Light Water Reactor Sustainability Program

Modifications to MELCOR 1.8.6 for modeling Accident Tolerant Fuel in Boiling Water Reactors

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Modifications to MELCOR 1.8.6 for modeling Accident Tolerant Fuel in Boiling Water Reactors

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ABSTRACT

This work describes further modifications made to a previously implemented User-Defined Generalized Coating (UDGC) model in MELCOR 1.8.6. The UDGC version of the code allows for the modeling of cladding and canister materials other than Zircaloy (without overwriting Zircaloy properties) as well as coated Zircaloy cladding and canisters, with the thermophysical and oxidation properties of the clad or coating material specified by the user. Specific changes outlined in this report are the extension of the UDGC models to BWR canisters, and generalization of the oxidation model for all UDGC components to accommodate different oxidation rate correlations in two different temperature ranges. User input requirements are specified and an example case is described that illustrates the potential impact of model assumptions.

CONTENTS

FIGURES

ACRONYMS

ATF   Accident-Tolerant Fuel

BWR   Boiling Water Reactor

CB   Canister, adjacent to control blade

CL   Cladding

CN   Canister, not adjacent to control blade

COR   Core package

HPCS   High-Pressure Coolant Spray-injection system

INL   Idaho National Laboratory

LWR   Light Water Reactor

NRC   Nuclear Regulatory Commission

NS   Non-supporting Structure

OS   Other Structure

RCIC   Reactor Core Isolation Cooling system

SS   Supporting Structure

STSBO   Short-Term Station Blackout

UDGC   User-Defined Generalized Coating

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1. INTRODUCTION

Accident Tolerant Fuels (ATF) and cladding materials are being investigated as a way to provide a greater resistance to fuel degradation, oxidation, and melting under severe accident conditions. Scoping simulations performed using a severe accident analysis code can be used to investigate the influence and potential safety advantages of these advanced materials on beyond design basis accident progression and to identify any existing code limitations. To this end, in recent years INL has made a number of generalizations to the oxidation and material property models in the MELCOR code (developed by Sandia National Laboratories) that allow for modeling of alternate (i.e. not Zircaloy) cladding or duplex coated claddings consisting of a Zircaloy base structure and a metal coating of differing properties. The most recent of these, designated "UDGC" for User Defined Generalized Coating, allows for the modeling of any metal coating that follows parabolic oxidation kinetics, with the material properties and Arrhenius law oxidation rate parameters specified by the user.

The work described herein rectifies two shortcomings of the previous UDGC MELCOR model. First, the oxidation model has been generalized to allow for two different Arrhenius laws in two different temperature regions. This is intended to better capture the supposed oxidation kinetics of (for example) FeCrAl, which may be dominated by oxidation of different alloy constituents (e.g. Al or Fe) depending on the temperature. Second, the UDGC coating model has been applied additionally to MELCOR's BWR canister components, allowing for better assessment of BWR accident progression with ATF fuel, in which case the Zircaloy canisters would also presumably be coated. These models and the modified input file format necessary to invoke them are described in this report. Analyses making use of the new models to assess the potential benefits of ATF cladding on severe accident progression in BWRs, in concert with possible synergistic effects of extended Reactor Core Isolation Cooling (RCIC) system operation and additional containment heat sink options such as external flooding of the drywell head, are the topic of a subsequent report.

2. MODEL DESCRIPTION AND IMPLEMENTATION

MELCOR [1-2] is the primary code used by the Nuclear Regulatory Commission (NRC) to model and analyze the progression of severe accidents. MELCOR is being developed and maintained for the NRC by Sandia National Laboratories. MELCOR is a system-level severe accident analysis code that models the major thermal hydraulic and other phenomena occurring in such an event, including fuel heat-up, cladding oxidation, radionuclide release and transport, fuel melting and relocation, etc.

MELCOR is presently designed for current light water reactor (LWR) core material configurations. The thermal response (including oxidation, melting, relocation, etc.) of solid core materials is modeled by the COR package, in which the core is divided into a series of radial rings and axial levels. Each core cell (corresponding to a particular ring and level) contains some number of components, which for a BWR can include [1]:

- Fuel pellets;

- Cladding;

- BWR canister walls, split into two parts: one part adjacent (CB) and another part that is not adjacent (CN) to the control blade;

- "Supporting structure" (SS);

- "Nonsupporting structure" (NS);

- "Other structure" (OS).

Each component in each cell comprises some number of different material masses, which are a subset of [1]:

- UO_2

- Zircaloy

- ZrO_2

- Steel

- "Steel oxide"

- Control rod poison, either B4C or Ag-In-Cd

- Inconel

- Electric heating element material

Not all of the above materials are available to every component; for example the "cladding" component may only contain Zircaloy, ZrO_2, and Inconel. Generalization of the COR components to include coated claddings and specification of their oxidation properties is described in the following sections.
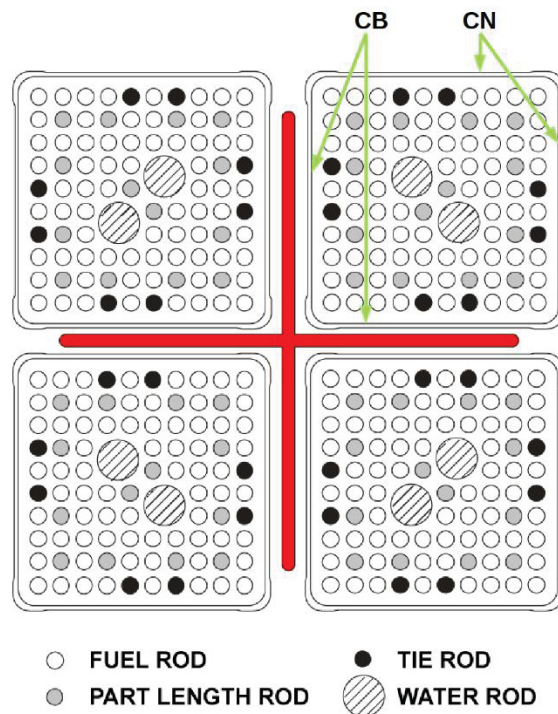

Figure 1. Cross-section of a BWR assembly. The cruciform-shaped control rod is red; the portions of a canister adjacent to (CB) and *not* adjacent to (CN) the control rod are labeled.

