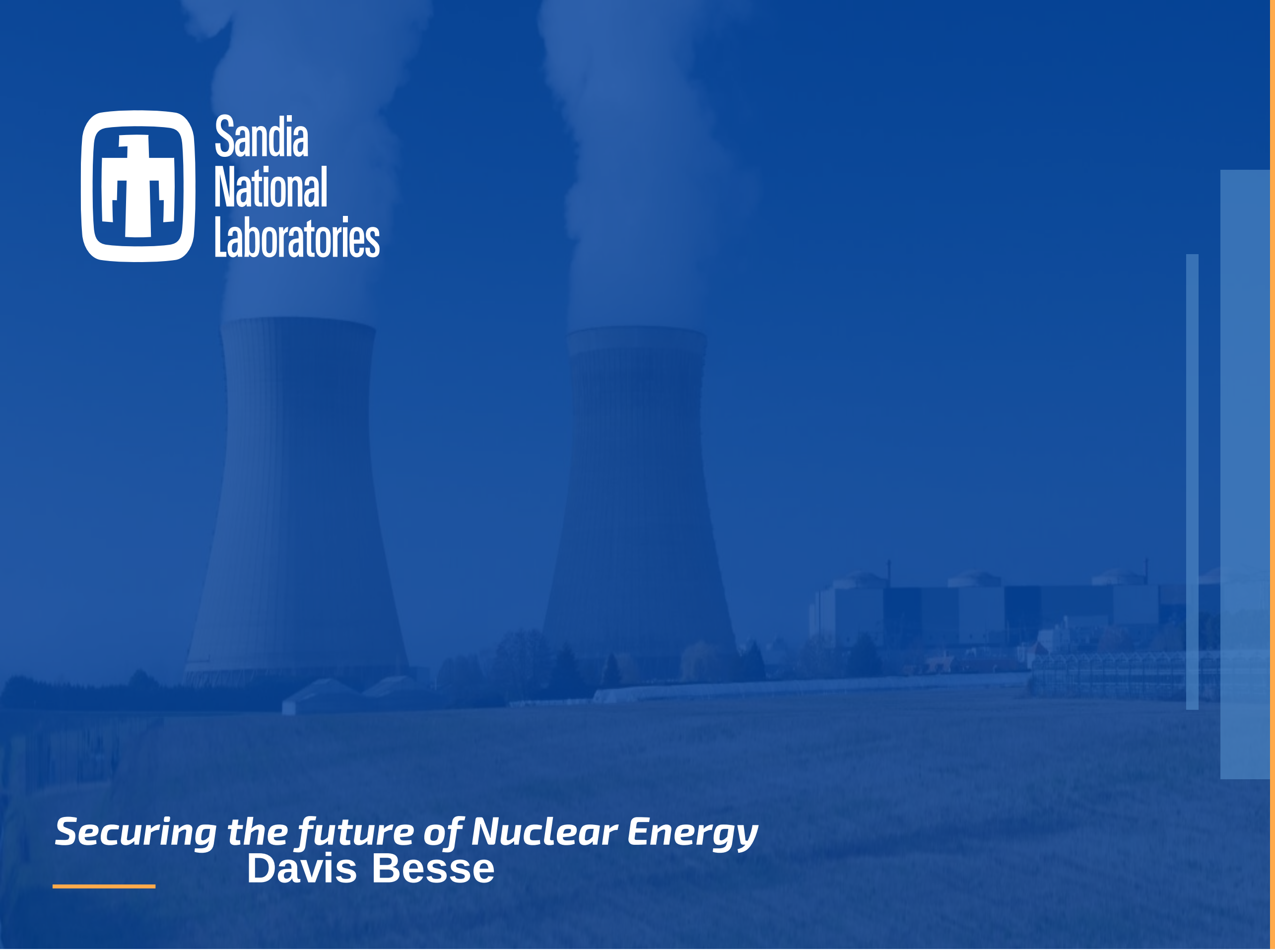


Sandia National Laboratories

*Securing the future of Nuclear Energy*

**Davis Besse**

# MELCOR Containment Models

2024 European MELCOR Users' Group Meeting

April 15th-18th, 2024

SAND2024-04300PE

# MELCOR Containment Models
## Overview of Presentation

- Present several containment-related models that have general applicability
  - Gas combustion models in the BUR package
  - Passive Autocatalytic Recombiner model, PAR
    - Part of Engineered Safety Features (ESF) Package
  - Fan cooler model, FCL (also part of ESF)
  - Spray models in the SPR package
    - Thermodynamics only at this point
  - Filter models
  - Sodium Fire Models
  - Other built-in models
    - Isolation condenser model
    - Condenser model
- Show simple example input
  - More flexibility is available, as described in code manuals
- Recent examples
  - MSRE
  - Reprocessing facility

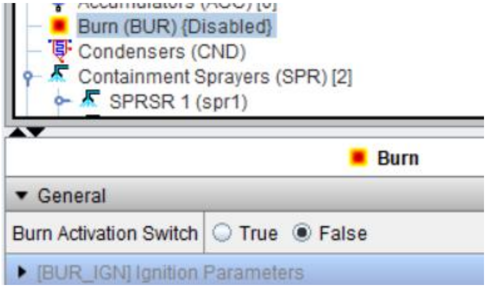
# MELCOR Gas Combustion Models Description

- Calculates burning of $H_2$ and CO
  - Does not treat burning of structures
  - Uses LeChatelier's formula for mixtures
  - Deflagration only, but can warn of possible detonation
- Models based on HECTR
  - Parametric representation (*not* detailed kinetics)
  - Criteria for ignition and inerting based on mole fractions
    - Different criteria with igniters on and off
  - Correlations for combustion velocity and completeness
    - Assumes duration is characteristic_dimension/velocity
    - Constant rate over duration of burn (with checks)
  - Criteria for propagation between connected volumes
    - Different for upward, horizontal, or downward

**BUR_INPUT 0**

| | |
|---|---|
| **0 or ACTIVE** | **BUR package is active.** |
| **1 or NOTACTIVE** | **BUR package is not active,** |

**(type = integer, default = 0, units = none)**



Burn (BUR) {Disabled}
Condensers (CND)
Containment Sprayers (SPR) [2]
SPRSR 1 (spr1)

Burn

General

Burn Activation Switch ○ True ● False

[BUR_IGN] Ignition Parameters

# Why We Care

- PWR Large Dry and Subatmospheric
  - Very low
- PWR Ice Condenser
  - High without mitigation
- BWR Mark I and Mark II
  - Inerted
  - Surrounding reactor building not inerted
- BWR Mark III
  - High without mitigation

**Fukushima Unit 1**

# MELCOR H2 Model Ignition

**Test for Sufficient Fuel – Uses LeChatelier's formula for mixture**

$$X_{H2} + X_{CO}\left(L_{H2,ign}/L_{CO,ign}\right) \geq L_{H2,ign}$$

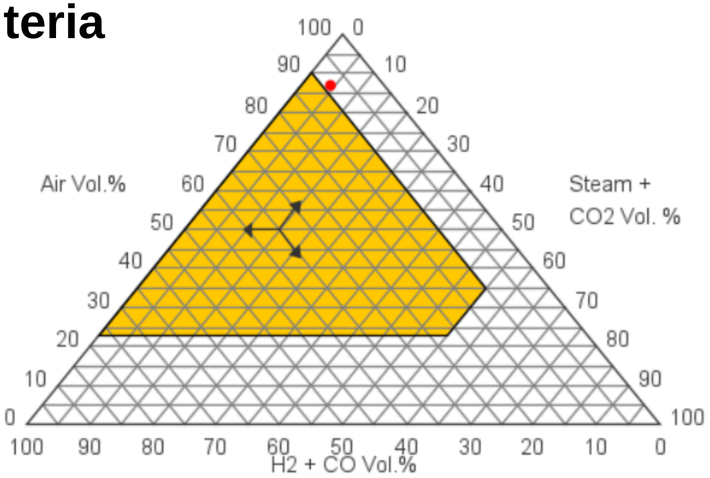
$$\frac{X_{H2}}{L_{H2,ign}} + \frac{X_{CO}}{L_{CO,ign}} \geq 1$$

**Ignition Criteria**

**Additional tests for sufficient oxygen and below inerting limits**

$$X_{O2} \geq \mathrm{XO2IG}$$

$$X_{H2O} + X_{CO2} < XMSCIG$$



**Combustion Ternary Plot**

## MELCOR Default Ignition and Propagation Limits

| Limits | Minimum H2<br>$L_{H2,ign}$ | Minimum CO<br>$L_{CO,ign}$ | Minimum O2<br>XO2IG | Maximum Diluent<br>XMSCIG |
|---|---|---|---|---|
| Ignition (Igniters) | 0.07 | 0.129 | ≥ 0.05 | < 0.55 |
| Ignition (no igniters) | 0.1 | 0.167 | ≥ 0.05 | < 0.55 |

# MELCOR H2 Model Propagation

$$\frac{X_{H2}}{L_{H2,prp}} + \frac{X_{CO}}{L_{CO,prp}} \geq 1$$

**Propagation Criteria**

**Use LeChatelier’s formula for mixture**

$$X_{SC} = X_{H2O} + X_{CO2} \quad \text{Diluent}$$

1. **Propagation occurs if the propagation criteria are satisfied in the connected control volume.**
2. **Propagation occurs through defined flow paths.**
3. **If a flow path is not open, or if the flow path is covered by water, propagation is not allowed.**
    - **Uses flow path elevations & water levels**

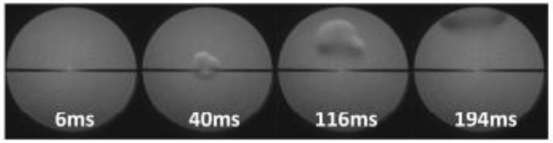
## MELCOR Propagation Limits

| **Limits** | Minimum $H_2$<br>$L_{H2,prp}$ | CO Limit<br>$L_{CO,prp}$ | Minimum $O_2$ | Maximum Diluent |
|---|---|---|---|---|
| **Upward Propagation** | **0.041** | **.125** | **≥ 0.05** | **< 0.55** |
| **Horizontal Propagation** | **0.06** | **.138** | **≥ 0.05** | **< 0.55** |
| **Downward Propagation** | **0.09** | **.15** | **≥ 0.05** | **< 0.55** |

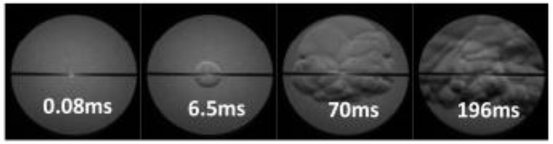
**A unique aspect of hydrogen is that the lean flammability limit is significantly different for upward, downward and sideways propagating flames. This is a buoyancy effect due to the low density of hydrogen relative to air.**

# Combustion Limits Tests

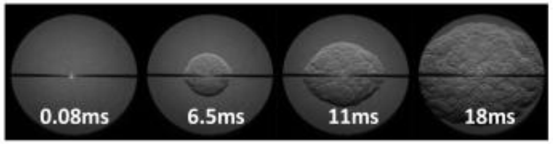
| | Lower Limit | Minimum O2 | Maximum Diluent |
|---|---|---|---|
| **Upward Propagation** | **0.041** | **≥ 0.05** | **< 0.55** |
| **Horizontal Propagation** | **0.06** | **≥ 0.05** | **< 0.55** |
| **Downward Propagation** | **0.09** | **≥ 0.05** | **< 0.55** |



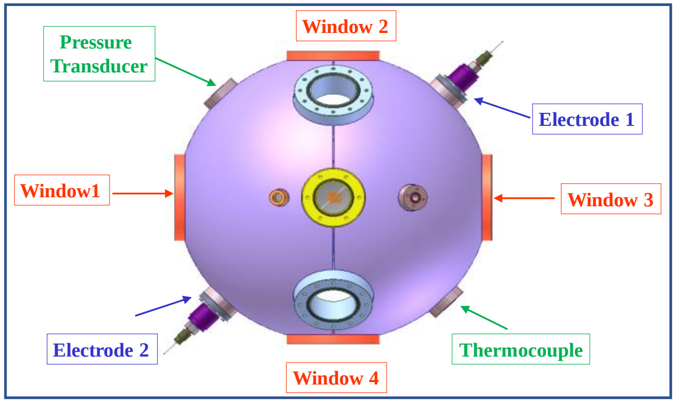
(a): 5.12%$H_2$+94.88%$O_2$-1bar-296K

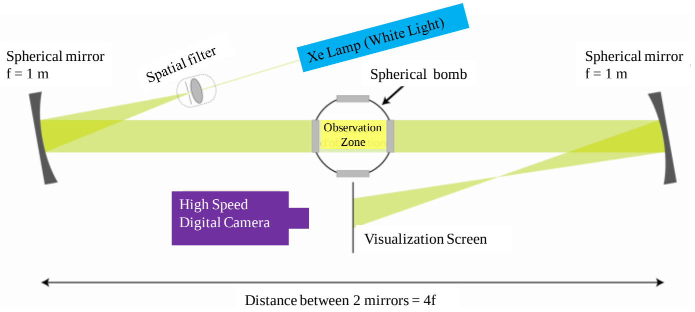


(b): 8.75%$H_2$+91.25%$O_2$-1bar-296K



(c): 12.75%$H_2$+87.25%$O_2$-1bar-296K





**K. N'Guessan, M. Idir, J. Pavageau, T. Cuvillier, N. Chaumeix. Evaluation of flammability limits of H_2/O_2/N_2 mixtures in conditions relevant to nuclear waste transportation. PATRAM 2016 - 18th International Symposium on the Packaging and Transportation of Radioactive Materials, Sep 2016, Kobe, Japan. ffcea-02438376f**

# MELCOR Gas Combustion Models
# Example Input

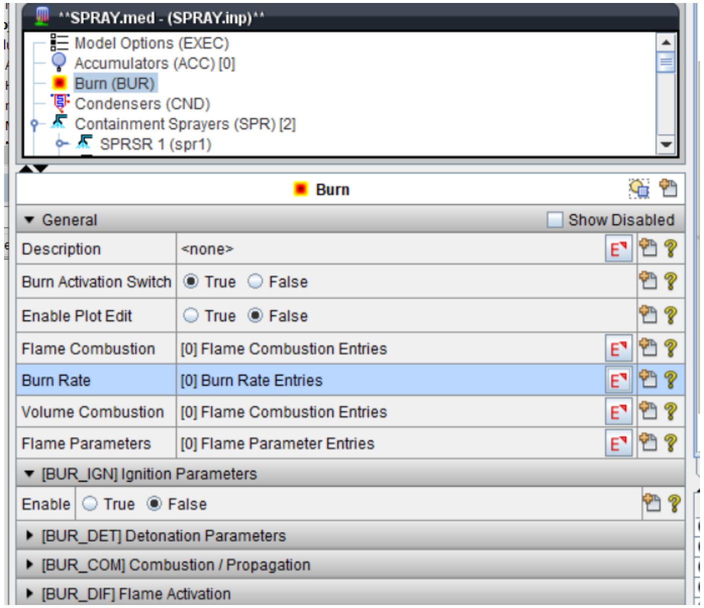
**Commonly-used optional input**

**Define igniters or prohibit burning in a volume**

- ASCII Input

```
BUR_BRT N
1 “CVnam” IGNITR  (CFNAME)  CDIM*  TFRAC*  CDDH  TFDH

BUR_PLT – Plot Edit Control

BUR_TIM – Burn Timestep Information
```

- SNAP Input



**SPRAY.med - (SPRAY.inp)**

- Model Options (EXEC)
- Accumulators (ACC) [0]
- Burn (BUR)
- Condensers (CND)
- Containment Sprayers (SPR) [2]
  - SPRSR 1 (spr1)

**Burn**

General ☐ Show Disabled

| | |
|---|---|
| Description | <none> |
| Burn Activation Switch | ● True ○ False |
| Enable Plot Edit | ○ True ● False |
| Flame Combustion | [0] Flame Combustion Entries |
| Burn Rate | [0] Burn Rate Entries |
| Volume Combustion | [0] Flame Combustion Entries |
| Flame Parameters | [0] Flame Parameter Entries |

[BUR_IGN] Ignition Parameters

| | |
|---|---|
| Enable | ○ True ● False |

[BUR_DET] Detonation Parameters

[BUR_COM] Combustion / Propagation

[BUR_DIF] Flame Activation

### TFRAC

**Time fraction of burn before propagation is allowed. It must satisfy 0.0 ≤ TFRAC ≤1. (default = 0.0)**

**The propagation delay is calculated to be**

$$t_{prp} = FRAC \cdot t_{comb}$$

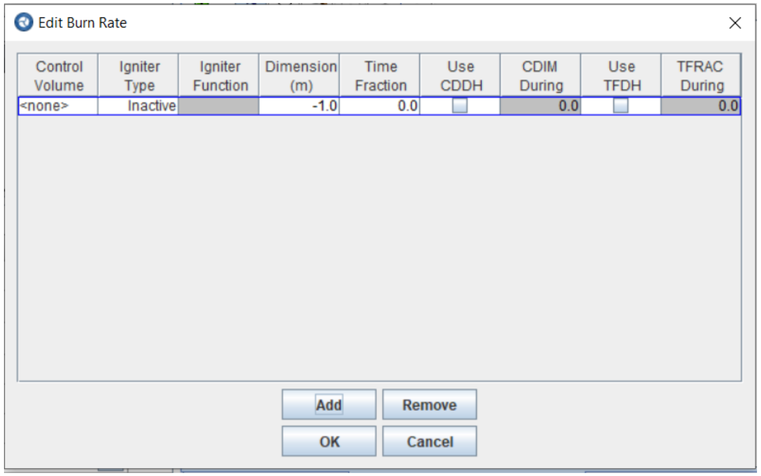
**where**

**FRAC = TFRAC, if DCH is not occurring in the control volume, or**
**= TFDH, if DCH is occurring in the control volume;**

