool temperature response. If code agreement improves relative to the best-estimate calculation, one may reasonably infer that the differences in code phenomenological models of the excluded aspect were in part to blame for disagreement. The above exposition of MELCOR and GOTHIC modeling serves as a launching point for further investigation. For compactness, not all the results from sensitivity calculations are included in plots. For clarity and ease of comparison, each plot includes the sensitivity run in question and best-estimate results.

For case 1 where only fan coolers are excluded, appreciable changes from the best-estimate results are not observed, i.e. the fan coolers do not meaningfully impact containment pressure or sump pool temperature response to a DEGB LOCA within the first 5000 s of the transient. There are noticeable increases in CV atmosphere/vapor temperatures without fan coolers, but this does not seem to impact CV pool/liquid temperatures significantly. The take-away from case 1 results is that fan coolers do not contribute considerably to code disagreement in terms of containment pressure and sump pool temperature.

Since fan coolers negligibly impact pressure and sump pool temperature, case 2 and case 3 results are virtually identical. Containment spray exclusion does of course lead to relatively higher pressure and sump pool temperature vs. best estimate. Code agreement in terms of pressure response is degraded somewhat when sprays are neglected. Both codes predict consistently higher pressures (between 2 and 5 psia higher) without sprays, as expected. This is evident from Figure 1. Code agreement in terms of sump pool temperature response both degrades and improves, depending on the problem time, when sprays are neglected. This is evident from Figure 2 as the dashed curves begin to move closer together at earlier times, yet never merge as the solid curves do. As expected, both codes predict higher sump pool temperatures without sprays. The take-away from case 2 and 3 results is that sprays have a mixed effect with respect to code disagreement. Their exclusion does not really eliminate the poor agreement for times between the break opening (300 s) and sump switchover (2580.8 s). Hence, though the sprays have a definite impact on code predictions of containment pressure and sump pool temperature response, they must not be the biggest contributor to disagreement between the predictions. Note for time after sump switchover, the containment sprays are seemingly responsible for the dissimilarity in best-estimate pressure curve shapes. The bump in the MELCOR best-estimate curve of Figure 1 is not reproduced in the black dashed curve.

Turning to case 4 wherein thermal surfaces are neglected, mixed effects are again observed with respect to code disagreement. Figures 3 and 4 show the pressure and sump pool temperature response when MELCOR excludes HSs and GOTHIC excludes TCs. From Figure 3, the initial pressure peaks are greater and pressure stays consistently higher as the only active suppressing agent is the containment

spray. From Figure 4, there is obviously better code-to-code agreement before sump switchover. Note also that MELCOR and GOTHIC curves swap positions relative to the best-estimate results where GOTHIC predicted a consistently higher temperature. When thermal surfaces are neglected, MELCOR predicts a higher pool temperature throughout the transient. Thus, MELCOR HSs have a stronger impact on MELCOR sump pool temperature than GOTHIC TCs have on GOTHIC sump pool temperature. The disagreement post sump switchover is likely due to ESF action, and this may be confirmed from sensitivity case 5. The important point of case 4 is that thermal surfaces are probably the prime causative factors for MELCOR-to-GOTHIC disagreement. To break the issue down further, one may take a closer look at indicators of atmosphere/structure heat transfer, pool/structure heat transfer, and condensation mass transfer and/or film effects.

Case 5 removes the influence of ESFs from the results of case 4. There is a drastic impact on containment pressure as no suppressants are available beyond the free hydrodynamic volume in containment. Figure 5 shows the pressure response and Figure 6 shows the sump pool temperature response. The only variable in play for case 5 is the break source, i.e. its enthalpy specification and its flashing treatment. This might in part explain the consistent  $\Delta T$  between the black and gray dashed curves of figure 6. The possibility remains that some as yet unidentified factor is influencing the comparative containment response, e.g. the MELCOR predictions of atmosphere/pool heat and mass transfer within CVs vs. the GOTHIC predictions of vapor/liquid heat and mass transfer within CVs.