2.1   Cladding and canister model extensions

The addition of UDGC coating to the above described COR package in MELCOR requires that 1) additional materials UDGC and UDGC-oxide be created; 2) The COR components "cladding" (CL), canisters adjacent to (CB) and not adjacent to (CN) control blades accept UDGC and UDGC-oxide masses as input in addition to Zircaloy, ZrO_2, and Inconel.

These changes have previously been made for the cladding (CL) component, and similar additions have now been made for both CN and CB canister components. The necessary changes include:

- Expanding arrays that store canister masses to include UDGC and UDGC-oxide, and modifying the code to properly read these additional masses from cards CORijjKCN and CORijjKCB (see Section 3 for complete input specifications);

- Inclusion of the UDGC and UDGC-oxide masses in the mass and energy conservation calculations;

- Addition of UDGC and UDGC-oxide masses in each cell to the output and plot files. The available plot variables are COR-MUDGC_ijj and COR-MUDGC-OX_ijj, where "ijj" is the COR cell.

In this latest revision of the code, the cladding and both canister components may therefore be composed of any combination of Zircaloy and UDGC (or Inconel, ZrO_2, or UDGC-oxide, though the latter two would not typically be part of an initial problem definition), including an entirely UDGC clad or canister, in which case zero mass must be specified for Zircaloy. To model a standard Zircaloy cladding or canister, the UDGC and UDGC oxide masses may be specified as zero or simply omitted. UDGC-coated Zircaloy clad/canisters will require non-zero masses for both, and the modifications include the necessary logic to oxidize the UDGC before Zircaloy (see Section 2.2 below).

An important difference exists between the cladding and canister components, namely that the latter may be exposed to steam or air on both sides. A standard Zircaloy canister, then, will consist of three regions: a Zircaloy core, and two oxide layers that grow independently on either side of it. The fluid volumes on either side of the canister would typically be modeled separately in MELCOR, so conditions may indeed differ on either side of the canister, though it is not clear to what extent they actually differ in practice. If a Zircaloy canister is simply to be replaced with a UDGC canister, the above logic does not change. If it is to be supplanted by a UDGC-coated Zircaloy canister, this would consist of 1) a Zircaloy core, 2) *a separate UDGC layer on either side*, and finally 3) a separate UDGC-oxide layer on either side, once these begin to form.

In the two above described configurations, the UDGC material must be either a single zone, bounded by UDGC-oxide layers, or two distinct zones, bounded by Zircaloy at the center, and UDGC-oxide layers on the other sides. Both configurations are not easily accommodated by the same model. For this reason, the simpler approach has been chosen for now, namely that the UDGC is treated as a single entity. For coated canisters, the entirety of the UDGC coating mass (both sides) should be entered on a single word as described in section 3. For this reason the UDGC coatings in a given core cell must necessarily melt and/or fail simultaneously. The oxide layer masses on either side of the canister are tracked separately in the same way that they are for the default Zircaloy canisters.

The material property data for most COR materials is built into the code; to use the UDGC model, all of the necessary properties (except emissivity, which is assumed to be identical to Zr and ZrO_2) must be specified via user input. The following must be specified for both UDGC and UDGC-oxide using tables [1], as described in section 3:

- Enthalpy (J/kg) vs. temperature (K)

- Temperature (K) vs. enthalpy (J/kg)

- Specific heat (J/kg-K) vs. temperature (K)

- Thermal conductivity (W/m-K) vs. temperature (K)

- Density (kg/m^3) vs. temperature (K)

The following constant values must additionally be specified [1] for each material as described in section 3:

- Density (kg/m^3)

- Melting temperature (K)

- Latent heat of fusion (J/kg)

Any of the above input left *un*specified will default to the built in properties of Zircaloy. This may be acceptable for some testing purposes, but in actual practice care should be exercised in ensuring complete entry of all of the above tables and values for the desired UDGC material.

It should also be noted that the same core materials are used by multiple core components, and therefore that the above properties entered for a UDGC (and its oxide) apply to both the cladding and canisters (both CN and CB varieties).

2.2   Oxidation model extensions

The UDGC oxidation model assumes that the UDGC material undergoes parabolic oxidation, i.e. that the square of the thickness x of the oxide layer that forms in a steam (or air) environment is proportional to the time t for which it is exposed:

$$x^2 = k_p t \tag{1}$$

The parabolic rate constant k_p is given by an Arrhenius law:

$$k_p = k_p^o \exp\left(-E_a/RT\right) \tag{2}$$

The new UDGC oxidation model mirrors the logic of MELCOR's Zircaloy oxidation model, in that it allows for a different Arrhenius law (different k_p^o and E_a) in each of two different temperature regions. The maximum temperature for region one and minimum temperature for region two must now be specified by the user. These need not be identical; a "gap" may exist between temperature regions, though they may not overlap. In the event of a gap between those values specified by the user, linear interpolation between the logarithms of the oxidation rates bounding this temperature gap is used to specify the oxidation rate constant. The same logic is used by default by MELCOR for zirconium oxidation.

Where both Zircaloy and UDGC masses are specified for cladding or canister components in a given core cell, the UDGC exists (e.g. as a coating) on top of the zirconium, and it is the UDGC material that oxidizes in the presence of steam or oxygen according to the above-described rate law. The presence of any UDGC or UDGC-oxide in a given core cell implies that none of the zirconium in the cell is yet exposed to the oxidizing environment, and so oxidation of this zirconium cannot occur until the UDGC and/or UDGC-oxide layer fails. This occurs either when the UDGC-oxide layer reaches its melting temperature, or when either the minimum thickness or maximum temperature specified in sensitivity coefficient array 1131 are exceeded [2]. Note that the coefficients in that array apply both to ZrO_2 and UDGC-oxide and cannot be changed independently. Also note that molten UDGC will otherwise be held in place by solid UDGC-oxide when the latter has a higher melting temperature. The same logic applies to standard Zircaloy cladding in MELCOR.

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If UDGC is the only cladding material in a core zone, then the same criteria apply to the failure of the entire rod. If Zircaloy is present, then the rod failure and candling criteria revert back to those for Zircaloy after the failure of the UDGC coating. The UDGC (and/or UDGC-oxide) material do not participate in candling or other material interaction phenomena, but are transferred directly to the debris bed in the corresponding volume, where any un-oxidized UDGC material will continue to undergo further oxidation by steam or air.

