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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 H₂ limit



MELCOR BurnPackage Methodology Sandia National Laboratories

- 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 specified 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 = $(X(t) - \text{BurnComplete}) / (\text{BurnDuration} - \text{TimeSpentBurning})$
 - **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 $\text{Const}(\text{def}=0.0) * \text{BurnDuration}$

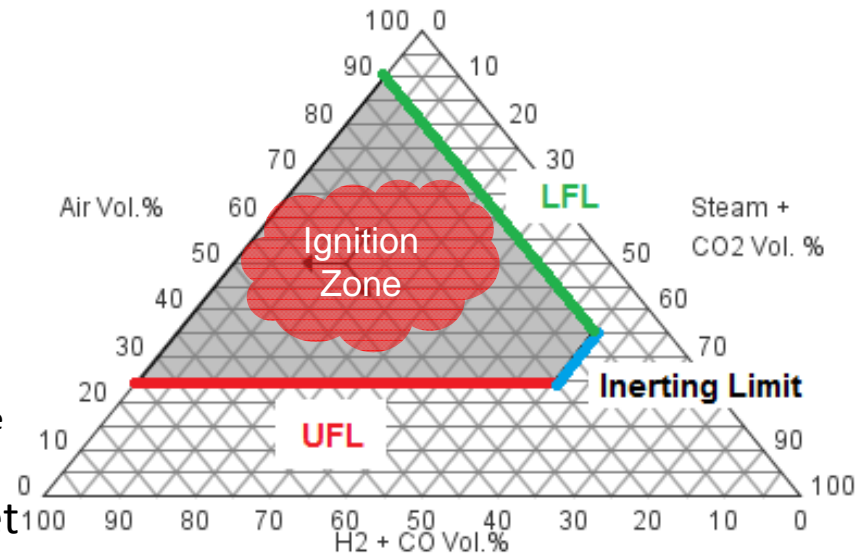
MELCOR BurnPackage Ignition Criteria

- Shapiro Model – Spontaneous Combustion

- Constant limits

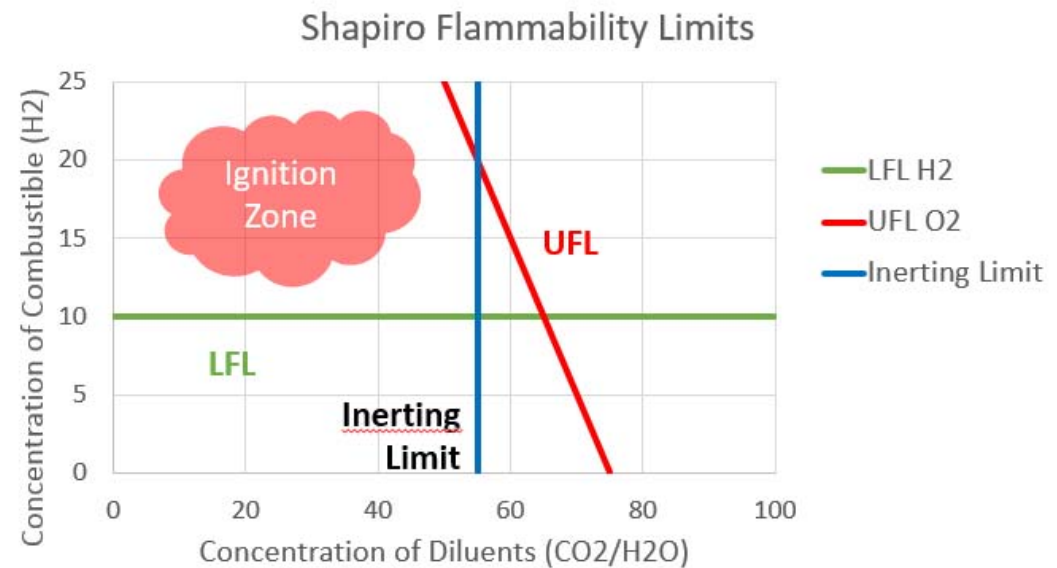
- Lower Flammability Limit (LFL)
 - 10% H₂ (+CO adjusted)
 - Upper Flammability Limit (UFL)
 - 5% O₂
 - Inerting Limit
 - 55% CO₂ + H₂O
 - Control volume mole fractions are evaluated against these limits