**TFRAC = propagation time fraction input on record BUR_BRT (default = 0)**

**TFDH = override value of TFRAC during DCH, input on record BUR_BRT (default = TFRAC).**

*Note that if TFRAC equals zero, propagation is possible as soon as a CV begins burning. If TFRAC equals 1.0, propagation is only considered at the end of the CV burn.*



Edit Burn Rate

| Control Volume | Igniter Type | Igniter Function | Dimension (m) | Time Fraction | Use CDDH | CDIM During | Use TFDH | TFRAC During |
|---|---|---|---|---|---|---|---|---|
| <none> | Inactive | | -1.0 | 0.0 | ☐ | 0.0 | ☐ | 0.0 |

# MELCOR Gas Combustion Models
# Other Optional Input - Primarily for specialists

## ASCII Input

**Ignition limits**

BUR_IGN/01

**Detonation warning parameters**

BUR_DET

**Completeness and propagation parameters**

BUR_COM

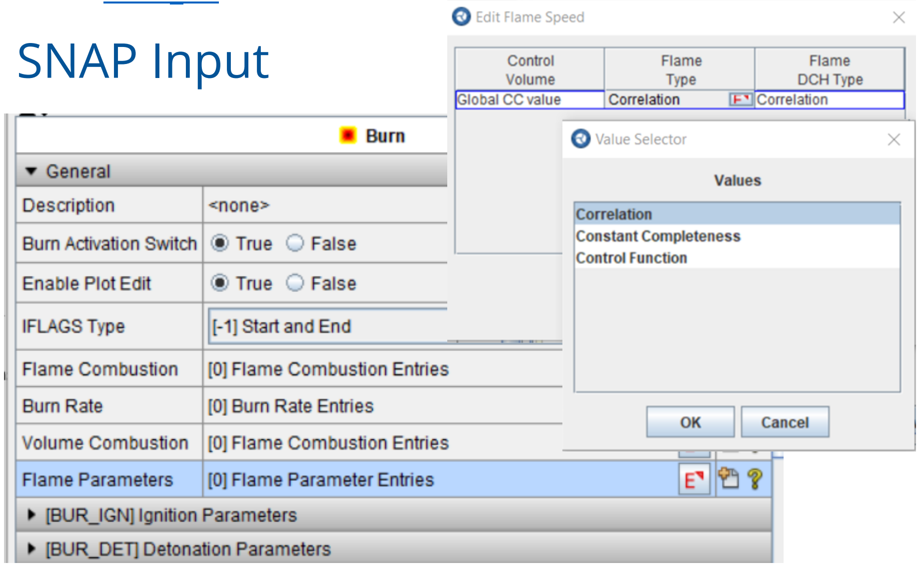
**Modify combustion completeness, by volume**

BUR_CC

**Modify flame speed, by volume**

BUR_FS*

- SNAP Input



**Burn**

▼ General

| | |
|---|---|
| Description | <none> |
| Burn Activation Switch | ● True ○ False |
| Enable Plot Edit | ● True ○ False |
| IFLAGS Type | [-1] Start and End |
| Flame Combustion | [0] Flame Combustion Entries |
| Burn Rate | [0] Burn Rate Entries |
| Volume Combustion | [0] Flame Combustion Entries |
| Flame Parameters | [0] Flame Parameter Entries |

▸ [BUR_IGN] Ignition Parameters

▸ [BUR_DET] Detonation Parameters

Edit Flame Speed

| Control Volume | Flame Type | Flame DCH Type |
|---|---|---|
| Global CC value | Correlation | Correlation |

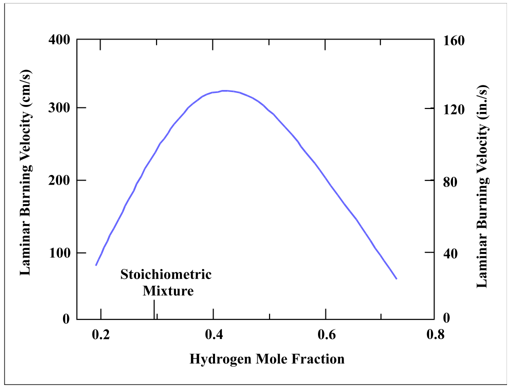
Value Selector

Values

- Correlation
- Constant Completeness
- Control Function

**Options for specifying how the flame speed is determined.**

1. **Calculate flame speed from control function.**
2. **Use correlation (sensitivity coefficient C2200).**
3. **Use constant value for flame speed.**



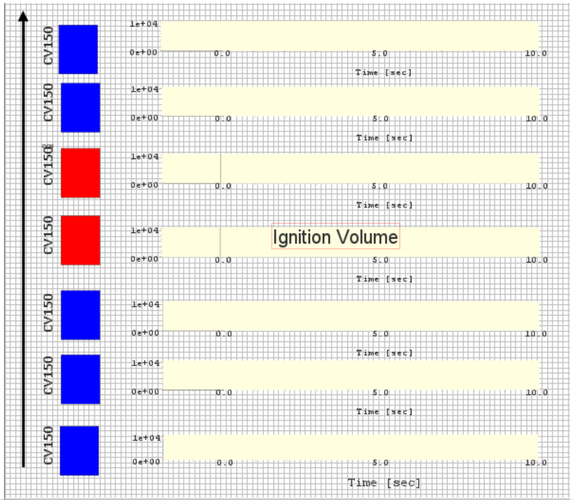
# SNAPlette: Burn Propagation

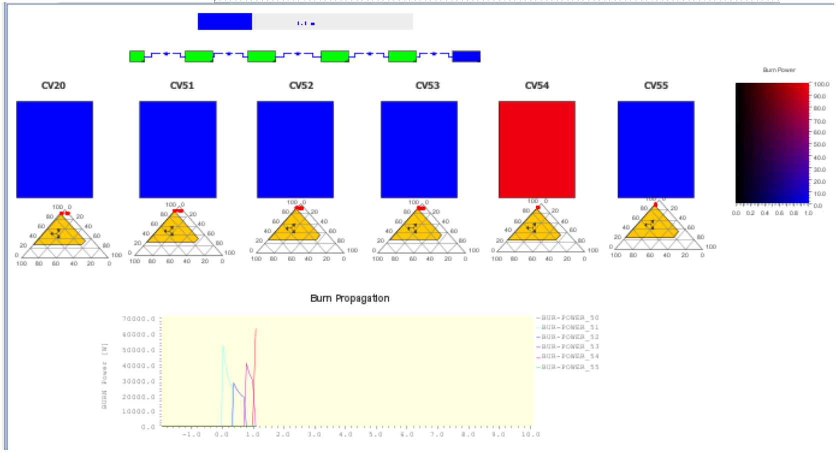
Model contains 2 independent BUR propagation calcs

1. First calc demonstrates horizontal burn propagation down a narrow pipe.
   - Represented by 6 identical volume CVs
   - Ignition only in left-most volume (CV50)
   - Propagation occurs only at end of CV burn
2. Second calculation demonstrates vertical burn propagation in a narrow pipe
   - Represented by 7 identical, vertically stacked volumes
   - Ignition only in the middle CV.
   - Propagation begins immediately on burning in adjacent cell
   - Both upwards & downward propagation are represented.

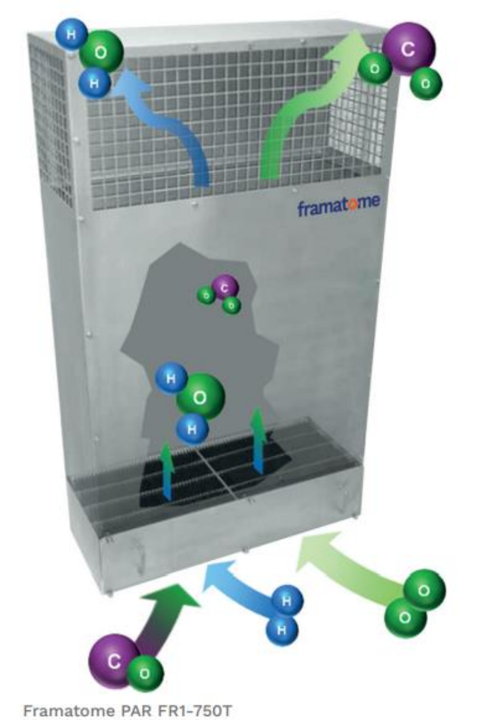
- Horizontal Burn
  - Things to Do
    - Note the movement of the deflagration down the pipe.
      - Can you see that propagation does not begin in a cell until it is complete in the burning adjacent cell.
      - How does changing TFRAC affect the power histories.
      - Examine the deflagration bean to be sure you understand how to create it.
    - Note the intensity of the burn (burn power) is greatest in the left-most and then the right-most CV. Is this what you would expect.
    - Note the control functions that activate when a burn is detected and stay active for 2 seconds. These CFs are used to reduce the time step and and send data to the plot file..
      - Change the time step and/or duration for the reduced time.
- Vertical Burn
  - Things to do
    - Note that the flame propagates upwards but not down
      - What parameters might you change to promote downward propagation?
    - Note that the H2 molar fraction in the upward cells drop significantly after the burns. There is smaller reduction inH2 molar fraction in lower cells.
    - Add a deflagration bean for CV150

- Input File
  - BUR_Prop.med
  - BUR_Prop_anim.med
- Job Stream/Data Source
  - Burn_Prop





# Passive Autocatalytic Recombiners (PARS)



Framatome PAR FR1-750T

- Removes hydrogen from containments through catalytic reactions
- Catalyst
  - Plates or pellets coated with platinum or palladium
  - Some potential for catalyst surface to be poisoned by aerosols, CO, fission products
- Passive
  - Reaction is spontaneous when hydrogen concentration reaches 1-2 percent.
    - Below flammability limits of 4 percent.
    - Relaxation time
      - Heat-up of surface by exothermic reaction
    - Startup delay time
      - May be delayed due to surface contamination (soot, CO, liquid film, etc.)
  - Flow of gas is sustained by reaction
    - Reaction energy heats gas creating chimney effect
    - Flow rates determined by PAR design (e.g. surface to volume ratios, etc.)
- Positioning of recombiners is important
  - To remove sufficient hydrogen from a large containment, multiple units are required
    - Olkiluoto 3 EPR requires 50 recombiners

# MELCOR Hydrogen Recombiner Model Description

- PAR is a sub-package in ESF Package
  - Simple parametric model of a passive autocatalytic recombiner for hydrogen removal
  - Calculates gas flow through recombiner
    - Flow rate from Fischer model
      - Coefficients can be changed through input
    - Option to define flow rate using a control function
      - Allows ultimate flexibility
  - Calculates catalytic recombination of $H_2$ and $O_2$
    - Efficiency constant or from control function
    - Startup and shutdown based on mole fractions
      - User-specified limits for $H_2$ and $O_2$
    - Associated heat generation delivered to atmosphere
  - Allow multiple units, different types

# MELCOR Hydrogen Recombiner Model Description (2)

**Fischer equations for a single step function in hydrogen concentration:**

$$R_H = \eta \ \rho_H Q \ f(t)$$

$$f(t) = \left[ 1 - e^{-\left[\frac{t-t_0}{\tau}\right]} \right]$$

$R_H$ = hydrogen reaction rate (kg/sec)
$\rho_h$ = hydrogen density of entering gas (kg/m3)
$\eta$ = hydrogen reaction efficiency (~0.85)
$Q$ = total gas-phase volumetric flow rate through the unit (m3/sec)
$\tau$ = characteristic heat-up time (~1800 sec)
$t_0$ = time of PAR initiation (s)
$t$ = time after PAR initiation (s)
$f(t)$ = relaxation time function during initial PAR heat-up

**The flow rate can be supplied by the user through a CF or it can be calculated:**

$$Q = a\, C_H^b$$

$C_H$ = hydrogen concentration (mole fraction)
$a$ = constant that depends on PAR unit design parameters (~0.67 kg/sec)
$b$ = exponent that depends on PAR unit design parameters (~0.307)

**Transient effects from multiple step changes in hydrogen concentration:**

$$Q_{new} = Q_{ss} \left[ 1 - e^{-\Delta t / \tau} \right] + Q_{old} e^{-\Delta t / \tau}$$

**Gas temperature change is calculated:**

$$\sum_{i=1}^{N} w_{i,in} h_{i,in} = \sum_{i=1}^{N} w_{i,out} h_{i,out}$$

**Reaction rates of species:**

$$\frac{dm(H_2)}{dt} = -R_H, \text{kg/s}$$

$$\frac{dm(H_2O)}{dt} = -\frac{M_{O_2}}{2M_{H_2}} * R_H, \ \text{kg/s}$$

$$\frac{dm(O_2)}{dt} = -\frac{M_{O_2}}{2M_{H_2}} * R_H, \text{kg/s}$$

$$\frac{dH}{dt} = \sum_{i=1}^{N} w_{i,in} h_{i,in} - \sum_{i=1}^{N} w_{i,out} h_{i,out}, \text{kg/s}$$

# MELCOR Hydrogen Recombiner Model Example Input

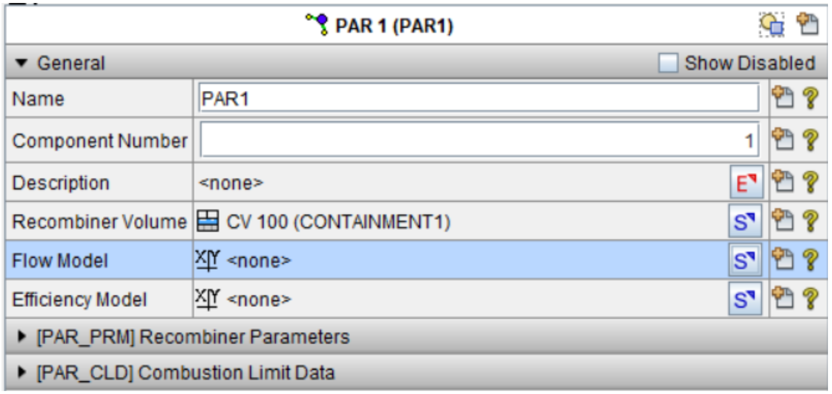
## ASCI Input

```
PAR identifies input for this model
PAR_ID    PAR1

PAR interface and control data (required)
PAR_ICI   IPAR    IPROPT* (CFNFLO) IETAPR (CFNEFF)

PAR Fischer model parameters (optional)
PAR_PRM   APAR   BPAR   EPAR   TAUPAR   TPARD   FPARD

PAR combustion limit data (optional
PAR_CLD   HPAR0*     HPARR     OPAR0     OPARR
```

**HPAR0**
**Minimum $H_2$ mole fraction for PAR startup (default = 0.02)**

**Note: Care must be exercised to ensure that the shutoff concentrations are always less than the startup concentrations. Also, the values here are for illustration only and are not based on any technical study.**

## SNAP Input



PAR 1 (PAR1)

General ☐ Show Disabled

| | |
|---|---|
| Name | PAR1 |
| Component Number | 1 |
| Description | <none> |
| Recombiner Volume | CV 100 (CONTAINMENT1) |
| Flow Model | <none> |
| Efficiency Model | <none> |

[PAR_PRM] Recombiner Parameters

[PAR_CLD] Combustion Limit Data

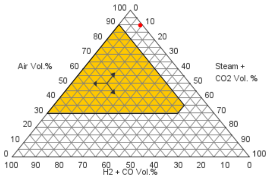
# SNAPlette: PAR Modeling

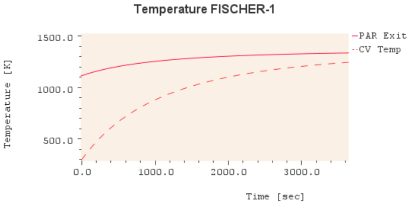
Model contains 8 independent and identical control volumes each with a unique PAR representation

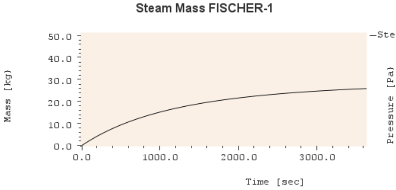
| CV | PAR Model | Delay (sec) | Relaxation Time (sec) | $H_2$ shutoff (mole %) |
|---|---|---|---|---|
| CV_FISCHER_1 | FISCHER-1 | 0.0 | 0.0 | 0 |
| CV_FISCHER_2 | FISCHER-2 | 0.0 | 180 | 0 |
| CV_FISCHER_3 | FISCHER-3 | 0.0 | 1800 | 0 |
| CV_FISCHER_11 | FISCHER-11 | 120. | 0 | 0 |
| CV_FISCHER_12 | FISCHER-12 | 120 | 180 | 0 |
| CV_FISCHER_13 | FISCHER-13 | 120 | 1800 | 0 |
| CV_FISCHER_21 | FISCHER-21 | 0 | 0 | 3 |
| CV_AREVA | AREVA | 0 | 0 | 0 |