Oxidation input for a UDGC is specified in sensitivity coefficient array 1001 as outlined in detail, and with an example, in Section 3. The following information must be specified, for both steam and air oxidation:

- Arrhenius law pre-factors (k_p^o), in kg^2-metal/m^4-s, for both temperature ranges;

- Arrhenius law activation temperatures (E_a), in K, for both temperature ranges;

- Maximum of the first temperature range, in K.

- Minimum of the second temperature range, in K. Must be greater than or equal to the preceding value.

- Heat of reaction, in J/kg-metal oxidized;

- Mass of metal oxide produced per mass of metal consumed (dimensionless);

- Mass of oxidizer (H_2O and O_2) consumed per mass of metal consumed (dimensionless);

- Mass of CO produced per mass of metal oxidized (dimensionless; for the steam reaction only).

The last three must be worked out from the stoichiometry of the oxidation reactions.

Example input is given in Section 3. The material properties used in the example input are those for FeCrAl and its oxide summarized previously in [3], but modified in the following ways to demonstrate the multi-region oxidation capability. First, the region 1 Arrhenius law pre-factor has been changed to 230.0 kg^2-**metal**/m^4-s in accordance with the values given in [4]:

$$k_p = 230.0 \frac{\text{kg}^2\text{metal}}{\text{m}^4\text{s}}\exp\left(-41376/T\right) \tag{3}$$

This reflects the proper conversion of previous measured FeCrAl oxidation rates, which in fact had units of kg^2-**oxide**/m^4-s, to the proper metal basis (kg^2-**metal**/m^4-s) as required by MELCOR. When using oxidation rate correlations from the literature, similar care should be exercised to ascertain whether these are based on the mass of oxygen consumed, mass of oxide generated, or mass of metal consumed, and to convert these to the latter when necessary.

Secondly, a different Arrhenius law is specified in temperature range 2, based on the assumption [4] that beyond some temperature at which the FeCrAl oxide layer (predominantly Al_2O_3) fails, oxidation proceeds as for stainless steel, dominated by the oxidation of iron. The correlation used in this temperature range is the MELCOR default for oxidation of stainless steel:

$$k_p = 2.42 \times 10^9 \frac{\text{kg}^2\text{metal}}{\text{m}^4\text{s}}\exp\left(-42400/T\right) \tag{4}$$

The first correlation applies up to 1763 K, and the second above 1783 K. In between these temperatures, the oxidation rate constant is determined by interpolating between the two correlations, as described above. Note that the nominal transition temperature, 1773 K [4], is not necessarily associated with failure of the FeCrAl oxide layer as predicted by MELCOR, which likely does not occur until the melting temperature of the oxide (1901 K in this case) is reached, as described above. Equation (4) implies a jump in the oxidation rate constant of almost seven orders of magnitude at the transition point (Figure 2); the implications of such an assumption are briefly explored in Section 4.
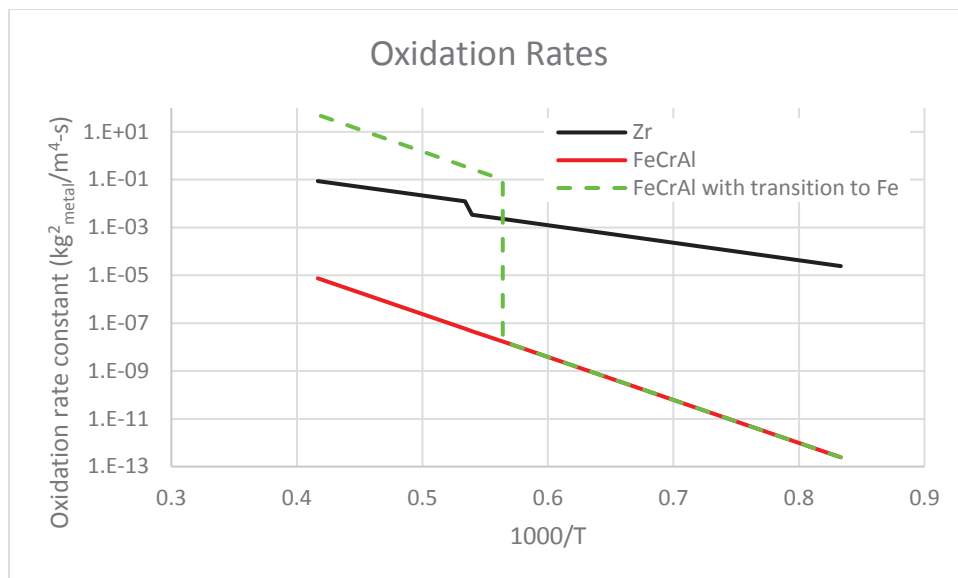
Figure 2. Oxidation rate constants for Zircaloy (from MELCOR) and FeCrAl as described by equations (3)-(4).

The example input for air oxidation essentially uses only the region 1 correlation, by setting the maximum temperature for range 1 and minimum temperature for range 2 to an unattainably high number (10,000 K).

As with the material property input, if any of the sensitivity coefficient input for UDGC oxidation described above (and in Section 3) is omitted, default Zircaloy values are used. Therefore, care should be taken to ensure that the oxidation parameters are completely specified for the material being modeled.

3. MELCOR USER INPUT

The UDGC models are invoked by 1) specifying non-zero masses for the UDGC or its oxide on cards CORijjKCL, CORijjKCN, and/or CORijjKCB, 2) specifying 16 additional sensitivity coefficients (in sensitivity coefficient array 1001) to define the oxidation parameters, and 3) defining the necessary material properties of the UDGC and its oxide (internally, new materials called UDGC and UDGC-OXIDE have been added to MELCOR's materials package). If left unspecified, the material properties default to those of Zircaloy that are already stored in the code. Excerpts from the MELCOR 1.8.6 user manual [1] appear below, with additional input specifications for the UDGC models added in blue text.

CORijjKCL – Cladding Component Masses
      $1 \leq i \leq$ NRAD, i is the radial ring number
      $1 \leq jj \leq$ NAXL, jj is the axial level number
      Optional

      This record specifies the initial masses of the cladding component in cell ijj. This record is not generally required, but component masses for at least one component must be entered if the new-format option is exercised for this cell. Three floating point fields are allowed on this record. If any fields on this record are missing or are set to –1.1 (or if the record is not present), the corresponding values from reference cell IREFN are used if IREFN is defined; otherwise, the values are set to zero.