Figure 1. Case 2 and 3 of sensitivity study, containment pressure response



Figure 2. Case 2 and 3 of sensitivity study, containment sump pool temperature response



Figure 3. Case 4 of sensitivity study, containment pressure response



Figure 4. Case 4 of sensitivity study, containment sump pool temperature response



Figure 5. Case 5 of sensitivity study, containment pressure response



Figure 6. Case 5 of sensitivity study, containment sump pool temperature response

### 6. Discussion

Some highlights of the analysis thus far:

- Fan coolers have minimal impact on comparative containment response for a DEGB LOCA
- Sprays have mixed effects on comparative containment response:
  - Agreement is not materially improved between 300 s and 2580.8 s
  - The qualitative disagreement in best-estimate pressure curve shape is explained by sprays
- Thermal surface effects are the greatest contributor to disagreement on sump pool temperature
- Under exclusion of thermal surfaces and ESFs, disagreements are still evident, accounted for by:
  - o The break source (enthalpy specification and/or flashing treatment), or

• Some unexplored effect, e.g. intra-CV heat/mass transfer between pool and atmosphere The final bullet points above imply that more investigation is warranted for thermal surface heat transfer and for break source flashing. It is illuminating to compare code predictions for thermal surface heat transfer coefficients and total water and steam mass fractions.

For the largest outer walls of containment, Figure 7 shows atmosphere (steam/air) heat transfer coefficients and obviously there is considerable disagreement - one to two orders of magnitude – between MELCOR and GOTHIC results for these thermal surfaces. This is quantitative proof of code differences with respect to atmosphere/surface heat transfer. GOTHIC heat transfer coefficients are much larger than those of MELCOR in this case. Note the data in Figure 7 were taken from sensitivity case 3 where all ESFs are excluded. Comparing code predictions for pool/surface heat transfer in Figure 8, the roles are reversed as MELCOR heat transfer coefficients are larger than those of GOTHIC for much of the transient. Such a discrepancy in pool/floor heat transfer is manifest in sump pool temperature curves, e.g. of Figure 2 above. This is quantitative confirmation that the particular thermal surface effect of pool/floor heat transfer is crucial to comparative containment response. Figure 8 data is from sensitivity case 3.



Figure 7. Code predictions of heat transfer coefficients, outer containment walls to CV atmospheres



Figure 8. Code predictions of heat transfer coefficients, compartment floors to CV pools



Figure 9. Relative fractions of liquid water and vapor (steam) in containment, total over all CVs

The mass fractions plotted in Figure 9 (taken from sensitivity case 3) are those of liquid and steam considering all CV contents in the computational domain. Thus the denominator of each fraction is the sum of liquid and steam mass in all CVs. The numerator of the liquid fraction is the sum of all liquid in all CVs, whereas the numerator of the steam fraction is the sum of all steam in all CVs. These fractions, in the short term after the break opens, give some quantitative insight into how MELCOR and GOTHIC predict the liquid/steam partition upon flashing. As can be seen from the inset of Figure 9, GOTHIC predicts a larger fractional liquid inventory vs. MELCOR by about 10% shortly after the break. Therefore, in the GOTHIC simulation a comparatively greater amount of high temperature liquid water enters the sump pool straight from the break by way of the lower compartment. This high temperature water has little opportunity to cool before entering the sump, hence the higher sump pool/floor heat transfer coefficients and the comparatively greater mass of hot water straight from the break, the comparatively higher GOTHIC sump pool temperature (under best-estimate conditions) makes physical sense.

#### 7. Conclusions

There are discernable differences in the methods by which MELCOR and GOTHIC treat source flashing, thermal surface effects, and Engineered Safety Features. From the sensitivity calculations, one can surmise causes for observed disagreements in the best estimate containment response according to MELCOR and to GOTHIC. Regarding the fan coolers, one concludes from sensitivity cases 2 and 3 that their impact is minimal and they contribute little to code disagreement. Regarding the sprays, one concludes from sensitivity cases 2 and 3 that they contribute significantly to code disagreement only after sump switchover time. Regarding the thermal surfaces, one concludes from sensitivity case 5 that they are the most influential factor with respect to code disagreement. The order-of-magnitude differences in atmosphere/surface heat transfer coefficients (larger for GOTHIC) and in pool/surface heat transfer coefficients (larger for MELCOR) help to explain code disagreement on sump pool temperature under

best-estimate conditions. Regarding break source flashing, one concludes that it contributes to code disagreement on sump pool temperature under best-estimate conditions.

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