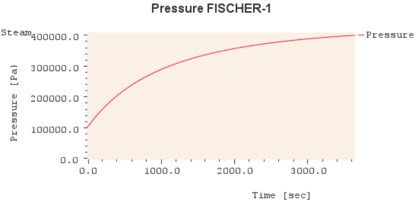
- Things to observe
  - Hydrogen concentration is reduced below flammable limits
  - Hydrogen mass loss is faster for lower heat-up time
  - Time delay results in slight lag in response
  - Steam concentration increases
  - PAR immediately stops when H2 < 3%
- Things to do
  - Demonstrate that steam is being produced
  - Show that a PAR operates below flammability limits
  - Show temperature exiting PAR & temperature of CV
  - Show pressure response
  - Examine the Alt Model and the AREVA model is implemented for CV_AREVA
    - Note that the ideal reaction rate (100% efficiency) is used for the flow model and the efficiency is then applied after

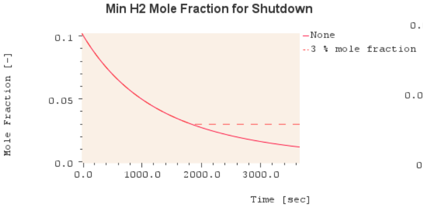
- Input File
  - PAR.med
  - PAR_anim.med
- Job Stream/Data Source
  - PARS

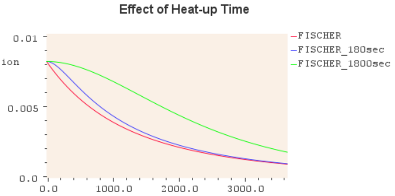


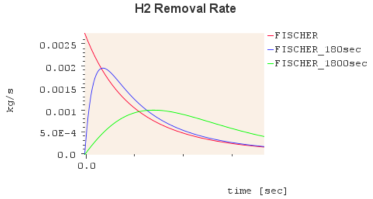


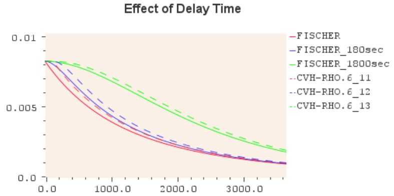












# MELCOR Fan Cooler Model Description

- FCL is a sub-package in ESF Package
- Two Fan Cooler Models Implemented in MELCOR
  - “MARCH” parametric FCL model
  - “CONTAIN” mechanistic fan cooler model (Default)

## ASCII

**FCL_ID  Fan1  CONTAIN**

**FCNAME**

**Fan cooler name.**

**FCMODEL**

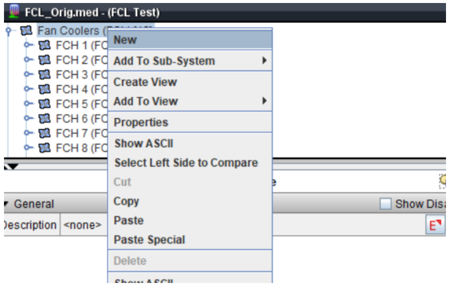
**Fan Cooler Model to be used**

**“MECHANISTIC” or “CONTAIN” - mechanistic fan cooler model**

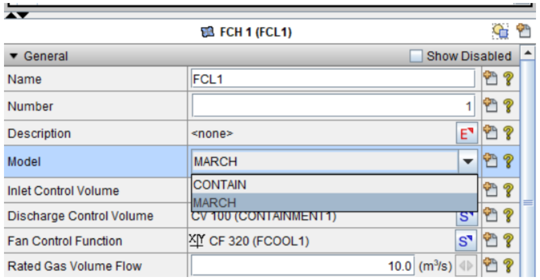
**“MARCH”– old MARCH modeling**

## SNAP

**Add FCL**



**Select Model**



FCH 1 (FCL1)

Name: FCL1
Number: 1
Description: <none>
Model: MARCH
CONTAIN
MARCH
Inlet Control Volume:
Discharge Control Volume: CV 100 (CONTAINMENT1)
Fan Control Function: CF 320 (FCOOL1)
Rated Gas Volume Flow: 10.0 ($m^3/s$)

# MELCOR Parametric Fan Cooler Model

- Based on MARCH 2.0 model, with extensions
  - Empirical relation for total effective heat transfer coefficient from Oconee FSAR
  - Rated operating condition used to infer
    - Temperature change of gas and coolant
    - Effective area for heat transfer
  - Total heat transfer interpreted as sum of sensible heat and condensation
    - Based on average of inlet and outlet temperatures
    - Correlation coefficients accessible as SC array 9001
- Heat/mass transfer calculated at actual operating conditions
  - Cooler can be turned on or off
  - User can specify off-rated flows, coolant temperature
  - Gas inlet temperature and composition taken from CVH
  - Outlet volume can be different than inlet volume
    - FCL defines sinks and sources to CVH

# MELCOR Fan Cooler Model Example Input (2)

## ASCII Input

FCL interface and control data. (required)

FCL_ICI ICVI ICVD CFName

FCL rated flows and temperatures (required)

FCL_RFT XVFGSR XMFSER TSECIR TPR

FCL additional rated conditions (required)

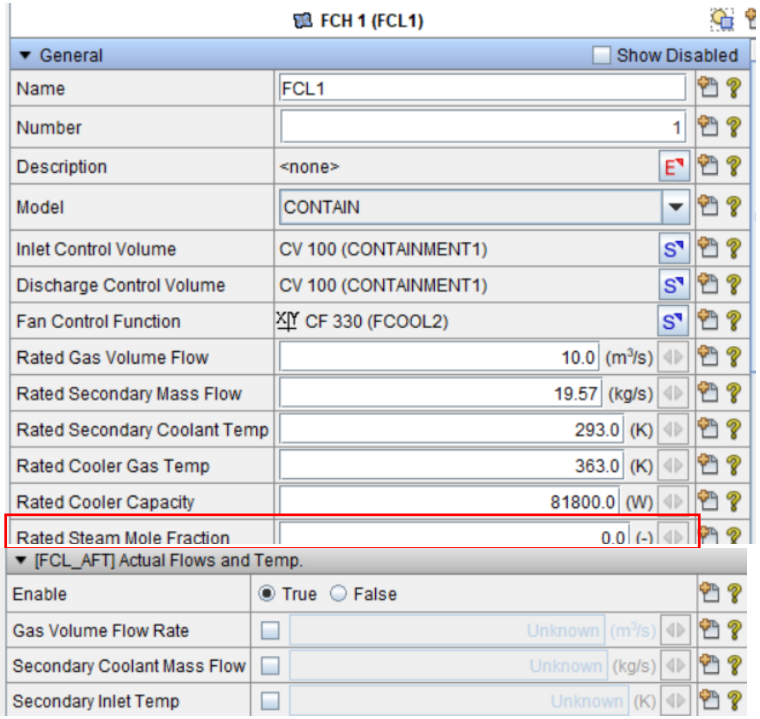
FCL_ARC QRAT$^*$ FMLSTR

FCL off-rated operation (optional)

FCL_AFT XVFGSI XMFSEC TSECIN

**FMLSTR**
**Steam mole fraction at rated conditions.**

## SNAP Input



FCH 1 (FCL1)

General ☐ Show Disabled

| | | |
|---|---|---|
| Name | FCL1 | |
| Number | 1 | |
| Description | <none> | |
| Model | CONTAIN | |
| Inlet Control Volume | CV 100 (CONTAINMENT1) | |
| Discharge Control Volume | CV 100 (CONTAINMENT1) | |
| Fan Control Function | CF 330 (FCOOL2) | |
| Rated Gas Volume Flow | 10.0 | ($m^3/s$) |
| Rated Secondary Mass Flow | 19.57 | (kg/s) |
| Rated Secondary Coolant Temp | 293.0 | (K) |
| Rated Cooler Gas Temp | 363.0 | (K) |
| Rated Cooler Capacity | 81800.0 | (W) |
| Rated Steam Mole Fraction | 0.0 | (-) |

[FCL_AFT] Actual Flows and Temp.

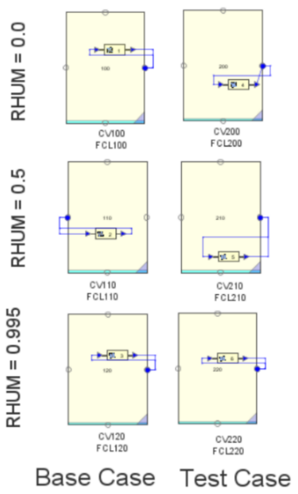
| | | | |
|---|---|---|---|
| Enable | ● True ○ False | | |
| Gas Volume Flow Rate | ☐ | Unknown | ($m^3/s$) |
| Secondary Coolant Mass Flow | ☐ | Unknown | (kg/s) |
| Secondary Inlet Temp | ☐ | Unknown | (K) |

# SNAPlette: Parametric Fan Cooler

Model contains a 3 independent CV/FCL models to assess the performance of the fan cooler model over a range of humidity (see diagram at right).

- All CVs are the same dimensions, temperatures, and NCG mole fractions.
- Fan coolers are identical parametric FCL models

A similar system of independent CV/FCL models are provided to make comparisons

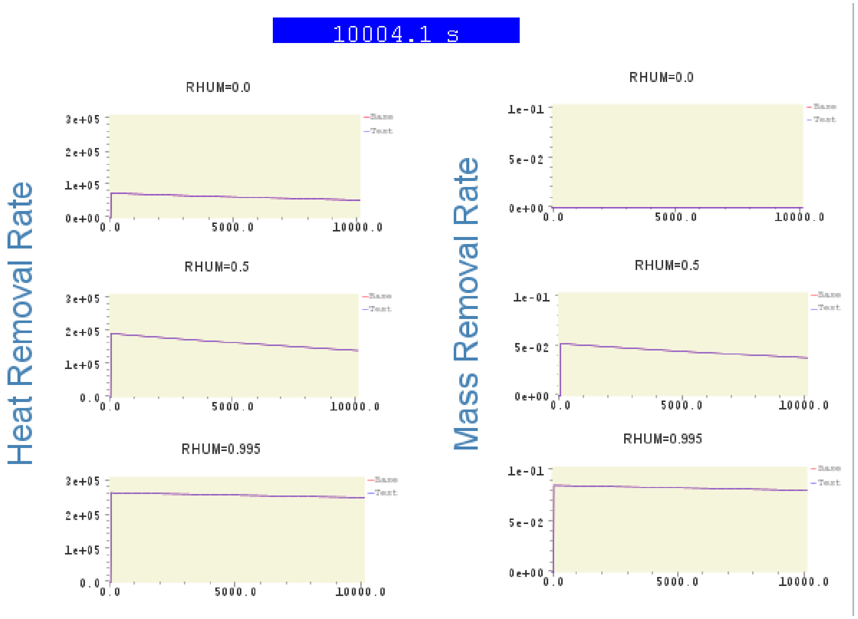


- Input File
  - FCL_Parametric.med
  - FCL_Parametric_anim.med
- Job Stream/Data Source
  - Fans2

Things to Observe

- Performance of the coolers improves with humidity in the environment
- For the case of 0.0 relative humidity, there is no condensation calculated.

- Things to do
  - Change the sensible heat transfer multiplier by 10% and observe the effect.
  - Change the atmosphere temperatures in the CV and observe the effect.
  - Change the actual fan cooler gas volumetric flow rate by 10% and observe the effect.
  - Change the number of coils in the FCL model and observe the change.



# Mechanistic Fan Cooler Model

- Based on CONTAIN mechanistic Model*
  - Nusselt number correlation for flow over horizontal tubes.

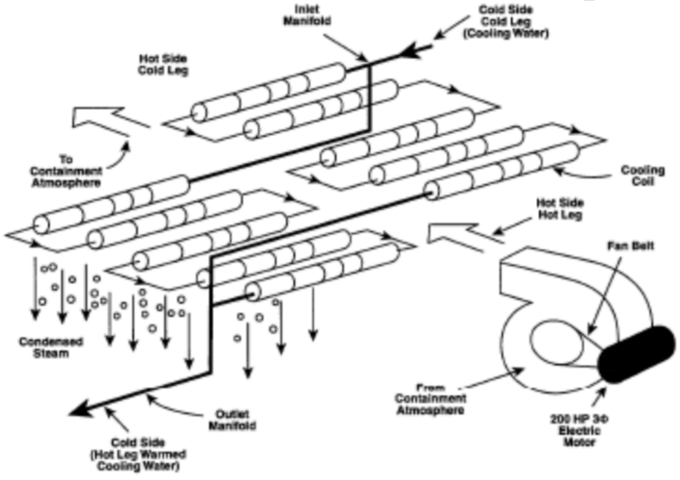
$$Nu = 0.33Re^{3/5}Pr^{1/3}$$

    - Valid for 10 or more transverse rows
    - 1.25<Pitch/D<1.5
  - Analogy between heat and mass transfer

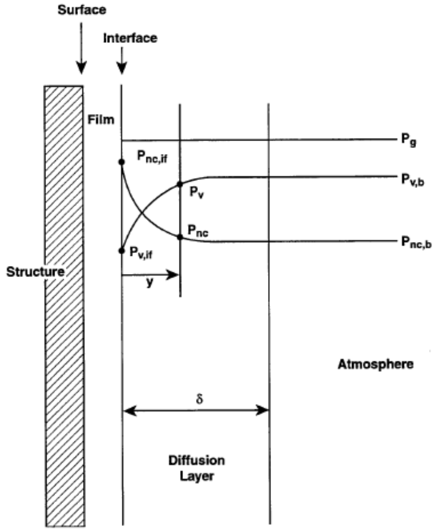
$$Sh = 0.33Re^{3/5}Sc^{1/3}$$

  - Mass transfer driven by concentration gradient (partial pressures)

$$K_g = \frac{SH\ D_v\ ln\left[\frac{P_g - P_{v,b}}{P_g - P_{v,if}}\right]}{RT_{av}d_c\left[P_{v,if} - P_{v,b}\right]}$$



Note: arrows indicate direction of fluid flow



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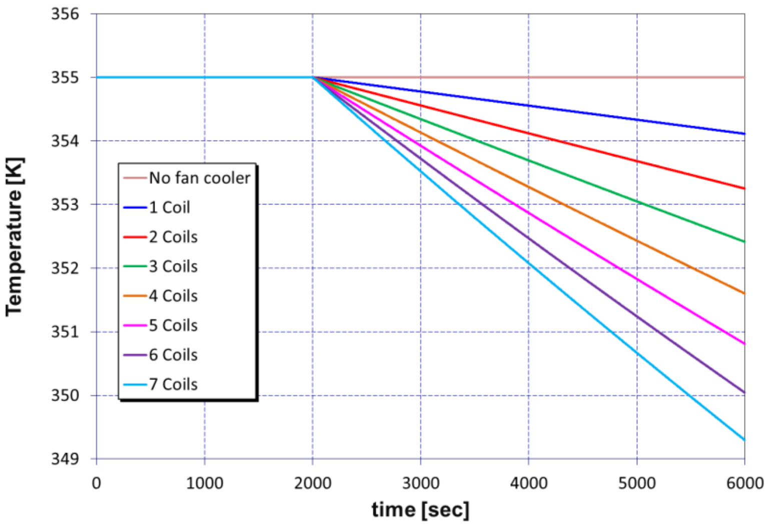
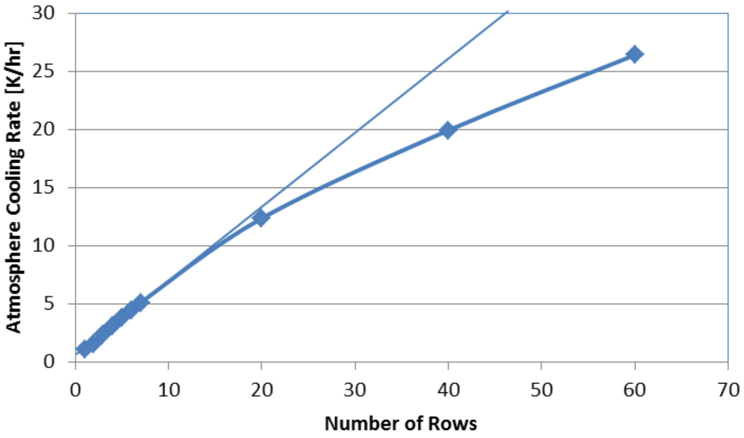
***Murata, et al, "Code Manual for CONTAIN 2.0: A computer Code for Nuclear Reactor Containment Analysis", NUREG/CR-6533, December 1997.**

# Mechanistic Fan Cooler Model

- Iterative solution is necessary
  - First row of coils seen by incoming air/steam mixture is at the outlet of the coils.
  - Coolant exit temperature is estimated from March model
  - Coolant conditions for coil row inlet / gas outlet calculated
  - Repeated for next coil row
  - Coolant inlet temperature and exhaust gas temp calculated.
  - If calculated inlet temperature different from inlet value procedure is repeated with modified estimate
- Efficiency of cooler decreases with number of rows