(1) XMCLZR - Mass of Zircaloy in the cell cladding component.
    (type = real, default = –1.1, units = kg)
(2) XMCLIN - Mass of Inconel associated with the cell cladding component
    (e.g., PWR grid spacers).
    (type = real, default = –1.1, units = kg)
(3) XMCLZX - Mass of ZrO2 in the cell cladding component.
    (type = real, default = –1.1, units = kg)

For the User Defined Generalized Coating (UDGC) version:

(4) XMCLGC - Mass of UDGC material in the cell cladding component.
    (type = real, default = –1.1, units = kg)
(5) XMCLGX - Mass of UDGC-oxide in the cell cladding component.
    (type = real, default = –1.1, units = kg)

This record specifies the initial masses of the cladding component in cell ijj. This record is not generally required, but component masses for at least one component must be entered if the new-format option is exercised for this cell. Five floating point fields are allowed on this record. If any fields on this record are missing or are set to –1.1 (or if the record is not present), the corresponding values from reference cell IREFN are used if IREFN is defined; otherwise, the values are set to zero. If the user wishes the UDGC material to constitute the entire cladding, then the only non-zero mass that the user should enter is that for the UDGC material.

CORijjKCN – Canister (CN) Component Masses
    1 ≤ i ≤ NRAD, i is the radial ring number
    1 ≤ jj ≤ NAXL, jj is the axial level number
    Optional

This record specifies the initial masses of the canister (CN) component (the portion not adjacent to a control blade) in cell ijj. This record is not generally required, but component masses for at least one component must be entered if the new-format option is exercised for this cell. Three floating-point fields are allowed on this record. If any fields on this record are missing or are set to –1.1 (or if the record is not present), the corresponding values from reference cell IREFN are used if IREFN is defined; otherwise, the values are set to zero.

(1) XMCNZR - Mass of Zircaloy in the cell canister (CN) component.
    (type = real, default = –1.1, units = kg)
(2) XMCNXI - Mass of ZrO2 on the inside surface of the cell canister (CN)
    component.
    (type = real, default = –1.1, units = kg)
(3) XMCNXO - Mass of ZrO2 on the outside surface of the cell canister (CN)
    component.
    (type = real, default = –1.1, units = kg)

For the User Defined Generalized Coating (UDGC) version:

(4) XMCNGC - Mass of UDGC in the cell canister (CN) component.
    (type = real, default = –1.1, units = kg)
(5) XMCNGXI - Mass of UDGC-oxide on the inside surface of the cell canister (CN)

component.
(6) XMCNGXO - Mass of UDGC-oxide on the outside surface of the cell canister (CN)
component.
(type = real, default = –1.1, units = kg)

CORijjKCB – Canister (CB) Component Masses
1 ≤ i ≤ NRAD, i is the radial ring number
1 ≤ jj ≤ NAXL, jj is the axial level number
Optional

This record specifies the initial masses of the canister CB component (the portion adjacent to a control blade) in cell ijj. This record is not generally required, but component masses for at least one component must be entered if the new-format option is exercised for this cell. Three floating-point fields are allowed on this record. If any fields on this record are missing or are set to –1.1 (or if the record is not present), the corresponding values from reference cell IREFN are used if IREFN is defined; otherwise, the values are set to zero.

(1) XMCBZR - Mass of Zircaloy in the cell canister (CB) component.
(type = real, default = –1.1, units = kg)
(2) XMCBXI - Mass of ZrO_2 on the inside surface of the cell canister (CB)
component.
(type = real, default = –1.1, units = kg)
(3) XMCBXO - Mass of ZrO_2 on the outside surface of the cell canister (CB)
component.
(type = real, default = –1.1, units = kg)

For the User Defined Generalized Coating (UDGC) version:

(4) XMCBGC - Mass of UDGC in the cell canister (CB) component.
(type = real, default = –1.1, units = kg)
(5) XMCBGXI - Mass of UDGC-oxide on the inside surface of the cell canister (CB)
component.
(type = real, default = –1.1, units = kg)
(6) XMCBGXO - Mass of UDGC-oxide on the outside surface of the cell canister (CB)
component.
(type = real, default = –1.1, units = kg)

Oxidation parameters for the UDGC material must also be defined. The logic of the modified code will oxidize the UDGC material first, using the additional user-specified oxidation constants in sensitivity coefficient array 1001 listed below (input in blue text is required for the UDGC model).

1001 – Zircaloy Oxidation Rate Constant Coefficients

These coefficients are used to calculate the rate constant for oxidation of Zircaloy by parabolic kinetics. The rate constant K (kg^2/m^4-s) as a function of temperature T (K), where I = 1 for oxidation by H_2O and I = 2 for oxidation by O_2.

(1,I) - low temperature range constant coefficient
(default = 29.6 for I = 1, 50.4 for I = 2; units = $kg^2(Zr)/m^4$–s, equiv = none)

       (2,I) - low temperature range exponential constant
            (default = 16820.0 for I = 1, 14630.0 for I = 2; units = K, equiv = none)
       (3,I) - high temperature range constant coefficient
            (default = 87.9 for I = 1, 0.0 for I = 2; units = $kg^2(Zr)/m^4$–s, equiv = none)
       (4,I) - high temperature range exponential constant
            (default = 16610.0 for I = 1, 0.0 for I = 2; units = K, equiv = none)
       (5,I) - upper temperature boundary for low temperature range
            (default = 1853.0 for I = 1, 10000.0 for I = 2; units = K, equiv = none)
       (6,I) - lower temperature boundary for high temperature range
            (default = 1873.0 for I = 1, 10000.0 for I = 2; units = K, equiv = none)

For the UDGC version of MELCOR the following input is required:

       (7,I) - low temperature range constant coefficient
            (default = 0.0 for I = 1, 0.0 for I = 2; units = $kg^2(UDGC)/m^4$–s, equiv = none)
       (8,I) - low temperature range exponential constant
            (default = 0.0 for I = 1, 0.0 for I = 2; units = K, equiv = none)
       (9,I) - high temperature range constant coefficient
            (default = 0.0 for I = 1, 0.0 for I = 2; units = $kg^2(UDGC)/m^4$–s, equiv = none)
      (10,I)- high temperature range exponential constant
            (default = 0.0 for I = 1, 0.0 for I = 2; units = K, equiv = none)
      (11,I)- upper temperature boundary for low temperature range
            (default = 1853.0 for I = 1, 10000.0 for I = 2; units = K, equiv = none)
      (12,I)- lower temperature boundary for high temperature range
            (default = 1873.0 for I = 1, 10000.0 for I = 2; units = K, equiv = none)
      (13,I)- heat of oxidation reaction (J/kg-UDGC metal oxidized)
            (default = 0.0 for I = 1, 0.0 for I = 2; units = $kg^2(UDGC)/m^4$–s)
      (14,I) - mass of UDGC metal oxide produced/mass UDGC metal oxidized, I=1 and
            mass CO produced/mass UDGC metal oxidized, I=2
            (default = 0.0 for I = 1, 0.0 for I = 2; units = none)
      (15,I) - mass H_2O consumed/mass UDGC metal oxidized, I=1, and
            mass O_2 consumed/mass UDGC metal oxidized, I=2
            (default = 0.0 for I = 1, 0.0 for I = 2; units = none)

It should be emphasized that the reaction rate constant must be based on the mass of metal (UDGC) consumed, not the mass of oxide formed (or oxygen mass gained). Care should be exercised in converting any correlations found in the literature to this basis for use in MELCOR.