- 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%

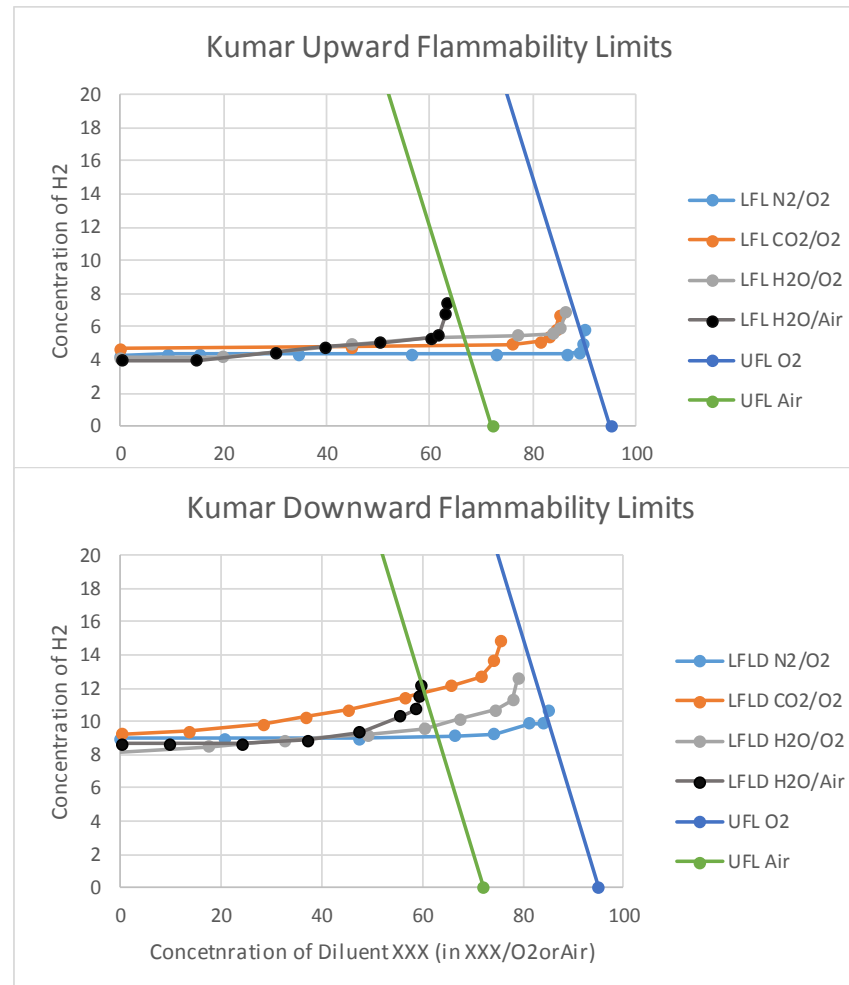


Kumar-Inspired Model

- 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 than 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/H₂O ratio)
 - Create control function logic which combines ignition criteria and ignition source
 - H₂ + CO limit; O₂ limit
 - Hot jet temperature at break site
 - Debris in cavity

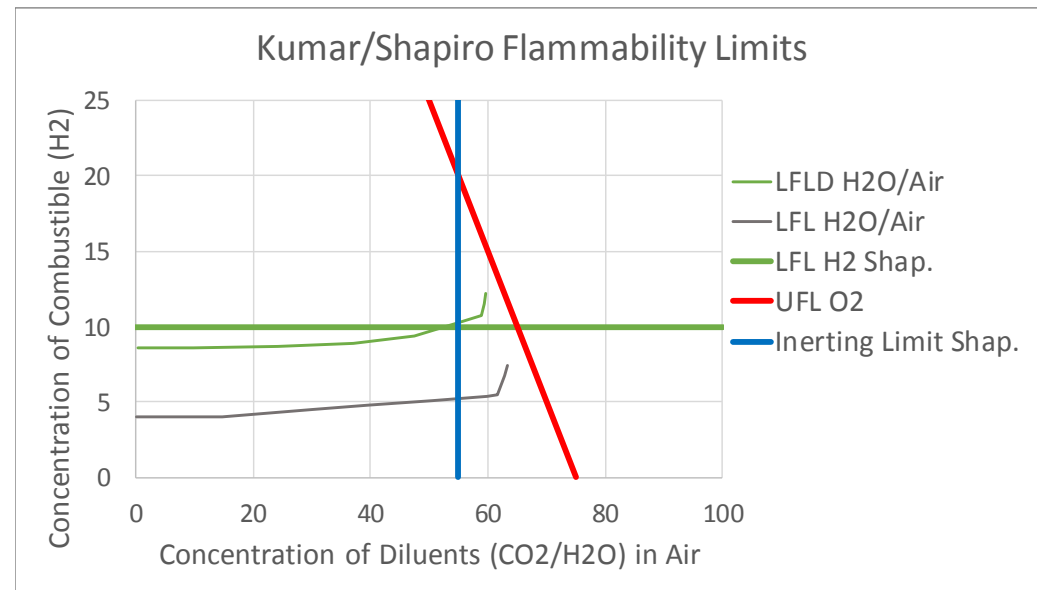
Imposing Data

- Kumar investigated various systems to determine up/downward limits
 - $H_2 - N_2 - O_2$
 - $H_2 - CO_2 - O_2$
 - $H_2 - H_2O - O_2$
 - $H_2 - H_2O - Air$
- Kumar purports 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