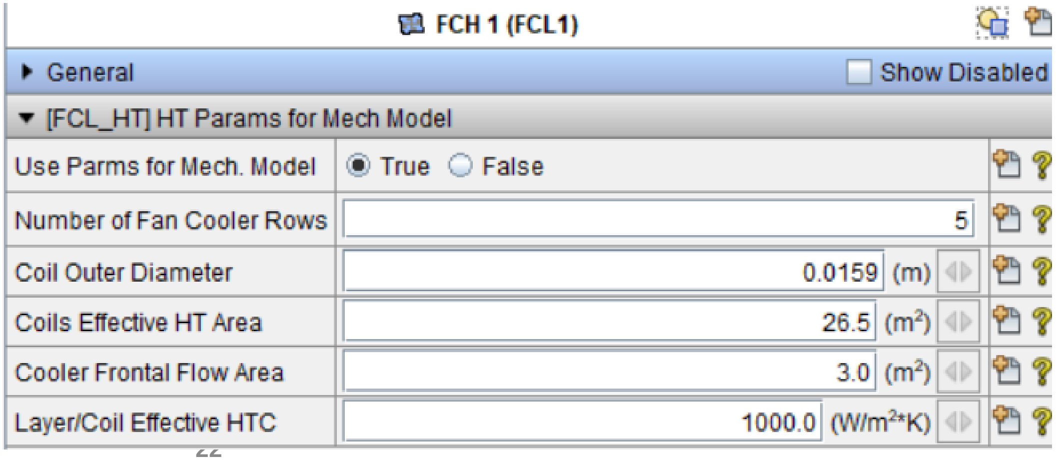


# Mechanistic Fan Cooler Model Input

- FCL_ICI, FCL_RFT, ARC still required
  - User specifies CVs, associated with FCL, on/off control, rated primary & secondary flows and rated fan and secondary inlet temperatures, and rated fan cooler capacity (W),
- Off-rated parameters not specified

and

- FCL_HT NCOILS DCOIL AREAHT AREAFL HTCEFF
  - NCOILS - Fan cooler number of coil rows from front to back of cooler
  - DCOIL - OUTER DIAMETER OF FAN COOLER COIL (M)
  - AREAHT - EFFECTIVE HEAT TRANSFER AREA FOR ONE ROW OF COILS (M**2)
  - AREAFL - FLOW AREA OF COOLER (FRONTAL) (M**2)
  - HTCEFF - HEAT TRANSFER COEFFICIENT THRU BOUNDARY LAYER AND COIL (W/M**2 K)



FCH 1 (FCL1)

[FCL_HT] HT Params for Mech Model

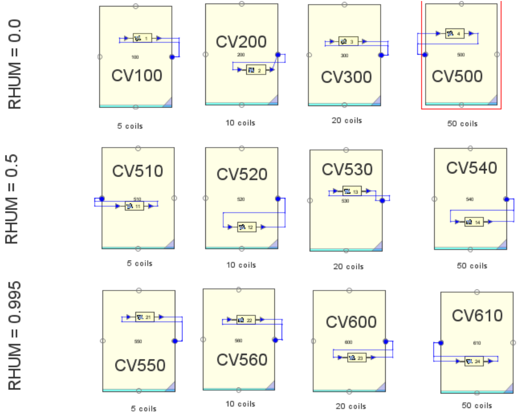
| | |
|---|---|
| Use Parms for Mech. Model | ● True ○ False |
| Number of Fan Cooler Rows | 5 |
| Coil Outer Diameter | 0.0159 (m) |
| Coils Effective HT Area | 26.5 ($m^2$) |
| Cooler Frontal Flow Area | 3.0 ($m^2$) |
| Layer/Coil Effective HTC | 1000.0 ($W/m^2*K$) |

# SNAPlette: Mechanistic Fan Cooler

Model contains a matrix of independent CV/FCL models to assess the performance of the fan cooler model over a range of humidity and # of coil rows (see diagram at right).

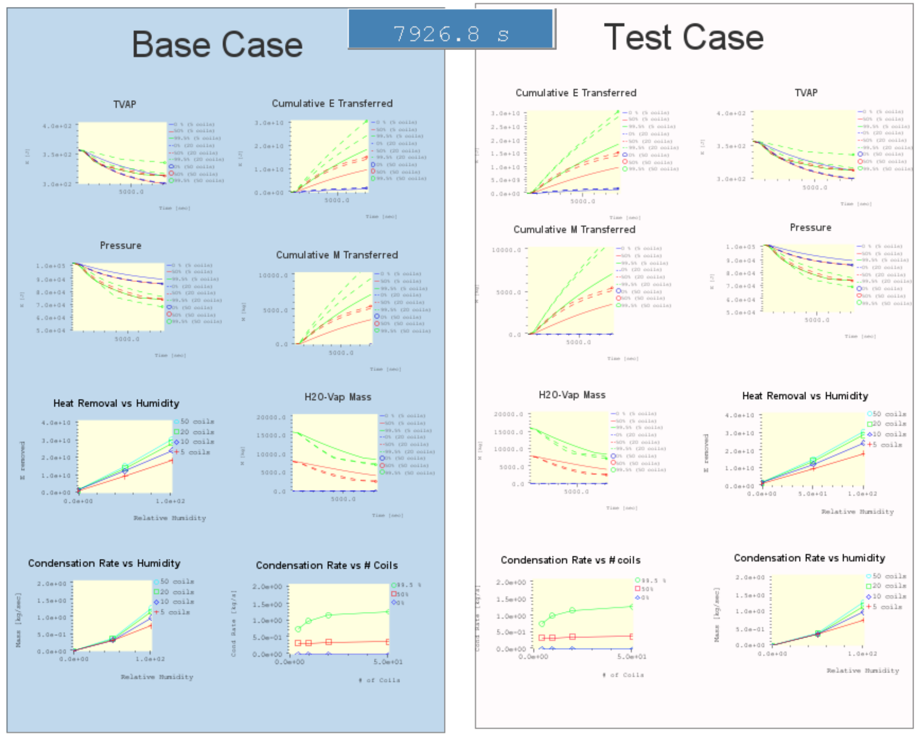
- All CVs are the same dimensions, temperatures, and NCG mole fractions.
- Fan coolers are identical except for the number of coils

A similar matrix of independent CV/FCL models are provided to make comparisons



- Input File
  - FCL_Mech.med
  - FCL_Mech_anim.med
- Job Stream/Data Source
  - FANS

- Observations on Base Case
  - The performance of the fan cooler does not appreciable improve with more coils beyond 20 coils
  - The performance of the fan improves significantly as humidity increases.
  - Containment pressure decrease is most significant for high humidity.
- Things to try
  - Make a 20% change to the coil effective HTC and see how the comparisons change.
  - Connect the fan cooler discharge to a large boundary condition CV



# MELCOR Containment Spray Model Description

- SPR package models interactions between falling droplets and volume atmospheres
  - Heat and mass transfer
  - Aerosol removal
- Sprays can be injected in any volume
  - Specify source elevation, water temperature and flow rate
  - Specify droplet size
    - Distribution allowed, but not recommended for aerosol removal calculations
  - Sprays can be on or off
  - More than one spray train is permitted

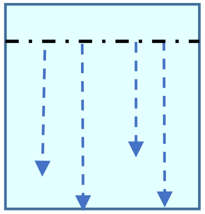
**Original modeling based on HECTR code**

# MELCOR Containment Spray Model Description (2)

- Source of spray water can be the following:
  - An external source
  - Taken from the pool of some control volume
    - May specify elevation range and action on dryout
  - From "rain" of water condensed on heat structures
    - Will return to this later
- Droplets reaching bottom of volume
  - Can be carried over to another control volume
  - Can be deposited into the pool in that volume
  - Can be deposited into a designated "sump" volume
  - User input determines fractional disposition
    - Default is to deposit all into local pool
- Droplets *cannot* be deposited on surfaces
- User specifies initial droplet temperature and flow rate
  - Can be controlled by a Control Function
- User turns sprays on and off with a CF

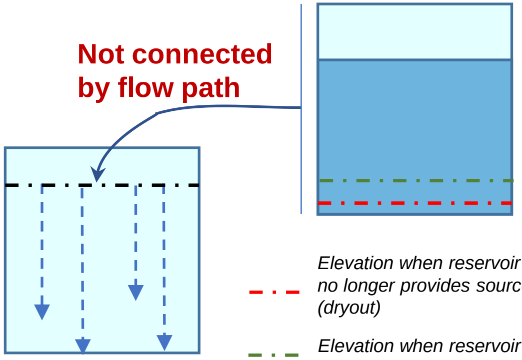
## External Source

*User specifies temperature & flow rate of water droplets*



## Reservoir CV Source

- *User specifies temperature (can be CF that takes on temperature of pool) & flow rate of water droplets*
- *User provides a CV representing a reservoir for the spray*

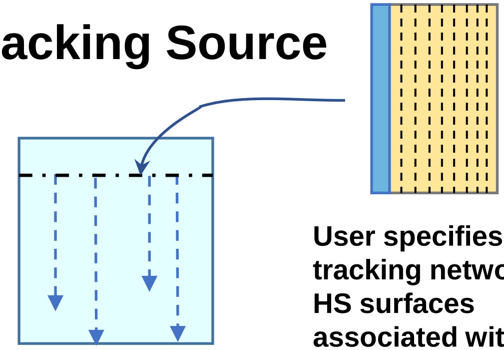


*Elevation when reservoir no longer provides source (dryout)*

*Elevation when reservoir no longer resumes spray after dryout*

## HS - Film Tracking Source

*Temperature and flow rates taken from film tracking model.*



**User specifies film tracking network & HS surfaces associated with 'spray'**

# MELCOR Containment Spray Model Example Input

- ASCII Input

SPR_ID identifies input for spray sources

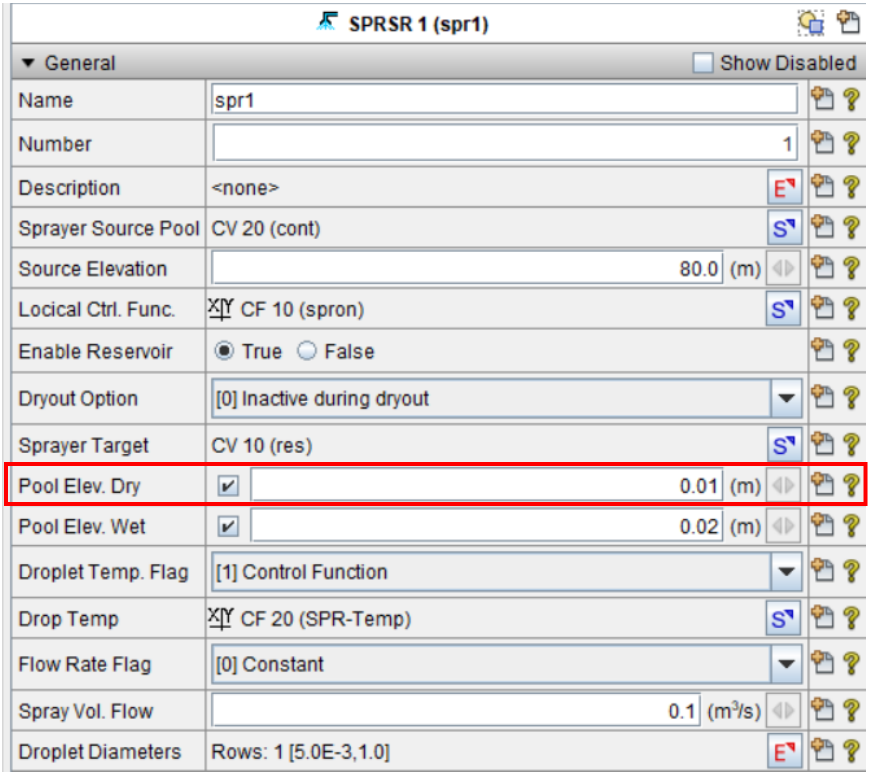
SPR_ID ‘spr1’ cont 80. CF spron

SPR Spray reservoir data input

SPR_SRD 0 res .01 .02

**ELDRY**
**Reservoir pool elevation at dryout.**
**default = CVBOT + 0.01*(CVTOP – CVBOT))**

- SNAP Input



SPRSR 1 (spr1)

General ☐ Show Disabled

| | |
|---|---|
| Name | spr1 |
| Number | 1 |
| Description | <none> |
| Sprayer Source Pool | CV 20 (cont) |
| Source Elevation | 80.0 (m) |
| Locical Ctrl. Func. | CF 10 (spron) |
| Enable Reservoir | ● True ○ False |
| Dryout Option | [0] Inactive during dryout |
| Sprayer Target | CV 10 (res) |
| Pool Elev. Dry | ☑ 0.01 (m) |
| Pool Elev. Wet | ☑ 0.02 (m) |
| Droplet Temp. Flag | [1] Control Function |
| Drop Temp | CF 20 (SPR-Temp) |
| Flow Rate Flag | [0] Constant |
| Spray Vol. Flow | 0.1 ($m^3/s$) |
| Droplet Diameters | Rows: 1 [5.0E-3,1.0] |

# MELCOR Containment Spray Model Droplet Input

- ASCII Input

```
SPR droplet temperature and flow
rate conditions
SPR_DTFR CF SPR-Temp Const 0.1
```

User can specify droplet size distribution

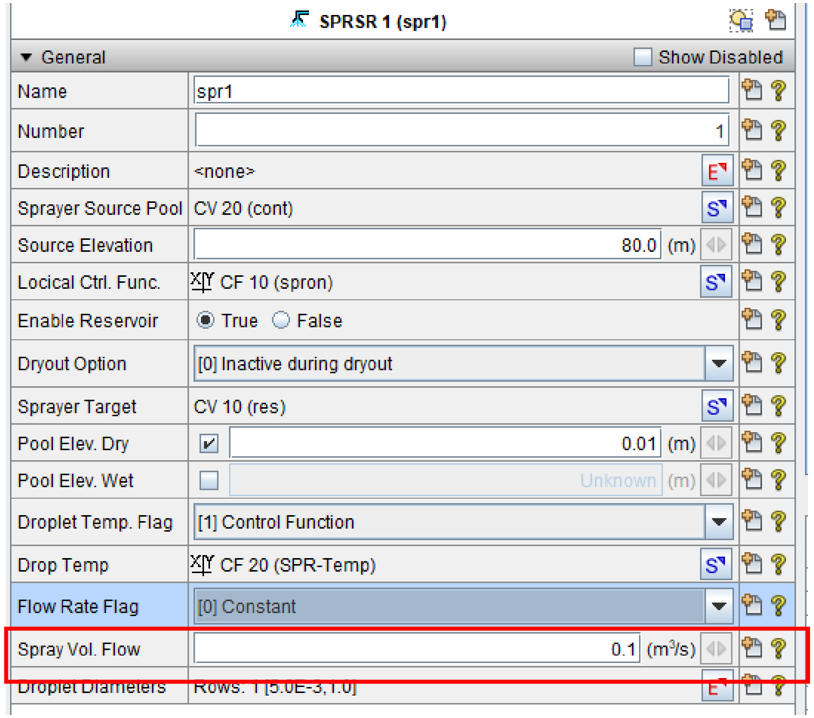
- Determines terminal velocity

```
SPR drop size distribution
SPR_DSD 1
        1  5.0E-4  1.0
```

**SPFLO**
**Total spray volumetric flow rate from this source. The value of SPFLO must be greater than or equal to zero. This field is required if KEYFL equals CONST or 0.**

**(type = real, default = none, units = m3/s)**

- SNAP Input



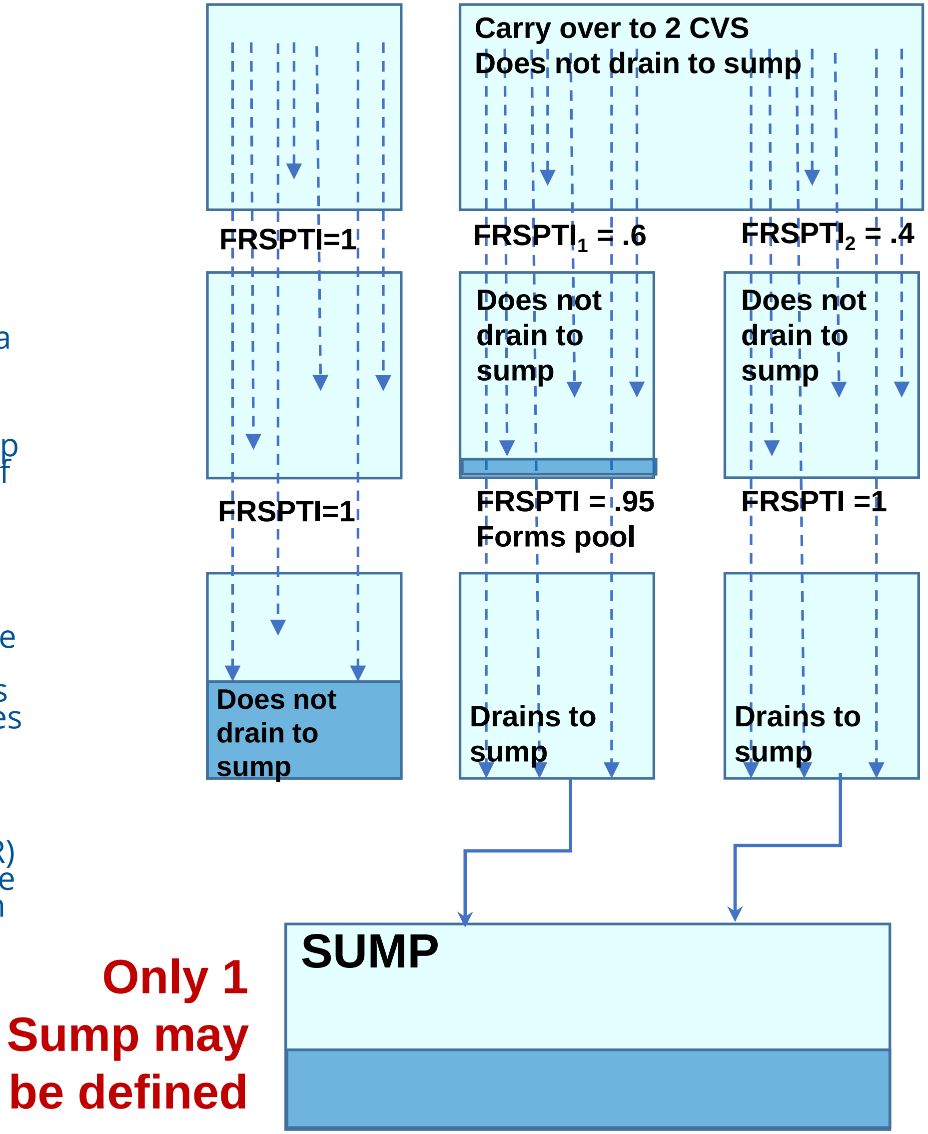
SPRSR 1 (spr1)