Also note that the default for these new sensitivity coefficients is zero. If 1001(7,I) is zero, then the modified version of MELCOR reverts to 1001(1-6,I) for oxidation constants of the UDGC material.

Examples of user input required to define a cladding coating material for the INL modified UDGC version of MELCOR 1.8.6 are shown below.

<u>Example core physics package input</u>

```
*               XMCLZR  XMCLIN  XMCLZX    XMCLGC  XMCLGX
COR101KCL     79.301        0.0        0.0      173.205        0.0
*
*         CANISTER (CHANNEL BOXES)
```

* 'CN' = not adjacent to blade
* 'CB' = adjacent to blade
*   XMCNZR XMCNXI XMCNXO XMCNGC   XMCNGXI   XMCNGXO
COR101KCN 145.66   0.00   0.00   15.00   0.0   0.0
*   XMCBZR XMCBXI XMCBXO XMCBGC   XMCBGXI   XMCBGXO
COR101KCB 145.66   0.00   0.00   15.00   0.0   0.0
*
*
************************************** Sensitivity coefficients for FeCrAl as a UDGC
sc00001 1001   230.0   7 1   * Pre-exponential UDGC H2O oxidation - region 1
sc00002 1001   6.6998   7 2   * Pre-exponential UDGC O2 oxidation
sc00003 1001   41376.0   8 1   * Exponential UDGC H2O oxidation
sc00004 1001   35355.7   8 2   * Exponential UDGC O2 oxidation
sc00005 1001   2.42E9 9 1   * Pre-exponential UDGC H2O oxidation - region 2
sc00006 1001   0.0   9 2   * Pre-exponential UDGC O2 oxidation
sc00007 1001   4.24E4 10 1   * Exponential UDGC H2O oxidation
sc00008 1001   0.0   10 2   * Exponential UDGC O2 oxidation
sc00009 1001   1763. 11 1   * Tmax H2O regime 1
sc00010 1001   10000. 11 2   * Tmax O2 regime 1 force use of only regime 1
sc00011 1001   1783. 12 1   * Tmin H2O regime 2
sc00012 1001   10000. 12 2   * Tmin O2 regime 2
sc00013 1001 1114105.0 13 1   * Heat of oxidation reaction H2O (J/kg-metal oxidized)
sc00014 1001 7507570.0 13 2   * Heat of oxidation reaction O2
sc00015 1001 1.3551506 14 1   * Mass (kg) of metal oxide produced/mass metal (kg) oxidized
sc00016 1001   0.0 14 2   * Mass (kg) CO produced/mass metal (kg) oxidized
sc00017 1001 0.3998968 15 1   * Mass (kg) H2O consumed/mass metal (kg) oxidized
sc00018 1001 0.3551506 15 2   * Mass (kg) O2 consumed/mass metal (kg) oxidized
*

Materials package input

MPMAT00100 'UDGC'   * Material properties for FeCrAl as a UDGC
MPMAT00101 ENH 001
MPMAT00102 TMP 002
MPMAT00103 CPS 003
MPMAT00104 THC 004
MPMAT00105 RHO 005
MPMAT00151 DEN   7100.0
MPMAT00152 MLT   1773.0
MPMAT00153 LHF 275000.0

*
TF00100 'UDGC h vs t' 19 1. 0.
TF00101 1   1
TF00111   300.0   139439.6
TF00112   400.0   188807.1
TF00113   500.0   243451.4
TF00114   600.0   302430.8
TF00115   700.0   364913.9
TF00116   773.0   412338.2
TF00117   823.0   446218.6
TF00118   873.0   482376.9

```
TF00119      923.0   518977.2
TF00120      973.0   554197.7
TF00121     1000.0   573005.4
TF00122     1200.0   714680.8
TF00123     1400.0   859912.9
TF00124     1600.0  1008674.8
TF00125     1700.0  1084758.2
TF00126     1773.0   1141298.3
TF00127    1773.01  1416298.3
TF00128     2000.0   1598231.9
TF00129     5000.0   4063812.5
*
TF00200 'UDGC t vs h' 19 1. 0.
TF00201  1  1
TF00211    139439.6      300.0
TF00212    188807.1      400.0
TF00213    243451.4      500.0
TF00214    302430.8      600.0
TF00215    364913.9      700.0
TF00216    412338.2      773.0
TF00217    446218.6      823.0
TF00218    482376.9      873.0
TF00219    518977.2      923.0
TF00220    554197.7      973.0
TF00221    573005.4     1000.0
TF00222    714680.8     1200.0
TF00223    859912.9     1400.0
TF00224   1008674.8     1600.0
TF00225   1084758.2     1700.0
TF00226   1141298.3     1773.0
TF00227   1416298.3    1773.01
TF00228   1598231.9     2000.0
TF00229   4063812.5     5000.0
*
TF00300 'UDGC cp vs t' 19 1. 0.
TF00311     300.00     464.80
TF00312     400.00     522.55
TF00313     500.00     570.33
TF00314     600.00     609.25
TF00315     700.00     640.41
TF00316     773.00     658.89
TF00317     823.00     696.33
TF00318     873.00     750.00
TF00319     923.00     714.01
TF00320     973.00     694.81
TF00321    1000.00     698.35
TF00322    1200.00     718.41
TF00323    1400.00     733.91
TF00324    1600.00     753.70
TF00325    1700.00     767.96
TF00326    1773.00     781.08
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TF00327   1773.01   781.08
TF00328   2000.00   821.60
TF00329   5000.00   821.60
*
TF00400 'UDGC k vs t' 15 1. 0.
TF00411      300.0  10.544
TF00412      400.0  12.574
TF00413      500.0  14.369
TF00414      600.0  15.982
TF00415      700.0  17.463
TF00416      800.0  18.863
TF00417      900.0  20.235
TF00418     1000.0  21.629
TF00419     1200.0  24.691
TF00420     1400.0  28.459
TF00421     1600.0  33.344
TF00422     1700.0  36.335
TF00423     1773.0  38.788
TF00424     2000.0  46.419
TF00425     5000.0  46.419
*
TF00500 'UDGC rho vs t' 2 1. 0.
TF00511   273.15   7098.5
TF00512   5000.0   7098.5
*
MPMAT00200 'UDGC-OXIDE'          * FeCrAl oxide
MPMAT00201 ENH 011
MPMAT00202 TMP 012
MPMAT00203 CPS 013
MPMAT00204 THC 014
MPMAT00205 RHO 015
MPMAT00251 DEN  5180.00
MPMAT00252 MLT  1901.00
MPMAT00253 LHF 687463.0
*
TF01100 'UDGCO h vs t' 4 1. 0.
TF01101  1  1
TF01111      300.0         0.
TF01112    1901.0  1440900.
TF01113   1901.01 2128363.
TF01114    3500.0 3567454.
*
TF01200 'UDGCO t vs h' 4 1. 0.
TF01201  1  1
TF01211          0.0    300.0
TF01212   1440900.0   1901.0
TF01213   2128363.0 1901.01
TF01214   3567454.0   3500.0
*
TF01300 'UDGCO cp vs t' 2 1. 0.
TF01311   273.15  900.0
```

```
TF01312  5000.0  900.0
*
TF01400 'UDGCO k vs t' 2 1. 0.
TF01411  273.15  4.0
TF01412  5000.0  4.0
*
TF01500 'UDGCO rho vs t' 2 1. 0.
TF01511  273.15  5180.0
TF01512  5000.0  5180.0
```

