Example of Modeling Methodologies Applied in SOARCA

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Hydrogen Deflagration

- Overview of the MELCOR Deflagration Modeling
  - Shapiro implementation of default limits
- Overview of the SOARCA Deflagration Modeling
  - Ignition source requirement
  - Application of a Kumar inspired methodology
    - Applies a directional component to ignition criteria
    - Temperature correction to combustion H$_2$ limit
Burns in MELCOR involve the following determinations:

- **Ignition Criteria** – Mole fraction criteria permitting a burn to occur
  - Two limits may be defined (burns may also be disallowed in user specifies volumes)
    - Spontaneous deflagrations / Igniter initiated deflagrations
      - Control function (CF) may be used to actuate an igniter
        - Recent SOARCA modeling use the igniter CFs to incorporate all of the ignition criteria

- **Burn Rate** – Moles of gases reacted during a time step (HECTR 1.5)
  - Burn Completeness – Mole fraction of combustible left at end of burn (solved at start of burn)
  - Burn Duration – Duration of a given burn (solved at the start of burn)
    - = Characteristic volume length / Flame Speed (HECTR Correlation)
  - Rate = (X(t) – BurnComplete)/(BurnDuration – TimeSpentBurning)

- **Propagation Criteria** – Mole fraction criteria permitting a burn to transfer to another control volume
  - Propagation directional ignition criteria (4%/6%/9%)
  - Ignition criteria check after Const(def=0.0)*BurnDuration
MELCOR BurnPackage Ignition Criteria

- Shapiro Model – Spontaneous Combustion
  - Constant limits
    - Lower Flammability Limit (LFL)
      - 10% H₂ (+CO adjusted)
    - Upper Flammability Limit (UFL)
      - 5% O₂
    - Inerting Limit
      - 55% CO₂ + H₂O
    - Control volume mole fractions are evaluated against these limits

- Note the use of “Air” implies set N₂/O₂ concentrations
Shapiro Model

- Shapiro Model – Depicted on an XY plot
  - LFL – 10% Hydrogen
  - UFL – 5% Oxygen (for 80/20 N2/O2 – 5% Oxygen corresponds to 25% “Air”)
  - Inerting Limit 55%
Kumar-Inspired Model

- Integrating directionality (up/down/horizontal) with ignition criteria
  - Performed for Uncertainty Analysis sampling in recent SOARCA studies
    - Uniform distribution for the three possible directions
  - Lower flammability limits vary with regard to relevant flame direction
    - Data from Kumar* was employed
      - Tabular functions using the diluent mole fractions to determine lower flammability limits
    - Upward directional flame front requires less hydrogen then downward traveling flame fronts
    - Horizontal is taken as the average between upward and downward propagation
  - Lower flammability limits vary with atmospheric temperature

- Known ignition sources employed
  - Disable spontaneous ignition criteria
  - Adjust igniter ignition criteria to reduced ignition criteria (maintain CO/H$_2$O ratio)
  - Create control function logic which combines ignition criteria and ignition source
    - $H_2 + CO$ limit; $O_2$ limit
    - Hot jet temperature at break site
    - Debris in cavity
Kumar investigated various systems to determine up/downward limits:
- \( \text{H}_2 - \text{N}_2 - \text{O}_2 \)
- \( \text{H}_2 - \text{CO}_2 - \text{O}_2 \)
- \( \text{H}_2 - \text{H}_2\text{O} - \text{O}_2 \)
- \( \text{H}_2 - \text{H}_2\text{O} - \text{Air} \)

Kumar purports \( \text{N}_2 \) may be treated as a diluent in context of paper.
SOARCA Compared to Default MELCOR Model

- Applies the Air data set for upward/downward and computes horizontal limit as the average from the up and downward ignition criteria limits
- Increases overall envelope supporting deflagrations
- Fidelity near inerting limit
Temperature Enhancement

- From Kumar
  - Up/downward augmentation to ignition criteria

\[ \text{LFL}_{\text{dir, aug}} = \text{LFL}_{\text{dir, Kumar}} + C_{\text{dir}} \times \Delta T_{\text{atm, Kumar}} \]

\[ C_{\text{dir}} = -1\%/100\text{C for downward and } -0.5\%/100\text{C for upward} \]

\[ \Delta T_{\text{atm, Kumar}} = \text{Delta between the present atmosphere temperature and the temperature at which the limit was determined} \]

\[ \Delta T_{\text{atm, Kumar}} = (T_{\text{atm}} - 295.15) \]
Fission Product Distribution with UA