$$LFL_{dir, aug} = LFL_{dir, Kumar} + C_{dir} * \Delta T_{atm, Kumar}$$

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

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

$$\Delta T_{atm, Kumar} = (T_{atm} - 295.15)$$

Fission Product Distribution with UA Sandia National Laboratories

- 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
 - Cs_2MoO_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 combine decay heat tables appropriately
 - Specify radioactive mass for Cs (CsOH), CsI, Mo, Cs₂MoO₄
- 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 Cs₂MoO₄
 - Specifying radioactive mass in the fuel
 - Class 7 – Mo decremented by formation of Cs₂MoO₄

SOARCA UA Fission Product Class Definition

- Pre-defined approximate compositions definition
 - Phebus test results provided evidence of the chemical form Cs_2MoO_4 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

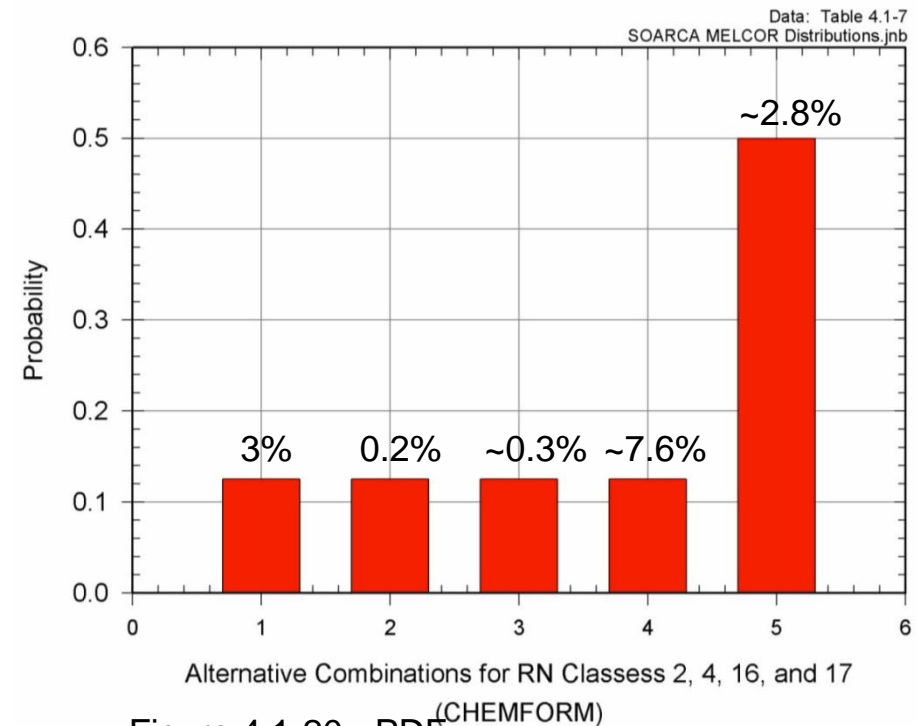
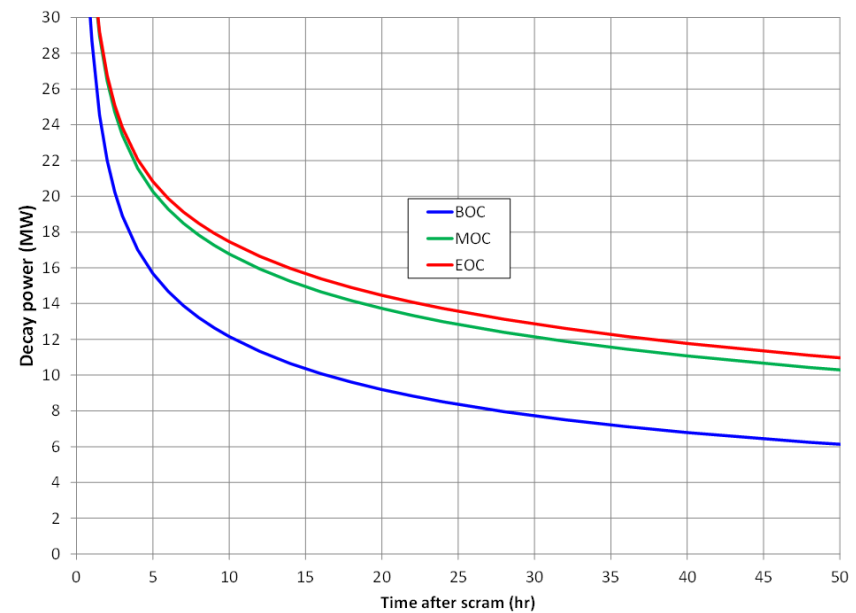