4. DEMONSTRATION AND SUMMARY

In order to demonstrate some of the functionality of the new models, some comparisons are made here between variations on a short-term station blackout (STSBO) accident, exercising variations on the new clad/canister and oxidation model inputs. These are based on a MELCOR model of LaSalle Unit 2, a ~1100 MWe (3500 MWth) BWR-5 with a Mark II containment. The MELCOR model has recently been adapted by the University of Wisconsin [5] and is based on earlier work published in [6]. The STSBO accident sequence assumes that DC power from batteries is not available at the start of the accident, thereby disabling all reactor safety systems. In addition, in this example it is assumed that the safety relief valve fails open after two hours due to excessive cycling at higher temperatures. The input of STSBO can be converted into a long-term station blackout by assuming that batteries are available until exhausted to provide DC power to allow for operation (instrumentation and control) of emergency cooling systems including the steam-driven High-Pressure Coolant Spray-Injection system (HPCS) and Reactor Core Isolation Cooling (RCIC) system. A detailed summary of the accident sequence is given in [5]. The cladding and canisters are made of Zircaloy with default MELCOR properties in this base case, referred to as "Zircaloy" in what follows.

Two variations on this base case are considered here. In both, all Zircaloy in cladding and canisters is replaced with an equal volume of FeCrAl (FeCrAl is slightly denser, so this constitutes a slightly larger mass for all such components). This is not intended to represent an actual ATF fuel design, but rather to simply illustrate the difference in accident progression resulting from replacement of material and oxidation properties alone, without accompanying modification of the geometry.

In the first variation (referred to in the figures as "FeCrAl - 2 reg."), the FeCrAl oxidation is as described at the end of Section 2.2, making use of equation (3) below 1763 K and equation (4) above 1783 K, and interpolating between the two between 1763 and 1783 K. In the second variation (referred to in the figures as "FeCrAl - 1 reg."), equation (3), which is based on actual FeCrAl oxidation data, is assumed to apply for all temperatures, similar to previous analyses made with the UDGC code prior to the implementation of multiple oxidation regions (e.g. [3]).