- Discuss sources for modeling in SOARCA and SOARCA UA
- Show probability density function for gaseous iodine
- Discuss input generation and deck management used to perform UA
SOARCA Fission Product Classes
Definition

- Modeling methodology draws from the following resources
  - Phebus experiments
    - $\text{Cs}_2\text{MoO}_4$ used across all of SOARCA
    - Gaseous iodine ($I_2$, methyl iodine neglected) only applied in SOARCA UA
      - Prior best-estimate SOARCA studies assume chemical form CsI only for iodine
        NUREG/CR-7155, "SOARCA Project – Uncertainty Analysis of the Unmitigated LTSBO of the Peach Bottom Atomic Power Station, Draft Report"
  - VERCORS, ORNL VI&HI, Phebus, and the CORSOR/ORNL-Booth release models
    - Modification of the Booth-ORNL model parameters
      NUREG/CR-7008, "MELCOR Best Practices as Applied in the SOARCA Project"
      Modification of CORSOR/Booth Parameters in MELCOR
  - NUREG-1465
    - Assumed gap fractions
Modeling Fission Products

- Pre-defined mass for all classes
  - No application of the class combination model
    - Prescriptive containment concentrations are being directly specified within the fuel
  - User must combines decay heat tables appropriately
  - Specify radioactive mass for Cs (CsOH), CsI, Mo, Cs$_2$MoO$_4$

- SOARCA practice
  - Class 2 – 5% of available Cs (all placed into the fuel gap)
  - Class 4 – 0%
  - Class 16 – All Iodine combined (5% placed into the fuel gap)
  - Class 17 – Remaining Cs combined to form Cs$_2$MoO$_4$
    - Specifying radioactive mass in the fuel
  - Class 7 – Mo decremented by formation of Cs$_2$MoO$_4$
SOARCA UA Fission Product Class Definition

- Pre-defined approximate compositions definition
  - Phebus test results provided evidence of the chemical form Cs₂MoO₄ and persistence of gaseous iodine which are used in the SOARCA UA
  - Combination n for iodine speciation
    - Average peak percentage of iodine observed as gaseous FTP0-3
    - 5th average over experiment

Figure 4.1-20 - PDF
SOARCA UA Total Decay Heat

- **Sampled – Time at Cycle**
  - Baseline decay heat power curves for scenario initiating at different times
  - Time of shutdown correspond to 7, 200, and 505 days for BOC, MOC, and EOC, respectively
Deck Organization Generation

**Input Files**

- MAIN.INP
- EXEC_INPUT
- CVH_INPUT
- COR_INPUT
- DCH_INPUT
- RN1_INPUT
- FL_INPUT

**Base Model Definition**

- UA Set (folder)
- RlzN.INP
  - Program MELCOR
  - Include /deck/Main.inp
    - CVH_INPUT
      - CVH_SC 3
        - 1
    - COR_INPUT
      - COR_SC 1
        - 1 1020 <rep-Cor-X1> 1
        - 2 1020 <rep-Cor-X2> 2
    - DCH_INPUT
      - Include /deck/DCH-RN/<REP-FileName> DCH_BLOCK
      - RN1_INPUT
        - Include /deck/DCH-RN/<Rep-FileName> RN1_Block

- DCH-RN (folder)
- (unique files generated)
  - DCH-RN-RlzN.INP

- CVH_INPUT
  - Include /deck/Containment.inp CVH_BLOCK
  - Include /deck/RCS-Loop-Z.inp CVH_Block
  - Include /deck/SG-Z.inp CVH_BLOCK
  - FL_INPUT
DCH-RN File Set

- Specifies total decay heat
- Class specific decay heat
- Class radioactive mass

```plaintext
DCH_EL 'I2' 100.0 10  ! Sampled value for mass
1 0.0e0 10.E5  ! Time of Cycle
2 2.0e0 9.5E5
3 ..
```
Conclusions

- Discussed the following:
  - Implementation of a Kumar-inspired deflagration model
    - Overview of the default Burn Package treatment
    - Modification of the LFL using Kumar’s data
  - Iodine class speciation
    - General SOARCA distribution of classes
    - SOARCA UA inclusion of Phebus results
  - Decay heat for different time of cycle
    - BOC, EOC, MOC
  - Possible deck configuration for UAs