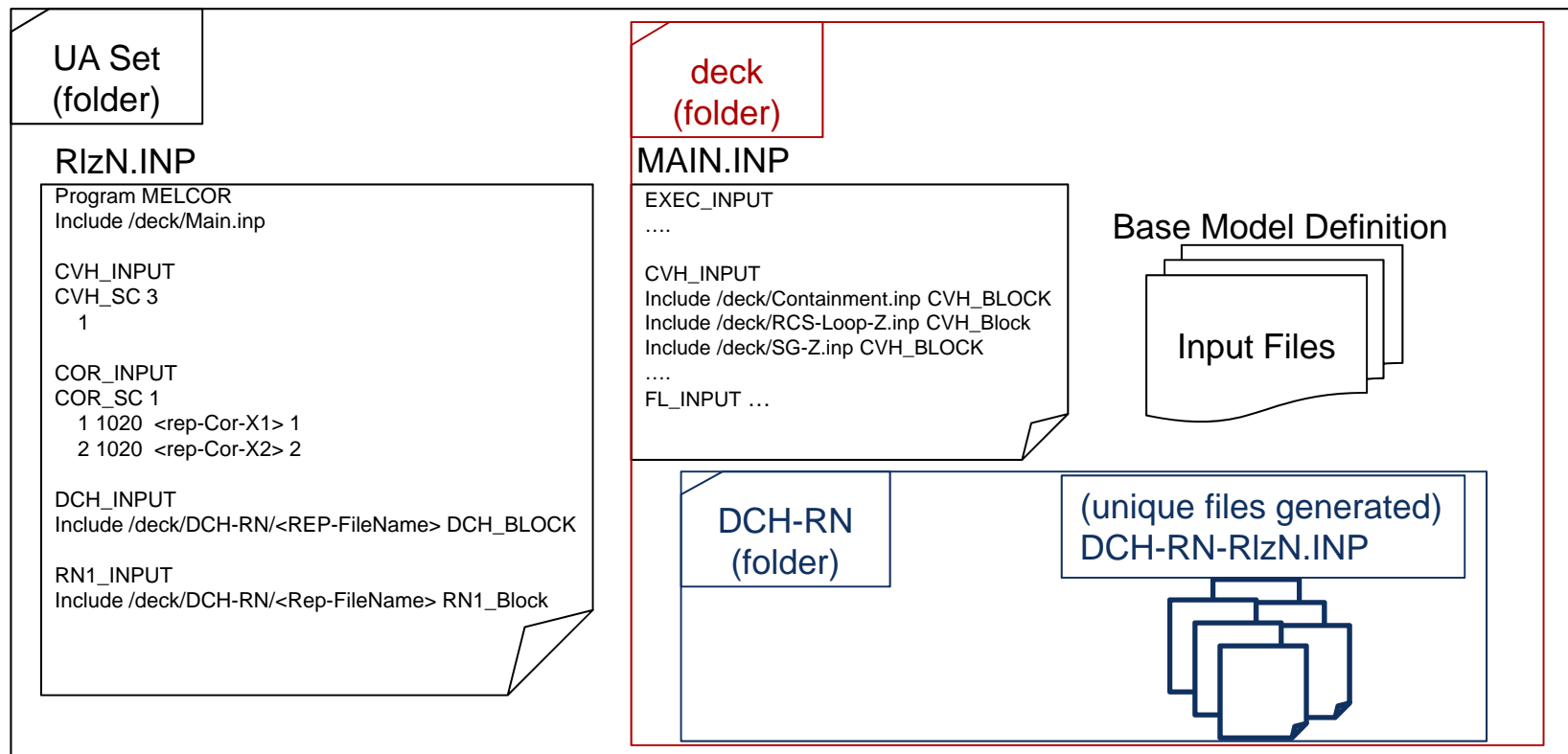
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SOARCA UA Total Decay Heat

- 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



DCH-RN File Set

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

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