The masses of either Zircaloy or FeCrAl in core cell 110 (near the center of the core, both radially and axially) in each case are shown in Figure 3. These material masses include both the cladding and canister components. It is seen that significant oxidation of Zircaloy begins at around 4000 seconds, with component failures occurring by about 5000 seconds. Subsequent spikes in the mass represent unoxidized material slumping down from higher core cells. For FeCrAl with two oxidation regions, significant oxidation occurs beginning at about 9600 seconds and continuing until component failures occur beginning at around 10200 seconds. For FeCrAl with only one oxidation region, there is no significant oxidation apparent prior to component failures at ~10500 seconds. This is confirmed by Figure 4, in which the corresponding oxide masses are plotted. The amount of oxide generated from FeCrAl with one oxidation region is very small compared to either FeCrAl with two oxidation regions or Zircaloy.
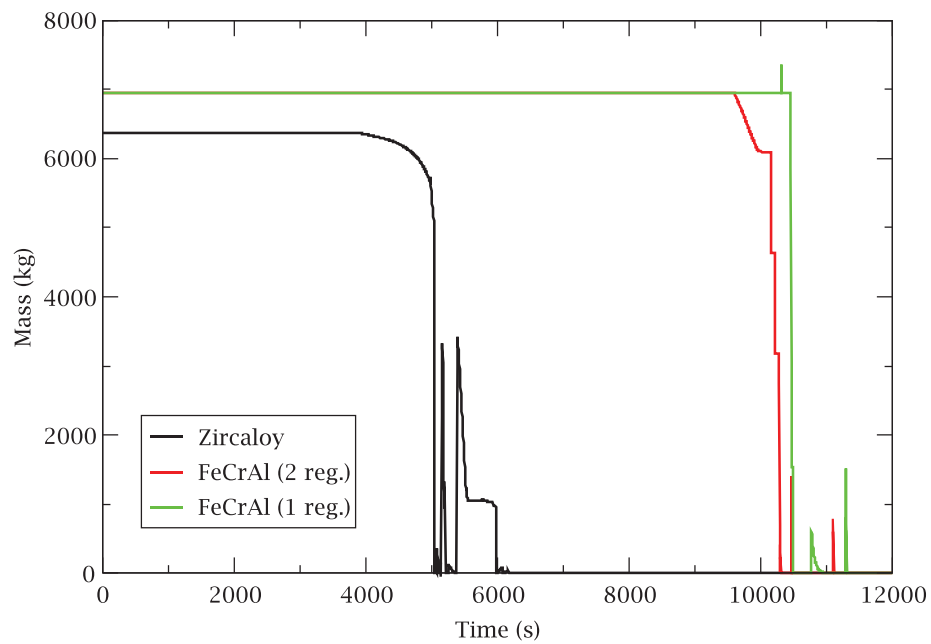
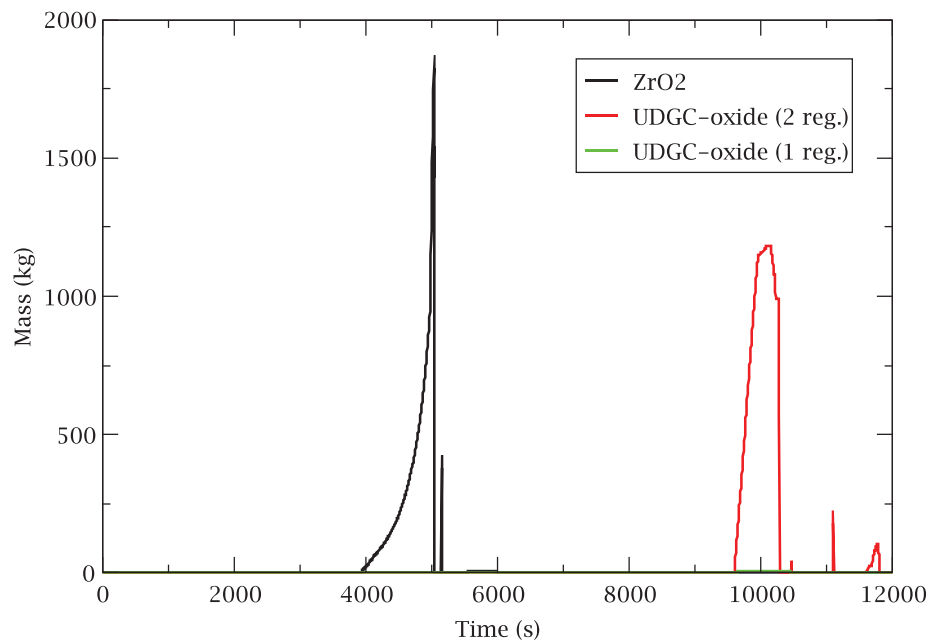Figure 3. Zircaloy and FeCrAl masses in core cell 110.

Figure 4. ZrO$_2$ and UDGC-oxide masses in core cell 110.

Further details of the Zircaloy and FeCrAl behavior are evident upon examination of their temperatures, as shown in Figure 5. Here the canister temperature begins to increase at about 3000 seconds, and at an increasing rate from 4000-5000 seconds as the material oxidizes. Failure occurs at 2100 K, the default maximum ZrO_2 temperature permitted to hold up molten Zr in canisters, as defined by sensitivity coefficient C1131(6) [1]. The lower oxidation rate of FeCrAl delays failure of the FeCrAl canisters in both instances by nearly two hours. They survive beyond depressurization of the reactor vessel at ~7200 seconds, at which point the temperature decreases before increasing again to the melting point of the FeCrAl, 1773 K at ~9800 seconds. Up to this point the temperatures in the "one region" and "two region" cases are identical, since only the region one oxidation correlation is used up to 1763 K. At this point the temperature is constant until the FeCrAl melts entirely, which occurs more quickly for the "two region" case as the higher oxidation rate correlation contributes at this point. In both cases, the molten FeCrAl is held up by the oxide layer for another 200 seconds or so, until the user-defined UDGC-oxide melt temperature (1901 K in this case) is reached, at which point the canister fails. The temperature trends and failure times for the cladding and both canister (CN and CB) components are similar.
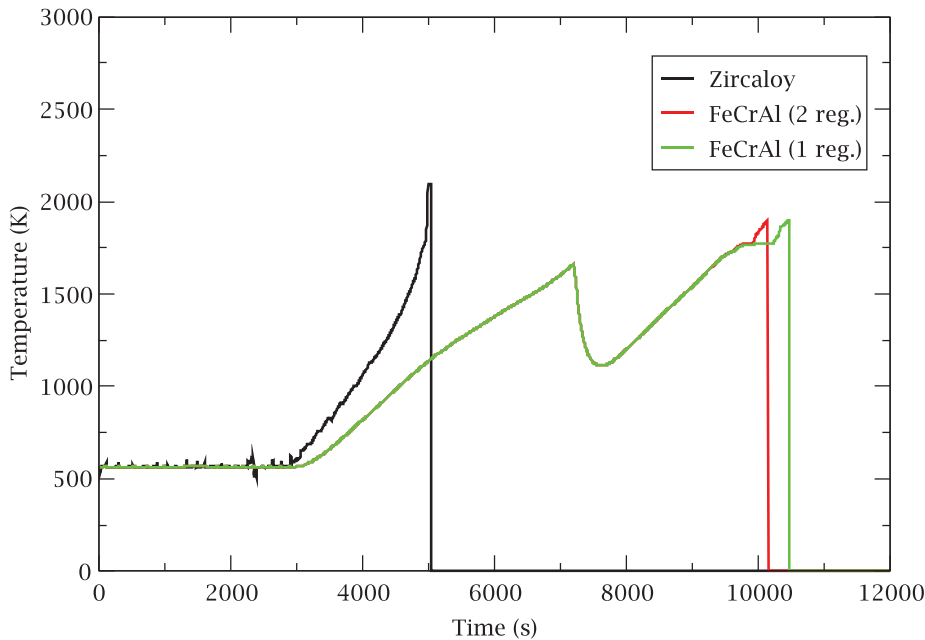

Figure 5. Canister (CB) temperatures in core cell 110.