General ☐ Show Disabled

| | |
|---|---|
| Name | spr1 |
| Number | 1 |
| Description | <none> |
| Sprayer Source Pool | CV 20 (cont) |
| Source Elevation | 80.0 (m) |
| Locical Ctrl. Func. | CF 10 (spron) |
| Enable Reservoir | ● True ○ False |
| Dryout Option | [0] Inactive during dryout |
| Sprayer Target | CV 10 (res) |
| Pool Elev. Dry | ☑ 0.01 (m) |
| Pool Elev. Wet | ☐ Unknown (m) |
| Droplet Temp. Flag | [1] Control Function |
| Drop Temp | CF 20 (SPR-Temp) |
| Flow Rate Flag | [0] Constant |
| Spray Vol. Flow | 0.1 ($m^3$/s) |
| Droplet Diameters | Rows: 1 [5.0E-3,1.0] |

# MELCOR Containment Spray Model
# Spray Junction Model

- User can override default disposition of droplets reaching bottom of control volume
- Specify fractions that are
  - Deposited into local pool (default)
  - Carried over to other volumes
    - Spray droplets reaching the bottom of a control volume may be carried over to other control volumes. The fraction of these droplets entering each subsequent control volume is specified by the user. If the sum of the specified fractions for a given from control volume is CAROVR, then CAROVR must be no greater than 1. If CAROVR is less than 1, and the from control volume is not in the list of control volumes emptying into the sump (see Section 2.1.3), then a fraction (1 – CAROVR) of the droplets is placed into the pool of the from control volume.
  - Transported directly to a designated sump volume
    - The user may optionally define the control volume that contains the sump. The sump is a pool into which spray droplets are deposited if the droplets reach the bottom of user-selected control volumes and are not carried over into other control volumes. The user may define a list of control volumes from which droplets enter the sump. If the sum of the transmission factors for a volume in that list is CAROVR, then a fraction (1 – CAROVR) of the droplets reaching the bottom of the volume is placed into the sump. At present, no more than one sump may be defined.



**Carry over to 2 CVS**
**Does not drain to sump**

**FRSPTI=1**

**FRSPTI$_1$ = .6**

**FRSPTI$_2$ = .4**

**Does not drain to sump**

**Does not drain to sump**

**FRSPTI=1**

**FRSPTI = .95**
**Forms pool**

**FRSPTI =1**

**Does not drain to sump**

**Drains to sump**

**Drains to sump**

**SUMP**

**Only 1 Sump may be defined**

## Mass Transfer

$$\frac{dm}{dt} = -2\pi\,\rho_g D\left(1 + 0.25\,Re^{1/2}\,S\,c^{1/3}\right)D_c\,ln\left(1 + B\right)$$

## Heat Transfer

$$\frac{dT}{dt} = \frac{1}{m\ c_{pl}}\left[\frac{c_{pv}\left(T - T_{cv}\right)}{\left(1 + B\right)^{1/Le} - 1} + h_{fg}\right]\frac{dm}{dt}$$

## Droplet Velocity

$$\frac{dz}{dt} = \left[\frac{4\left(\rho_d - \rho_g\right)g\ D}{3\rho_g C_d}\right]^{1/2}$$

## Mass Transfer Driving Force

$$B = \frac{x_b - x_i}{x_i - 1}$$

- m = droplet mass,
- $T, T_{cv}$ = droplet, control volume atmosphere temperatures,
- z = droplet fall height,
- $\rho_D$, $\rho_g$ = droplet, atmosphere densities,
- $C_{pl}$ = droplet specific heat capacity,
- $C_{pv}$ = control volume atmosphere specific heat capacity,
- $H_{fg}$ =latent heat of vaporization,
- D = droplet diameter,
- Re = Reynolds number,
- Sc = Schmidt number,
- Le = Lewis number,
- Dc = diffusion coefficient,
- $C_d$ = drag coefficient,
- Xb = H2O mass fraction in the bulk atmosphere
- Xi = H2O mass fraction at the liquid/atmosphere interface

Based on forced convection heat transfer and evaporation and condensation correlations that have been formulated specifically for high temprature atmospheres, such as might be encountered during a hydrogen burn [[i]]. The constants i have been implemented in sensitivity coefficient array 3001.

---

[i]. F. A. Williams, Combustion Theory, Addison-Wesley, Reading, MA (1965).

MELCOR

# Particulate Removal Rate

$$\frac{dM_k}{dt} = -\lambda_{k,i} M_k$$

# Removal Rate Constant

## Vapor Removal

$$E_{k,i} = 1 - \exp\left[-\frac{6\ k_g\ t_e}{2r_i\left(H + k_g / k_\ell\right)}\right]$$

$$k_\ell = \frac{\pi^2\ D_{k,\mathrm{H_2O}}}{3r_i} \qquad k_g = \frac{D_{k,gas}}{2r_i}\left(2.0 + 0.060\ \mathrm{Re}^{1/2}\ Sc^{1/3}\right)$$

## Aerosol Removal

$$\lambda_{k,i} = \frac{3F_i h E_{i,j}}{4Vr_i}$$

**<0.1 micron (Diffusion)**

$$\varepsilon_{diff} = 3.02\,\mathrm{Re}^{1/6}\,Pe^{-2/3} + 1.14\,(\mathrm{Re}/Pe)^{1/3} I + 0.57\,\mathrm{Re}^{1/3} I^2$$

**1 to 10 microns (Diffusiophoresis)**

$$\varepsilon_{diffusio} = \frac{4}{3}\frac{r_d}{F\ h}\left[\frac{M_s^{1/2}}{X_s M_s^{1/2} + X_g M_g^{1/2}}\right]\frac{W_s}{cM_s}$$

**>10 microns (Impaction & Interception)**

|  | Viscous flow around a sphere | Potential flow around a sphere |
|---|---|---|
| **Interception** | $\varepsilon_{In,vis} = (1+I)^2\left[1 - \frac{3}{2(1+I)} + \frac{1}{2(1+I)^3}\right]$ | $\varepsilon_{In,Pot} = (1+I)^2 - (1+I)^1$ |
| **Inertial Impaction** | $\varepsilon_{Im,Vis} = \left[1 + \frac{0.75\log_e(2\ Stk)}{Stk - 1.214}\right]^{-2}$ | $\varepsilon_{Im,Pot} = \left[\frac{Stk}{Stk + 0.5}\right]^2$ |

- Fi = volumetric flow rate for droplets of size i
- Ek,I = adsorption efficiency for vapor class k
- H = partition coefficient for partition of the vapor between spray water and gas
- V = volume of control volume
- $r_i$ = drop radius
- $t_e$ = drop exposure time
- $D_{k,gas}$ = diffusivity of vapor k through bulk gas
- $D_{k,H2O}$ = diffusion constant for vapor k in liquid water
- Re = Reynolds number,
- Sc = Schmidt number,
- Vd = drop velocity
- kg, the gas boundary layer mass transfer coefficient
- $K_l$ is the liquid boundary layer mass transfer coefficient

# MELCOR Containment Spray Model
# Spray Junction Model Input

## ASCII Input

```
SPR_JUN N ! KCVFM   KCVTO   FRSPTI
        1  CV1     CV2     1.0
        .  .       .        .
        .  .       .        .
        N  .       .        .
```

***KCVFM***

*From control volume name for this junction.*

***KCVTO***

*To control volume name for this junction.*

***FRSPTI***

*Fraction of spray droplets reaching bottom of from volume that are to be transported into to volume. Must be between 0 and 1.*

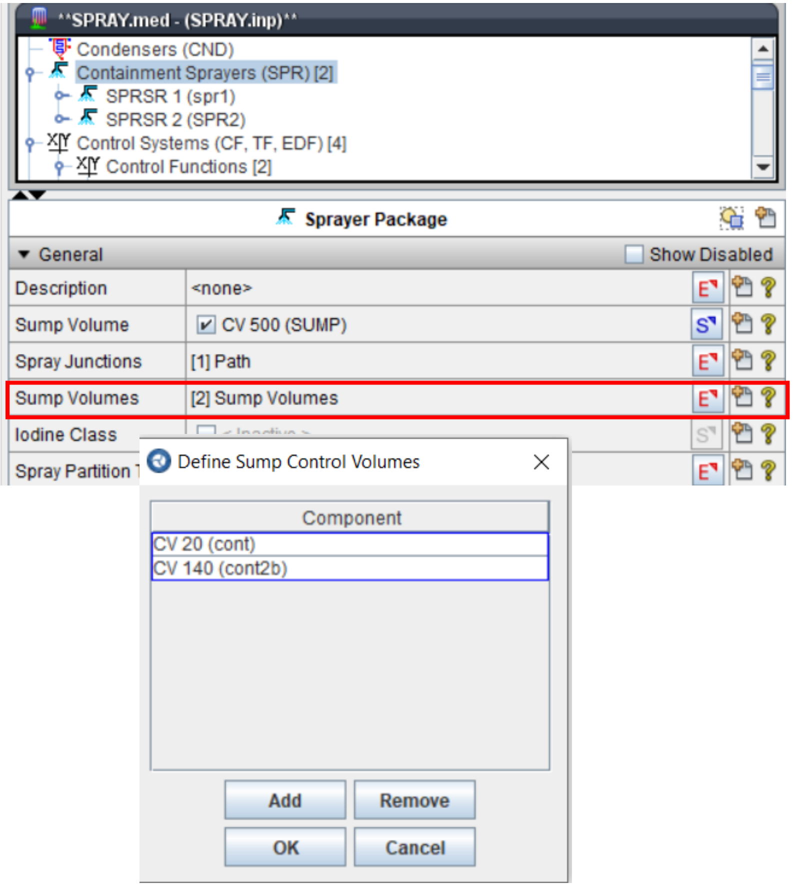
```
SPR_SUMP CVName
```

*Name of the control volume containing the sump.*

```
SPR_CV 1
        1    CVName1
        2    CVName2
```

*Control Volumes that Empty Sprays into Sump*

## SNAP Input



**SPRAY.med - (SPRAY.inp)**

- Condensers (CND)
- Containment Sprayers (SPR) [2]
  - SPRSR 1 (spr1)
  - SPRSR 2 (SPR2)
- Control Systems (CF, TF, EDF) [4]
  - Control Functions [2]

**Sprayer Package**

General ☐ Show Disabled

| | |
|---|---|
| Description | <none> |
| Sump Volume | ☑ CV 500 (SUMP) |
| Spray Junctions | [1] Path |
| Sump Volumes | [2] Sump Volumes |
| Iodine Class | ☐ < Inactive > |
| Spray Partition T | |

Define Sump Control Volumes

| Component |
|---|
| CV 20 (cont) |
| CV 140 (cont2b) |

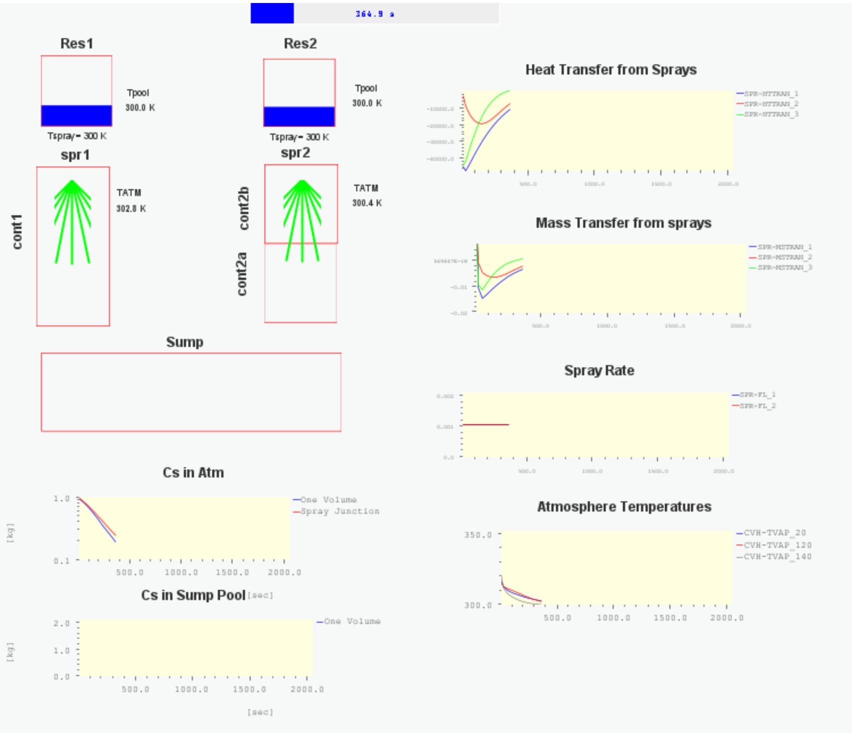
# SNAPlette: Spray Modeling

- Model contains 2 independent spray networks
  - Network 1 (spr1) –1 volume spray
    - Cont1 is volume where spray is associated.
    - Res1 is the reservoir volume for spr1
  - Network 2(spr2) -2 volume with spray connecting
    - Two equal volumes (cont2a & cont2b (upper))
      - Sum of two volumes is equal to cont1 and elevation is split equally
      - Idendical initial thermodynamic conditions & equivalent spray characteristics
  - Network 3 – This is identical to Network 1 but is used for comparisons
    - cont_test, res_test, spr_test
  - Atmospheric temperature is 380 K for contx volume
  - Sump volume is defined but not connected

- Input File
  - Spray.med
  - SPRAY_anim.med
- Job Stream/Data Source
  - spray

Things to consider

- Connect cont, cont2a, & cont_test to sump volume
  - Run before & after and inspect differences
- Activate RN package
  - Run before & after and inspect differences
- If time permits, reduce FNRSP on spray junction and verify formation of pool in cont2b
- Observations
  - Compare heat removal for single volume (spr1) to 2 volume (spr2)
  - Compare washout of Cs for two models
- Modify spr_test (make your own studies)
  - Add a deflagration component. Does steam condensation lead to combustible mixtures?
  - Change the droplet size
  - Change the droplet temperature to 320 K
    - Notice that the droplet temperature is not necessarily the same as the reservoir pool
      - Consider making the droplet temperature a CF based on reservoir pool temp
  - For spr_test, change the droplet temperature for spr_test without changing the pool temperature for Res_test



# New Spray Range Support

| | |
|---|---|
| SPR-HTTRAN(CV) | Rate of heat transfer from sprays to steam in control volume CV (either CVNAME or ICVNUM). (units = W) |
| SPR-MSTRAN(CV) | Rate of mass transfer from sprays to steam in volume CV (either CVNAME or ICVNUM). (units = kg/s) |

***To facilitate tracking the total heat or mass transfer from sprays in a collection of volumes, this control function now allows specification of a range instead of a single CV. The value returned is the mass (or energy transferred) from each CV in the range which can be used in vectorized control functions to sum over all volumes.***

**Example Input:**

```
CF_ID       'SPREtrans'   1030     ADD
CF_SAI 1.0 0.00
CF_UNITS 'KG'
CF_ARG 1
1   SPR-HTTRAN(#CVRANGE)    1.0    0.0

CF_RANGE  CVRANGE  CVOLUMES  1
CONSTRUCT  1
             1 CVTYPE='CTYP-4'
```

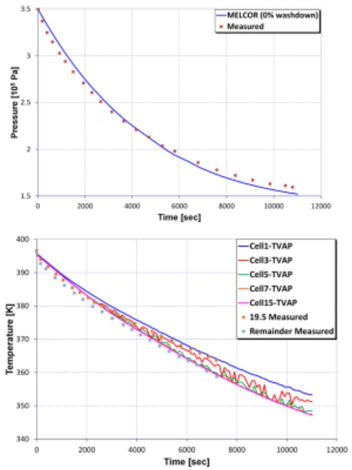
**Note: If a user includes a CV without any spray associated with it, the value returned by the CF for that element is zero.**

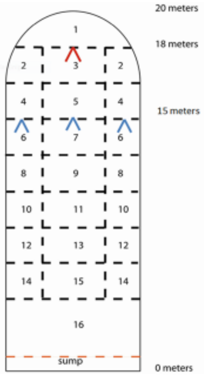
**Not yet supported in SNAP**

# Spray Assessments

- Multiple Assessments on Sprays
  - Thermal response of atmosphere
  - Pressure response of atmosphere
  - Radionuclide scrubbing
  - Effect on stratification in large containments

## JAERI Spray Test

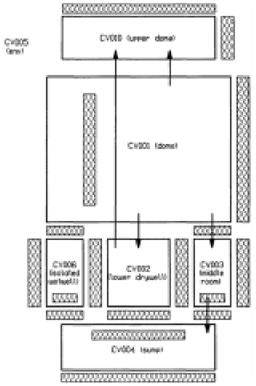


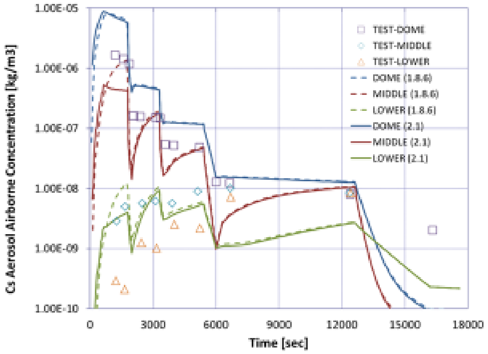


- Water spray tests conducted at the Japan Atomic Energy Research Institute (JAERI) during the late 1970's.
  - Confirm the effectiveness of pressure suppression through condensation by sprays that are often found in the containments of nuclear reactors.

## CSE-A9 Experiment

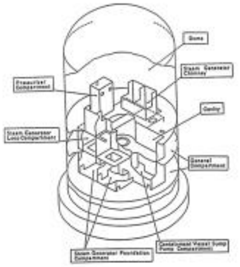
A series of water spray experiments were conducted as parts of the Containment Systems Experiment (CSE) program at Pacific Northwest Laboratories in the 1970s. The experiments were conducted to evaluate the performance of a containment spray engineered safety system as a means of removing fission products from the containment atmosphere. Measurements were obtained that provide a suitable basis for judging the ability of various mathematical models to predict spray performance in large nuclear power plants.

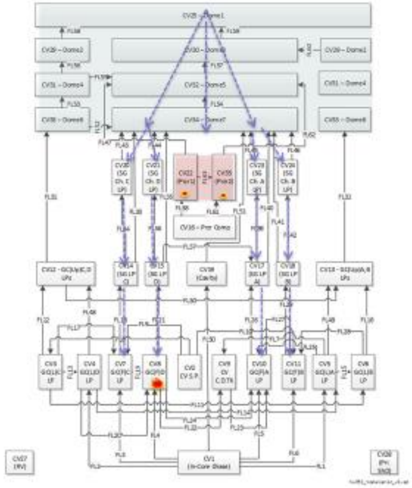




## NUPEC M-8-1, M-8-2, and M-7-1 experiments

- Validation objectives
  - Pressure response;
  - Temperature distribution and stratification
  - Hydrogen mixing
  - Spray modeling
  - Film Tracking Model
- Sprays
  - M-8-1 No Sprays
  - M-7-1 and M-8-2 Sprays modeled





# Multi HS Radiation Enclosure Model

- The space between surfaces may or may not be filled with a participating medium,
  - Participating gas may absorb, emit, and scatter radiation emitted by the surfaces.
- Each surface is assumed to be isothermal, opaque, diffuse, and gray, and are characterized by uniform radiosity.
  - The absorptivity (a) of a surface is equal to the emissivity (e) and the sum of the absorptivity and reflectivity (r) is 1.0

$$\varepsilon_i = \alpha_i = 1 - \rho_i$$

- Reciprocity is also assumed between surface pairs

$$\sum_{i=1}^{N} VF_{i,j} = 1.0$$

- It is assumed the sum of the view factors from a surface to all surfaces in the enclosure network, is equal to 1.0.
  - a surface may also radiate to itself.

**The surface radiosity is defined as the total heat flux that departs from an area (reflected and emitted)**

$$J_i = \rho_i \cdot G_i + \varepsilon_i E_{b,i}$$

**where**

**$G_i$= radiation flux incident on surface I from radiation from all other surfaces,**

**$E_{bi}$= blackbody emissive power of surface i, $\sigma T_i^4$**

$$J_i = (1-\varepsilon_i) \cdot \sum_j^N \left[F_{ij} \cdot \tau_{j,i} \cdot J_j\right] + \varepsilon_i \cdot \sigma \cdot T_i^4 + \rho_i \varepsilon_m E_{bm}$$

$$G_i = \sum_j^N \left[A_j \cdot F_{j,i} \cdot \tau_{j,i} \cdot J_j\right] / A_i + \varepsilon_m E_{bm}$$

$$q_i = A_i \left(J_i - G_i\right)$$

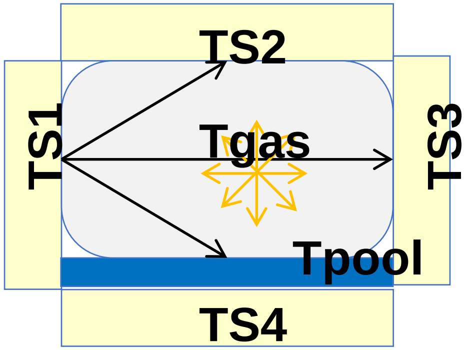
**$\tau_{j,i}$ is the transmissivity through gas**

# Multi HS Radiation Enclosure Model

- View factors can be control functions
  - Sum of view factors for a surface cannot exceed 1.0
- Radiation to pool surface
  - When pool covers a participating surface on a HS, the pool surface replaces that HS surface in the enclosure network.
- Aerosol cloud emissivity derived per Pilat and Ensor

$$\alpha_{\lambda m} = 4000 C_{\lambda m} f_m$$

  - Where $C_{\lambda m}$ is the user defined parameter kmx,
  - Input as part of the radiation enclosure model.
  - $f_m$ is the total aerosol mass concentration (kg/m$^3$) calculated by the code.
  - $C_{\lambda m}$ in this equation is provided to allow the user to account for the effects of wavelength, index of refraction, particle size distribution, and aerosol particle material density.
  - $C_{\lambda m}$ = 1, corresponds to soot-like particles with a density of 2000 kg/m$^3$



```
! #HS  NetName  #Net  NotUsed   KMX
HS_RAD  5  NET2 1  IGNOREPOOL -  0.25
  1 'top head'                   LEFT  EM1     20.3    0.05   0.3   0.15    0.5    0.0
  2 'walls-edge'  LEFT  EM1      7.62    0.1      -        -      0.3    -
  3 'vert-int'      LEFT  EM1      3.81    -        0.9    0.0        -     0.0
  4 'floor'          LEFT  0.65      20.3    0.0   0.25   0.25      0.0   0.5
  5 'horiz-int’    LEFT  EM1      3.81    0.0    0.5    0.0        0.5   0.0
```

**M. J. Pilat and D. S. Ensor, “Plume Opacity and Particulate Mass Concentration,” *Atmospheric Environment,* Vol. 4, pp. 163-173, 1970.**

# MELCOR Filter Models
## Description

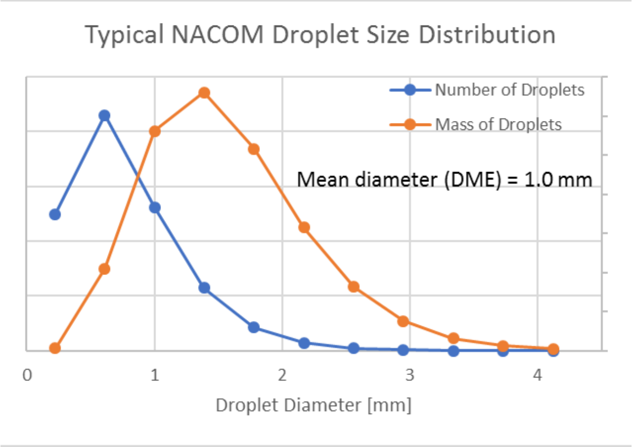
- FL & RN packages model filtration models
  - Aerosol filtration as a function of
    - Aerosol size
    - Chemical class
  - Aerosol filter degradation models
    - Increased filter resistance due to aerosol loading
    - Failure based on ΔP, temperature or other (CF based)
  - Vapor filtration as a function of
    - Chemical class
  - Vapor filter degradation models
    - Radiolytic desorption (Iodine model)
    - Thermal desorption (Iodine model)
    - Charcoal combustion due to decay heat or external heating
- Coupling to GRTR in progress
  - Sorption or hold-up in graphite structures and charcoal beds
  - All temperature releases

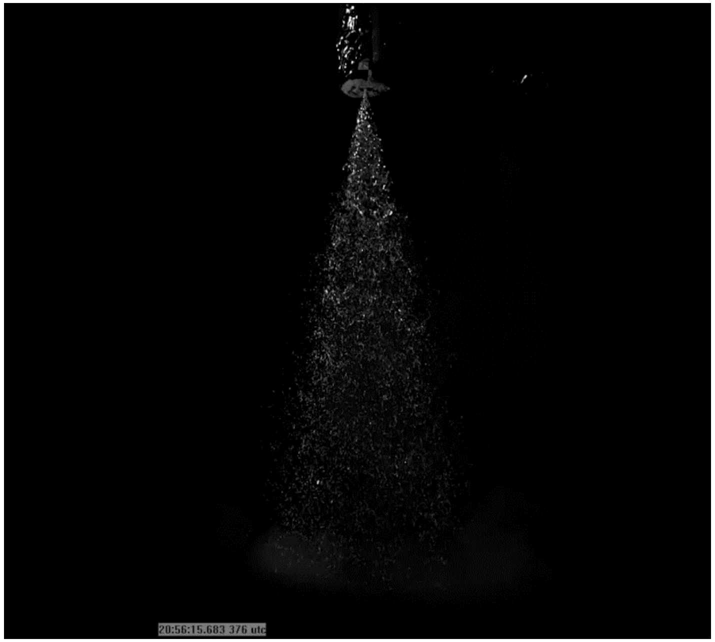
# Sodium Spray Fire Chemistry

- Based on NACOM spray model from BNL
  - Input requirement: fall height, mean diameter and source
  - Internal droplet size distribution (11 bins) from Nukiyama-Tanasama correlation
  - Reactions considered:
    - (S1) $2\,Na + {}^{1}/_{2}\,O_2 \rightarrow Na_2O$,
    - (S2) $2\,Na + O_2 \rightarrow Na_2O_2$
  - Fixed ratio of peroxide and monoxide

$$\frac{1.3478\cdot F_{Na_2O_2}}{1.6957-0.3479\cdot F_{Na_2O_2}}$$

  - Predicted quantities include:
    - Mass of Na (spray, burned, pool), $O_2$(consumed), $Na_2O_2$+ $Na_2O$(produced)
    - Energy of reactions
- Enhancements
  - Droplet acceleration model
  - Pre-ignition burn rate
  - Adjustment to heat of combustion to include heat of vaporization
    - $Na_2O$ from 9.18 to 13.71 MJ/kg of sodium
    - $Na_2O_2$ from 10.46 to 15.88 MJ/kg of sodium
- Missing from model
  - Maximum droplet size
  - Radiant heat loss from droplets
  - Swarm effects





# Sodium Pool Fire Model

- Based on SOFIRE II code from ANL
  - Reactions considered:
    - $2\,\mathrm{Na} + \mathrm{O_2} \rightarrow \mathrm{Na_2O_2}$, 10.97 MJ/kg
    - $4\,\mathrm{Na} + \mathrm{O_2} \rightarrow 2\,\mathrm{Na_2O}$, 9.05 MJ/kg
    - Half of the heat produced by these reactions is assigned to the sodium pool, while the other half is assigned to atmospheric gases above the pool.
  - Reactions depend on the oxygen diffusion as:

$$D = \frac{6.4315\times10^{-5}}{P} T^{1.823}$$

  - Input requirement:
    - F1 – fraction of $O_2$ consumed for monoxide, F2 – fraction of reaction heat to pool, F3 – fraction of peroxide mass to pool, & F4 – fraction of monoxide mass to pool
  - Predicted quantities:
    - Mass of Na(pool, burned), $O_2$(consumed), $Na_2O_2$+$Na_2O$(produced)
    - Energy of reactions
  - Model Extensions
    - Radiation Heat Transfer Between Heat Structures and Pool Surface
    - Heat Transfer Between Pool and Atmosphere
    - CONTAIN/LMR uses film temperature for evaluating many thermodynamic properties.
  - User controllable pool surface area
    - User-specified surface area (control function)

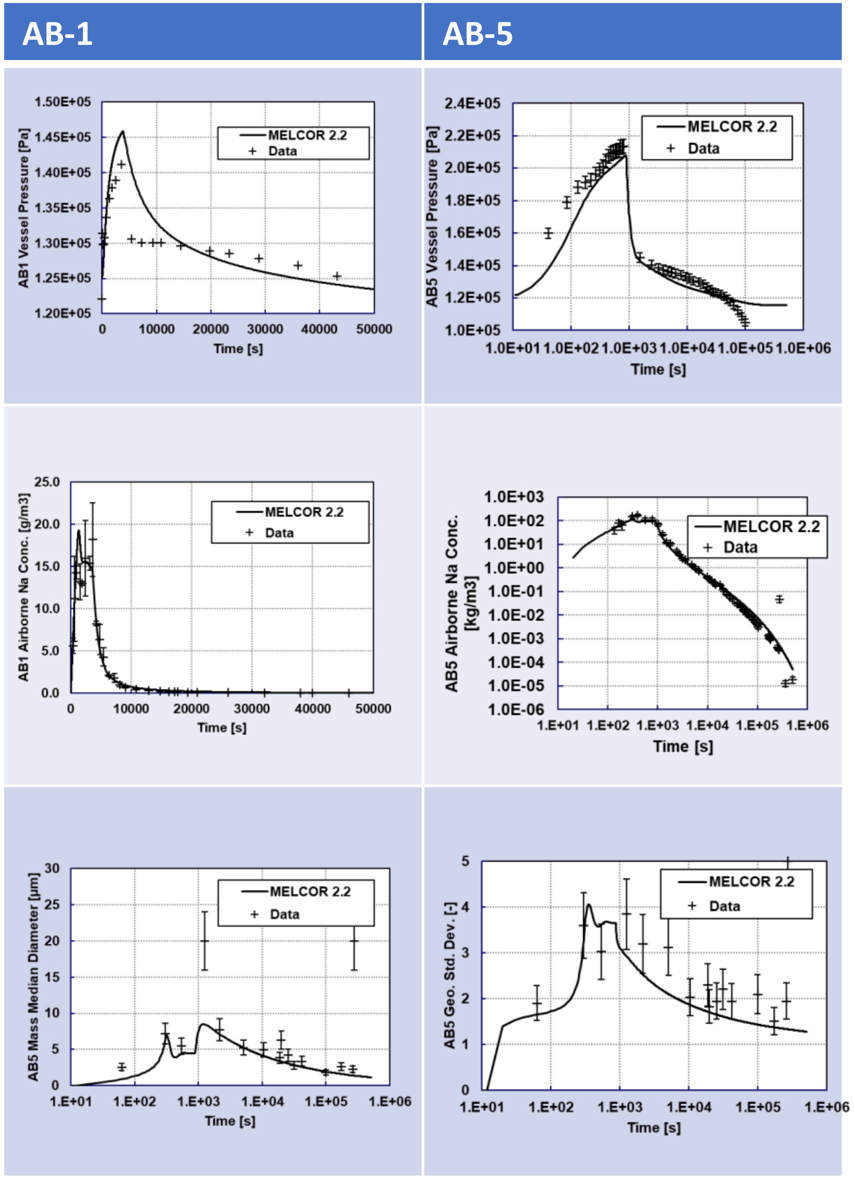
# Atmospheric Chemistry
# New in 2019 Code Release

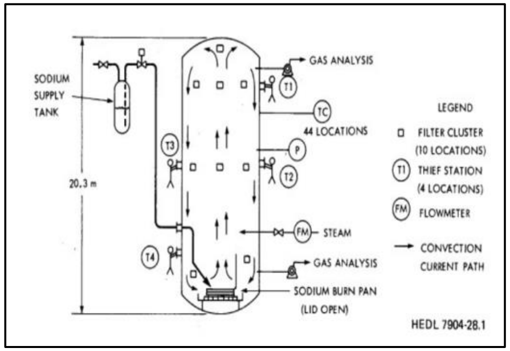
- A number of reactions have been considered:
  - $\mathrm{Na(l) + H_2O\ (l)\ \rightarrow NaOH(a) + \frac{1}{2}H_2}$
  - $\mathrm{2\ Na(g,l) + H_2O\ (g,l)\ \rightarrow Na_2O(a) +\ H_2}$
  - $\mathrm{2\ Na(g,l,a) + \frac{1}{2}O_2\ or\ O_2 \rightarrow Na_2O(a)\ or\ Na_2O_2(a)}$
  - $\mathrm{Na_2O_2(a) + 2\ Na(g,l) \rightarrow 2\ Na_2O(a)}$
  - $\mathrm{Na_2O(a) + H_2O\ (g,l)\ \rightarrow 2NaOH(a)}$
  - $\mathrm{Na_2O_2(a) + H_2O\ (g,l) \rightarrow 2NaOH(a) + 0.5O_2}$
- Kinetics of atmosphere gases are not explicitly modeled.
- All these reactions are assumed to occur in hierarchal order:
  - In the order listed above
  - By location of reactions
    - Atmosphere(g), aerosol, surfaces (i.e., HS)
- Outputs
  - Reaction number, reaction energy, byproducts (Na classes, $H_2$), gas and liquid consumed (Na, $H_2O$, $O_2$)