While the different assumptions regarding FeCrAl oxidation rates do not appear to significantly influence the accident up to the point of FeCrAl melting (and clad/canister failure), they have an enormous influence on the amount of hydrogen subsequently generated, as shown in Figure 6, which shows the amount of hydrogen generated strictly from Zircaloy and FeCrAl. Where the FeCrAl oxidation rate jumps to that of stainless steel (equation (4) at 1773 K, the total hydrogen generation is comparable to the Zircaloy case, though delayed a couple hours in time. If the oxidation rate follows equation (3) at all temperatures, very little hydrogen is generated from the FeCrAl— less than 4 kg, even after core melt and vessel failure. There is still a significant amount of hydrogen generated in this case from the stainless steel components in the core; the total hydrogen generated from all materials, which includes this contribution, is shown for each case in Figure 7.
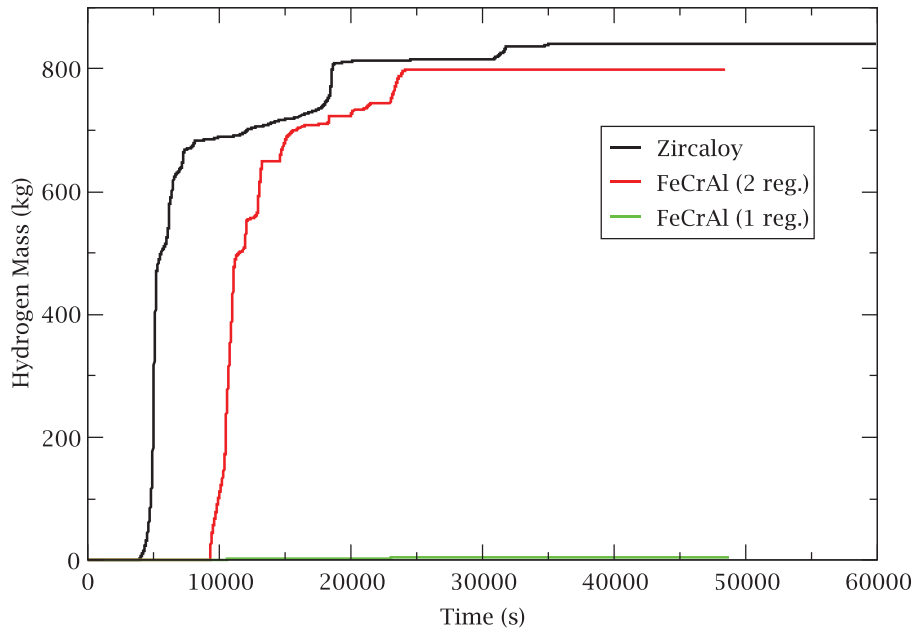
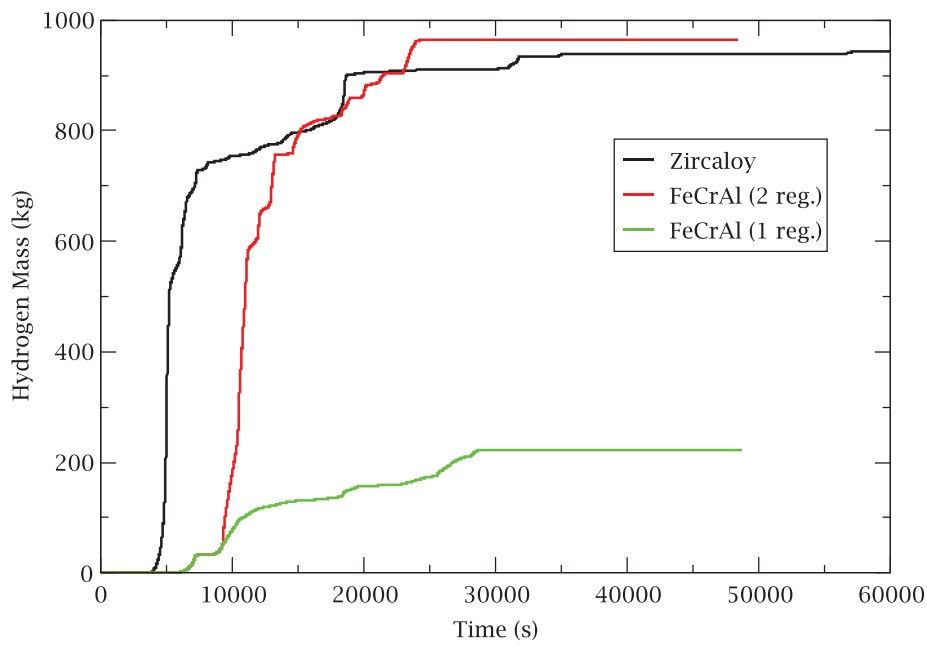Figure 6. Hydrogen generated from Zircaloy and FeCrAl oxidation.

Figure 7. Total hydrogen generated.

However, we need to note that MELCOR 1.8.6 only calculates the hydrogen generated in the core, not including the lower plenum, which means that hydrogen generation will not be calculated after the melting materials fall into the lower plenum. As shown in Figure 3, the falling time of melting materials is delayed in the FeCrAl cases, which means some of the hydrogen production in these cases may simply be due to the melting materials staying in the core longer.

This test case is meant to demonstrate the new functionality that has been added to the MELCOR models, and the potential importance of these generalizations to the resultant model predictions. It is not intended to represent an actual ATF fuel design and corresponding accident progression. Such analyses are the subject of a forthcoming report, in which the UDGC models described herein are applied along with different RCIC operation and drywell head cooling scenarios, to assess the impact that advances in all three areas might have on extending the coping time in a severe BWR accident.

REFERENCES

[1]   R. O. Gauntt et al., "MELCOR Computer Code Reference Manuals, Vol. 1: Primer and Users' Guide" NUREG/CR-6119, Vol. 1, Rev. 3, Version 1.8.6, September (2005).

[2]   R. O. Gauntt et al., "MELCOR Computer Code Reference Manuals, Vol. 2: Reference Manuals" NUREG/CR-6119, Vol. 2, Rev. 3, Version 1.8.6, September (2005).

[3]   P. W. Humrickhouse and B. J. Merrill, "Status Report on Modifications to MELCOR for modeling of Accident Tolerant Fuel (ATF)," INL/EXT-17-43162, August 2017.

[4]   K. R. Robb, J. W. McMurray, and K. A. Terrani, "Severe Accident Analysis of BWR Core Fueled with UO2/FeCrAl with Updated Materials and Melt Properties from Experiments," ORNL/TM-2016/237, June 2016.

[5]   R. Dailey, J. Wang, and M. L. Corradini, "Generic Boiling Water Reactor MELCOR Plant Model," UW-INES-18-100, September 2018.

[6]   C. J. Shaffer, L. A. Miller, and A. C. Payne, Jr., "Integrated Risk Assessment for the LaSalle Unit 2 Nuclear Power Plant, Vol. 3: MELCOR Code Calculations," NUREG/CR-5305, October 1992.