# AB1/AB5

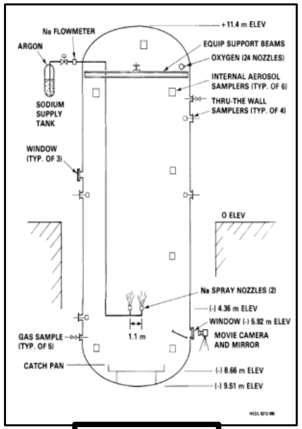
Validation

- Performed at Containment Systems Test Facility at Hanford Engineering Development Laboratory
  - AB1 – 1979
  - AB5 – 1983
- Experiments investigated aerosol behavior under liquid metal fast breeder reactor accident conditions
  - Provided experimental basis for evaluating adequacy of aerosol behavior codes
- Aerosols generated by sodium fires
  - AB1 – pool fire
  - AB5 – spray fire





AB1



AB5

# Other MELCOR Containment Models

## Description

- Two models developed for ESBWR but applicable to other advanced designs
- Passive Containment Cooling System (PCCS)
  - Allows input of performance data
    - Flow capacity versus ΔP
    - Efficiency versus non-condensable fraction
    - Efficiency versus absolute pressure
- Isolation condenser (ICS)
  - Allows input of performance data
    - Flow capacity versus ΔP
    - Efficiency versus non-condensable fraction
    - Efficiency versus absolute pressure
- Computationally efficient versus first principle calculations using CVH/FL/HS
  - Require performance data

# MELCOR Validation/Benchmark Reports

Validation

Tills, J., et al., “An Assessment of MELCOR 1.86: Design Basis Accident Tests of the Carolinas Virginia Tube Reactor (CVTR) Containment (Including Selected Separate Effects Tests),” SAND2008-1224, Sandia National Laboratories, Albuquerque, New Mexico, February, 2008.
*This report documents MELCOR code (Version 1.8.6) calculations for simulating the design basis accident tests performed in the CVTR containment facility. Additionally, a number of selected separate effects tests that emphasize phenomena occurring within the CVTR facility are calculated with the MELCOR code.*

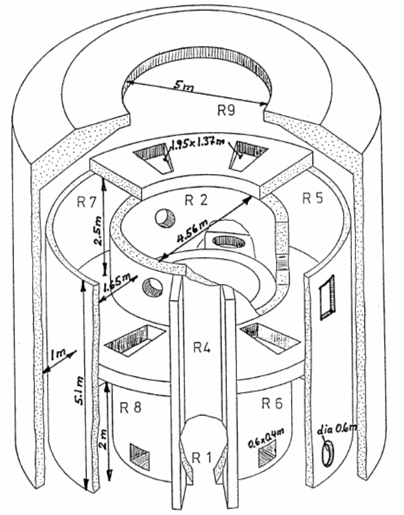
Tills, J., et al., “Application of the MELCOR Code to Design Basis PWR Large Dry Containment Analysis,” SAND2009-2858, Sandia National Laboratories, Albuquerque, New Mexico, May, 2009.
*This report documents MELCOR code demonstration calculations for postulated design basis accident with PWR large-dry containments. These calculations are compared to other calculations documented for the CONTAIN code. Appendices include a description of a containment blowdown model for short-term response during LOCA events and fan cooler performance modeling during design basis accident conditions.*

# DEMONA

- The DEMONA-B3 test was performed in the Battelle Model Containment (BMC) facility in Frankfurt, Germany
  - Examines containment-building response to severe accident conditions
  - Emphasis on characterizing the depletion rate of aerosols under varying humidity and thermal-hydraulic conditions
- Test B3 used non-hygroscopic aerosols
  - Aerosol injection rate = 3.575 g/s (215 g/min)
  - $SnO_2$/Sn molecular weight ratio of 1.27
  - Aerosol injection estimated to be log-normal distribution with 0.35 µm MMD and standard deviation of 2

# DEMONA

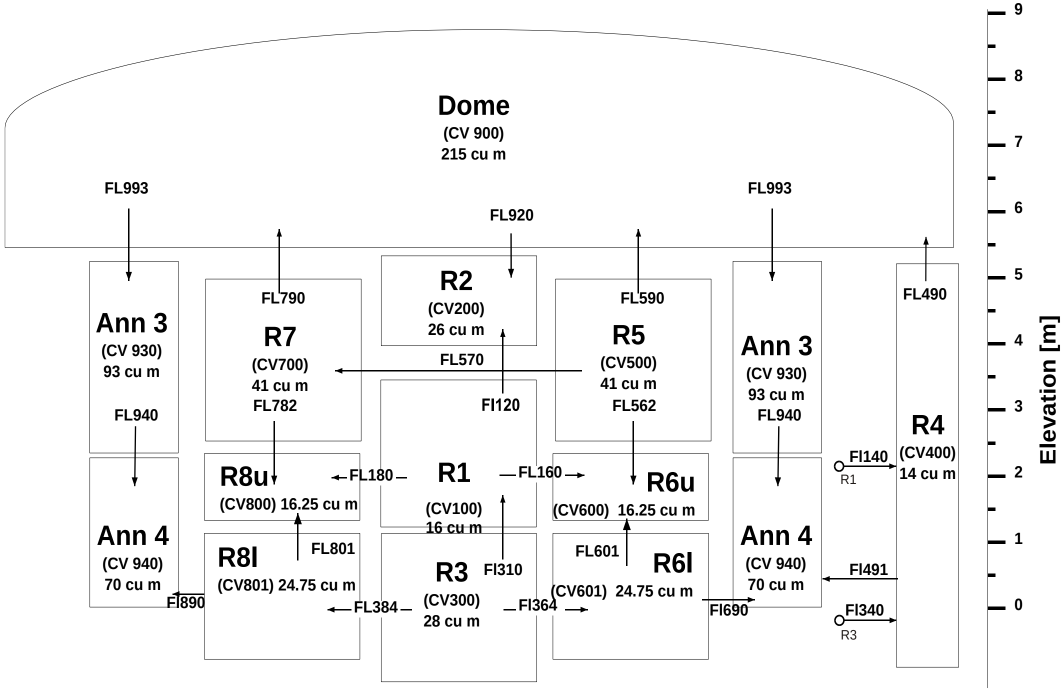
- Test B3 was conducted over a period of 3 days in 1986
    - Phase 1: purge air out to achieve a pure steam atmosphere (0.4-7.1 h)
    - Phase 2: Inject steam over 2 days to heat up BMC structure, at constant 1.7 bar
    - Phase 3: Hot air and aerosol injected from 48.4 to 49.3 h, raising the pressure to 3 bar (partial pressures, air 1.3 bar, steam 1.7 bar, & peak aerosol concentration was 9 g/m$^3$
    - Phase 4: Aerosol depletion 49.3-71.1 h
    - Phase 5: Cooldown (this was ignored in modeling)



# DEMONA

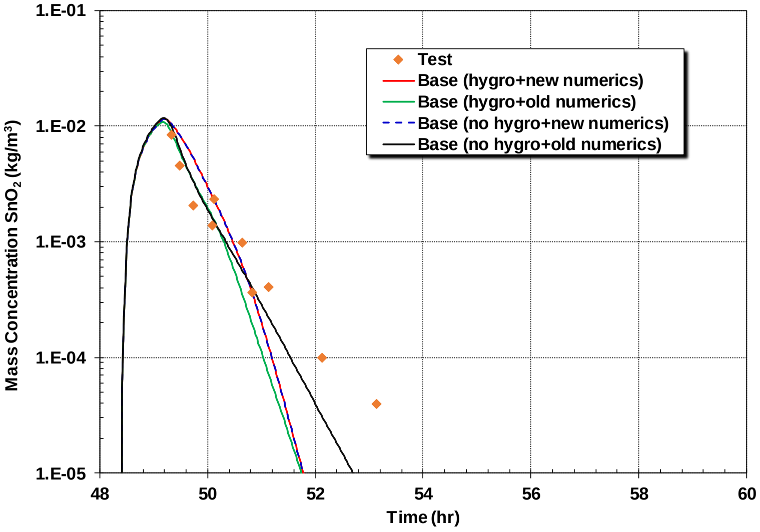
Validation

- MELCOR Nodalization



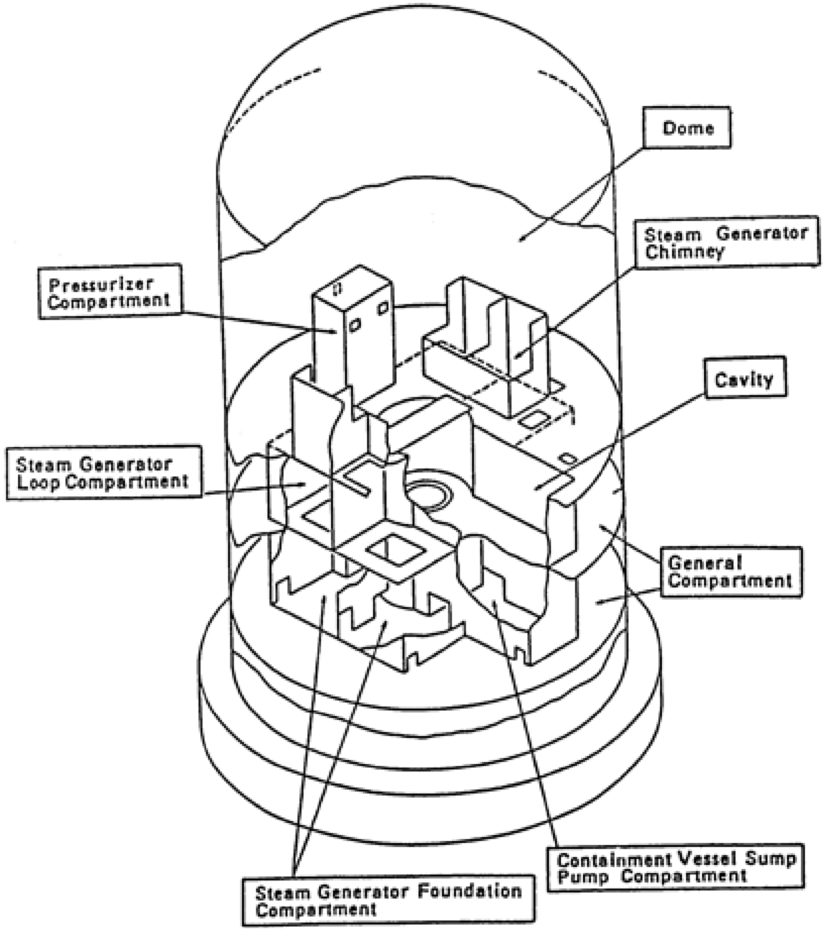
# DEMONA

- Base case and sensitivities
  - With and without new aerosol physics
  - With and without hygroscopic model



# NUPEC M-7-1, M-8-1, and M-8-2

- Validation objectives
  - Pressure response;
  - Temperature distribution and stratification
  - Hydrogen mixing
  - Spray modeling
  - Film Tracking Model
- ¼ Scale Containment
  - 10.8 m OD domed cylinder,
  - 17.4 m high
  - 25 interconnected compartments (28 total)
- Sprays
  - M-8-1 No Sprays
  - M-7-1 and M-8-2 Sprays modeled



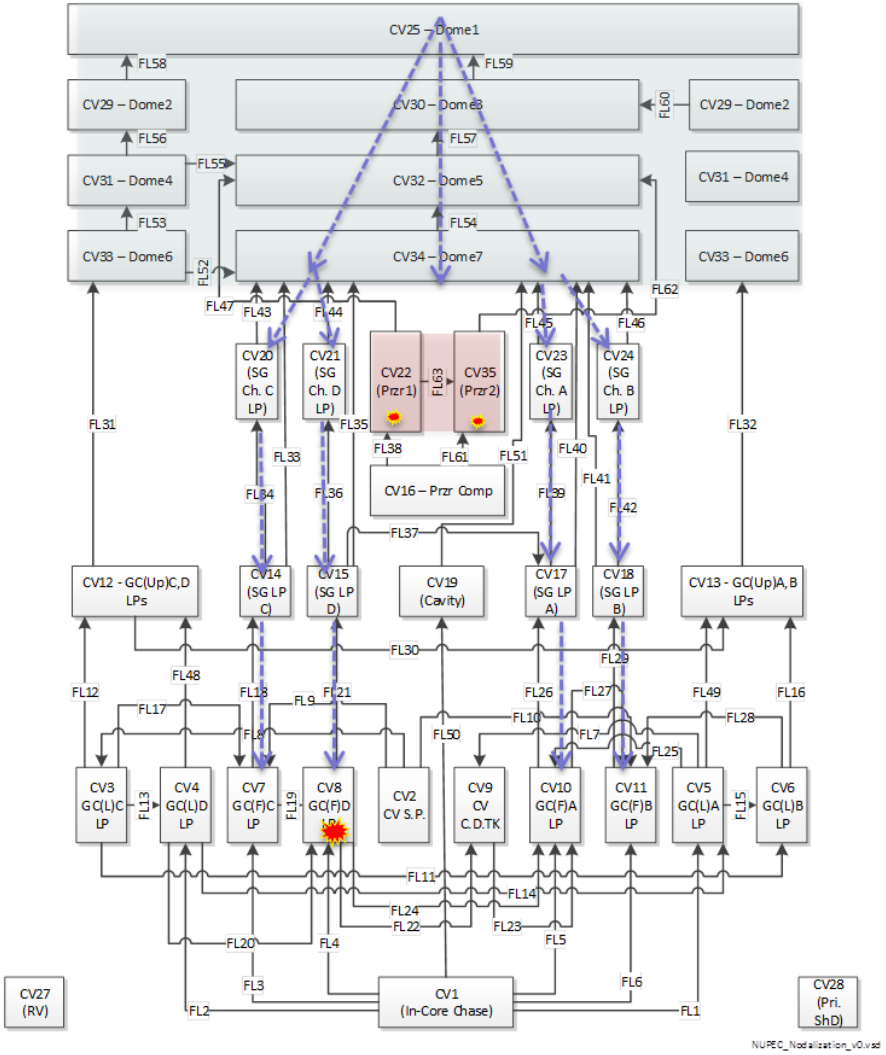
# NUPEC Tests

| Test | Injection Location | Initial Conditions | Relative Humidity | Helium Source | Steam Source | Containment Sprays |
|---|---|---|---|---|---|---|
| M-7-1 | Bottom of SG Comp D (8) | 343 K, 146 kPa | 0.95 | 0→0.03 kg/s→0<br>283 K | 0.08 kg/s→0.03 kg/s<br>383 K | 19.4 $m^3/s$<br>313 K |
| M-8-1 | Upper Pressurizer Comp (22) | 303 K, 101 kPa | 0.7 | 0.027 kg/s<br>283 K | 0.33 kg/s,<br>388 K | *None* |
| M-8-2 | Upper Pressurizer Comp (22) | 343 K, 146 kPa | 0.95 | 0→0.03 kg/s→0<br>283 K | 0.08 kg/s→0.03 kg/s<br>363 K | 19.4 $m^3/s$<br>313 K |

# NUPEC MELCOR Nodalization

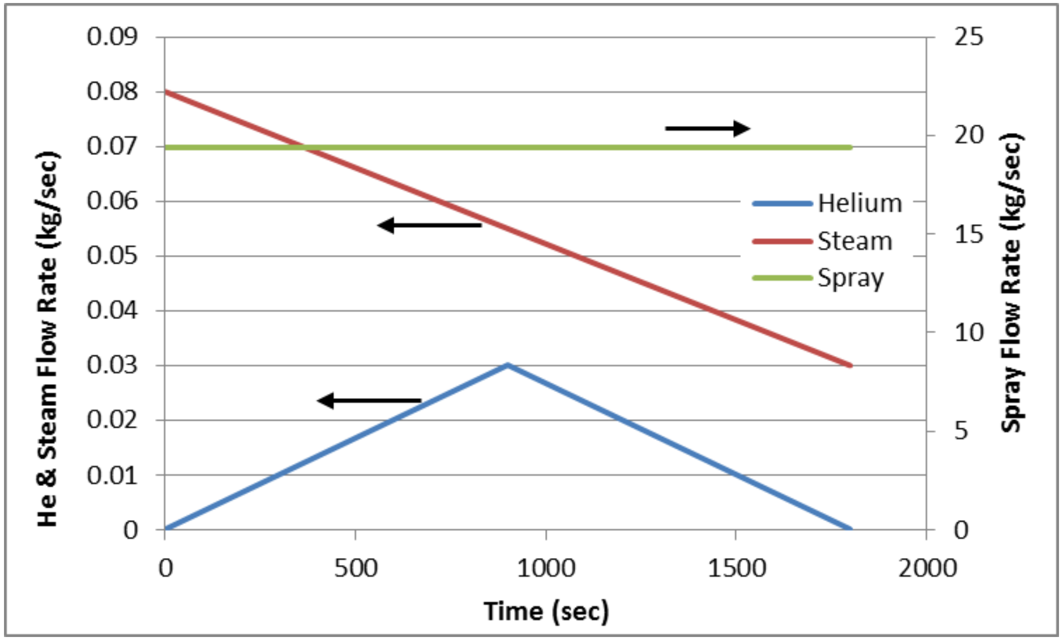
Validation

- Total of 35 CVs
  - Dome compartment subdivided into 7 CVs (green)
    - Allows convection loops
  - Upper pressurizer subdivided into two CVs (red)
    - Allows circulation from upper pressure compartment to lower compartment (dead end)
  - All other compartments represented by a single CV
- M-8-1 & M-8-2 He source in Pressurizer Compartment (CV 22 and CV 35)
- M-7-1 He source in CV8
- Spray junctions (M-8-2) shown by dashed arrows
  - Sprays not active in M-8-1



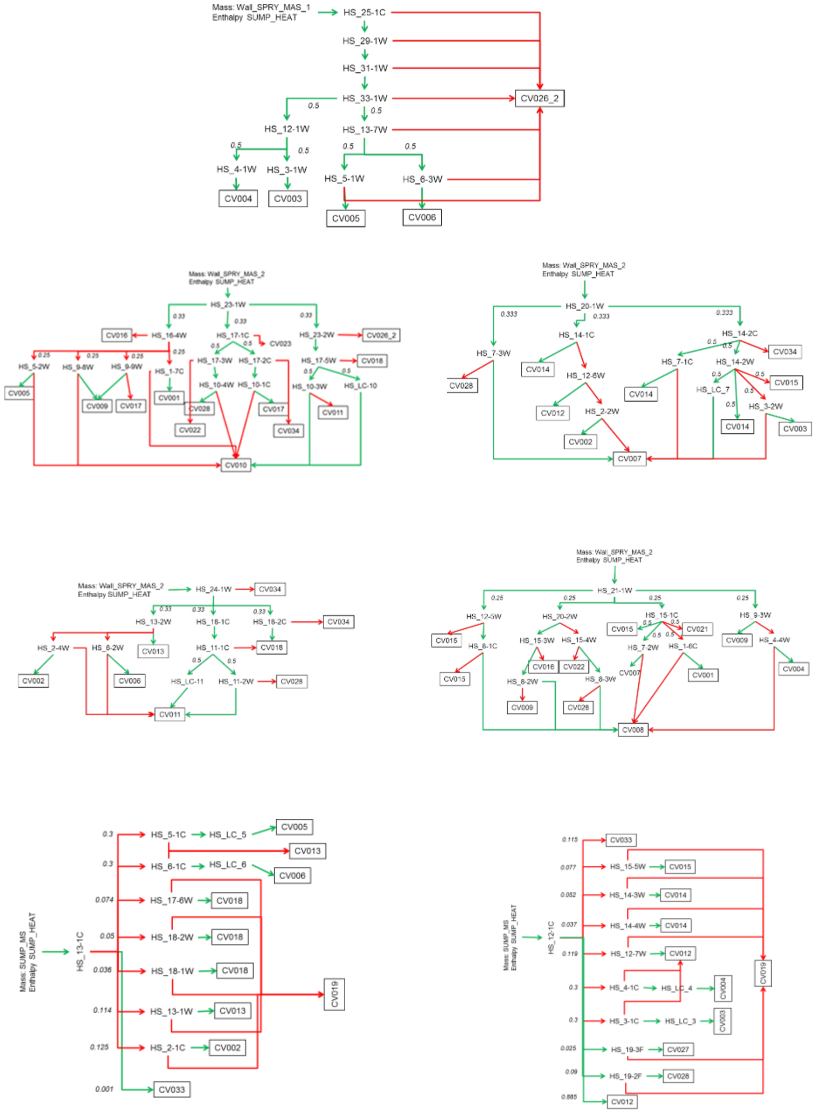
# He, Steam, and Spray Sources

- Steam released into a compartment to simulate break of a steam generator system. Total helium volume was decided by volumetric scaling of hydrogen release from 10% Zr-H2O reaction
  - CVH mass and energy sources in a CV
- At the same time, containment spray was activated to simulate the impact of spray water on mixing.



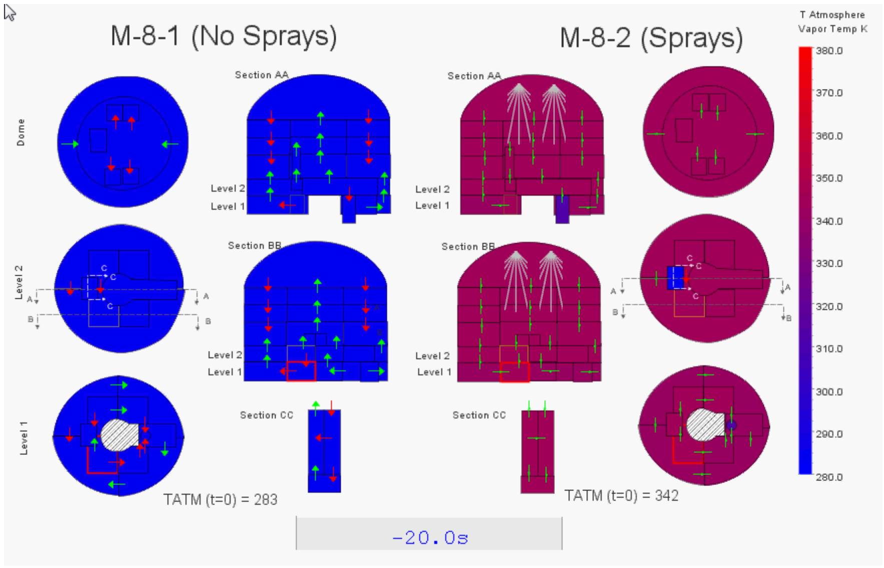
# HS Film-Tracking Networks

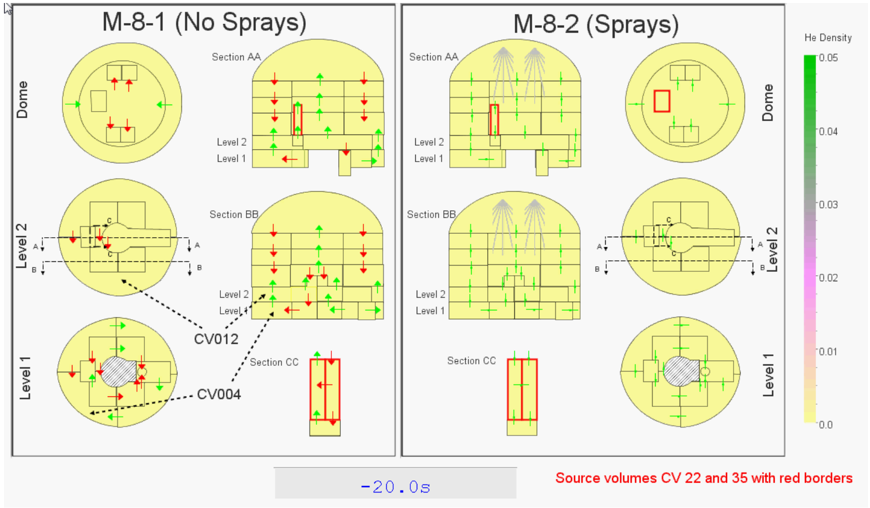
- Spray water is diverted onto seven separate film flow networks
  - Allows flow down each of the four steam generator compartments
  - Also models water draining down the containment walls from the dome
- Motivation: Since the heat structure film temperature and the spray temperature were close, it was expected that this model would better represent the uniform cooling of both structures and gases observed in the test



# Temperature and He Concentration Distributions

- SNAP representation based on MELCOR nodalization and NUPEC drawings.
- Temperature stratification occurs for M-8-1
  - No sprays
- Enhanced mixing for M-8-2
  - Sprays active
- Similarly, stratification of helium in the upper dome is much more significant for M-8-1 than M-8-2
- Mixing is greater for central compartments where the spray is active and is less effective in outer, lower compartments



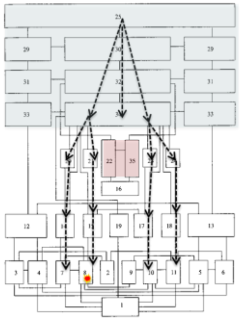
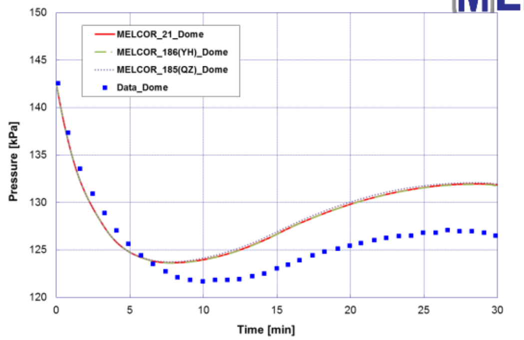
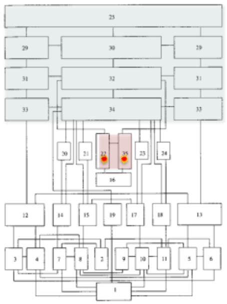
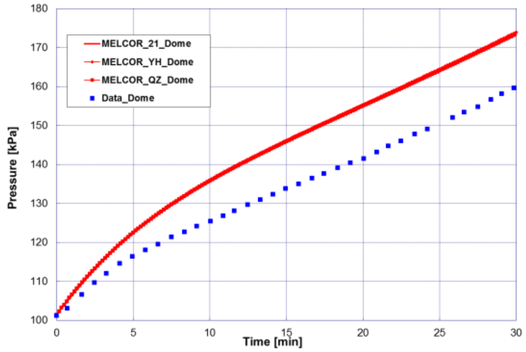
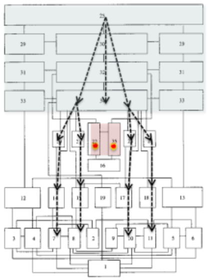
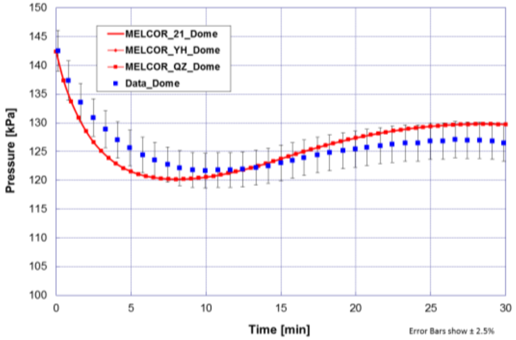


Source volumes CV 22 and 35 with red borders

# Pressure Response

Validation

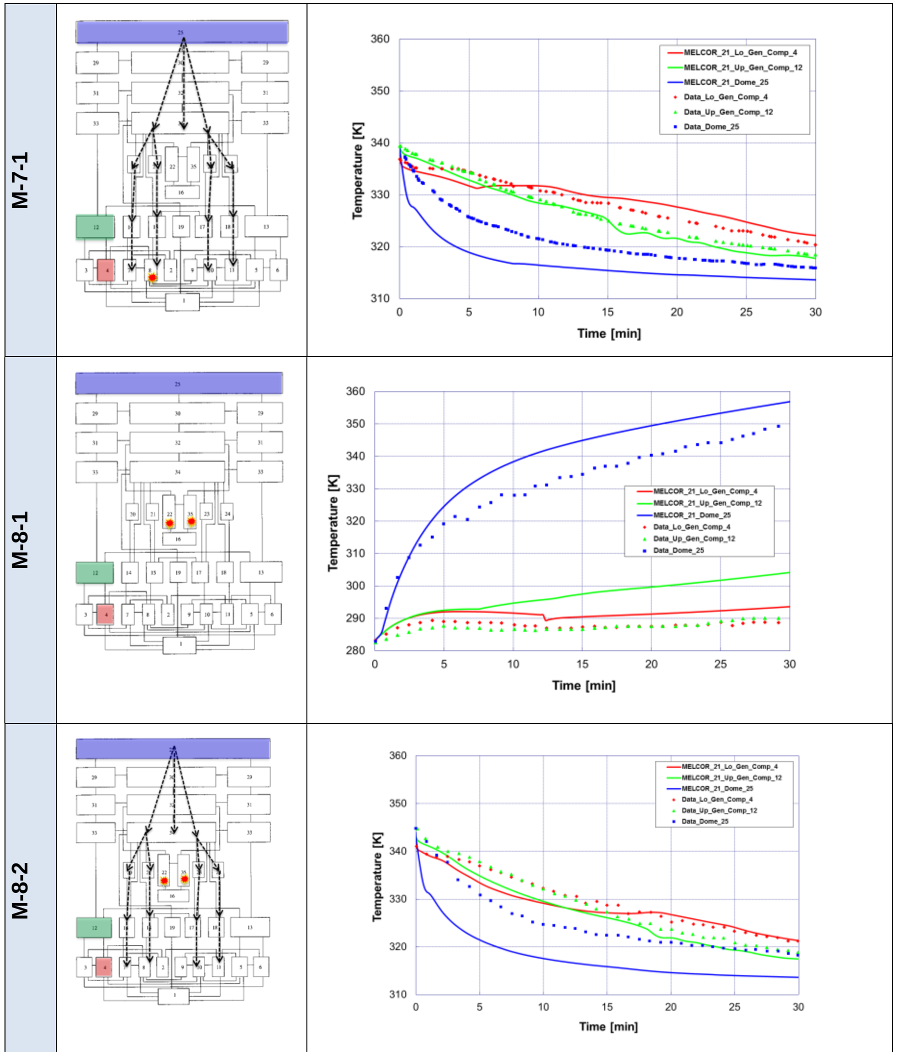
- Pressure calculated for M-7-1 exceeds experiment pressure
- M-8-1 without sprays shows excessive pressure

| | | |
|---|---|---|
| **M-7-1** |  |  |
| **M-8-1** |  |  |
| **M-8-2** |  |  |

# Temperature distribution  vert. distribution of general region

Validation

- Calculated temperature in dome is less than measured data for spray tests
  - Cooling from spray is overpredicted slightly by MELCOR
- Calculated temperature in dome is greater than data without sprays.
  - Stratification may be slightly overpredicted.

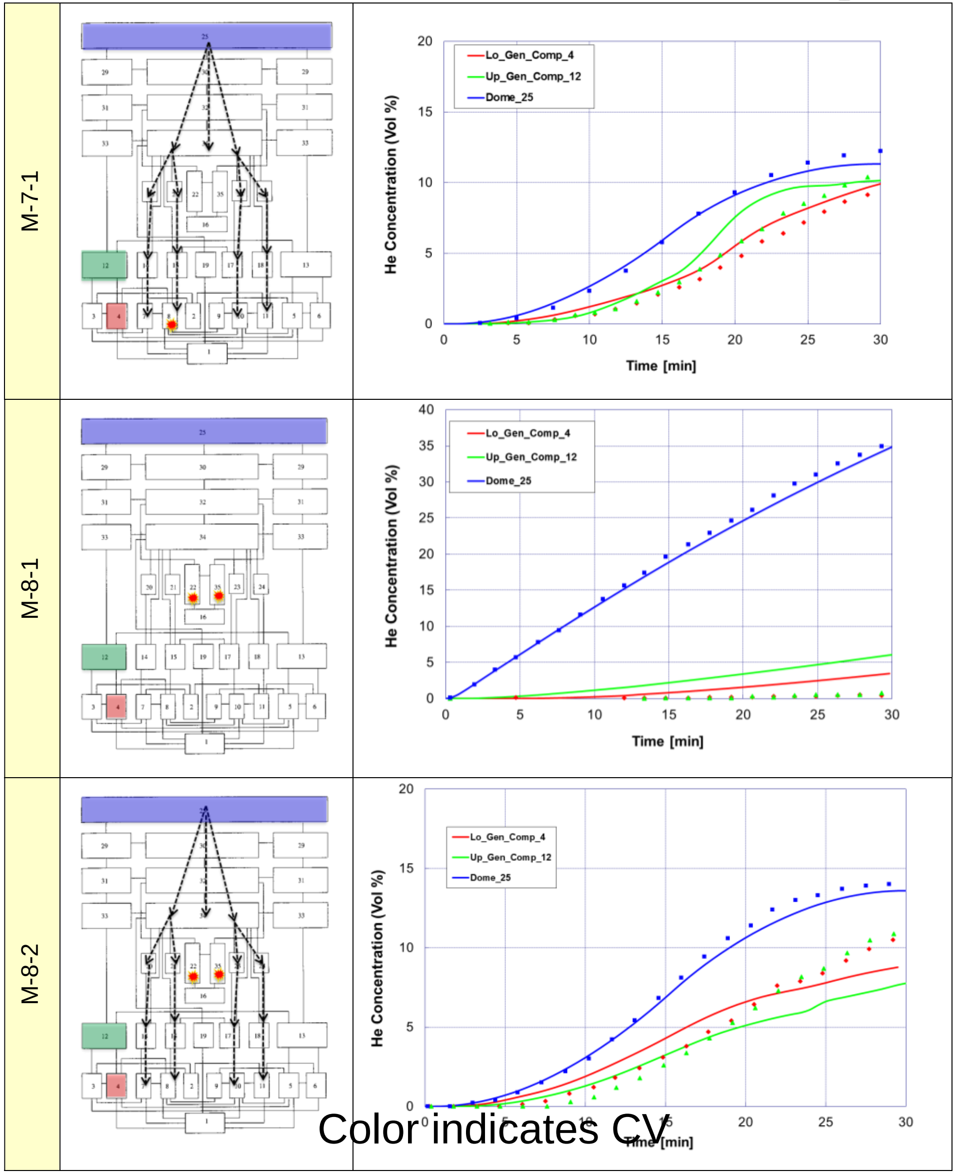


Color indicates CV

# He Concentrations for vert. distribution of general region

Validation

- Without sprays
  - MELCOR significantly overpredicts concentration in lower general compartments
- With sprays
  - He concentration well-predicted for all compartments

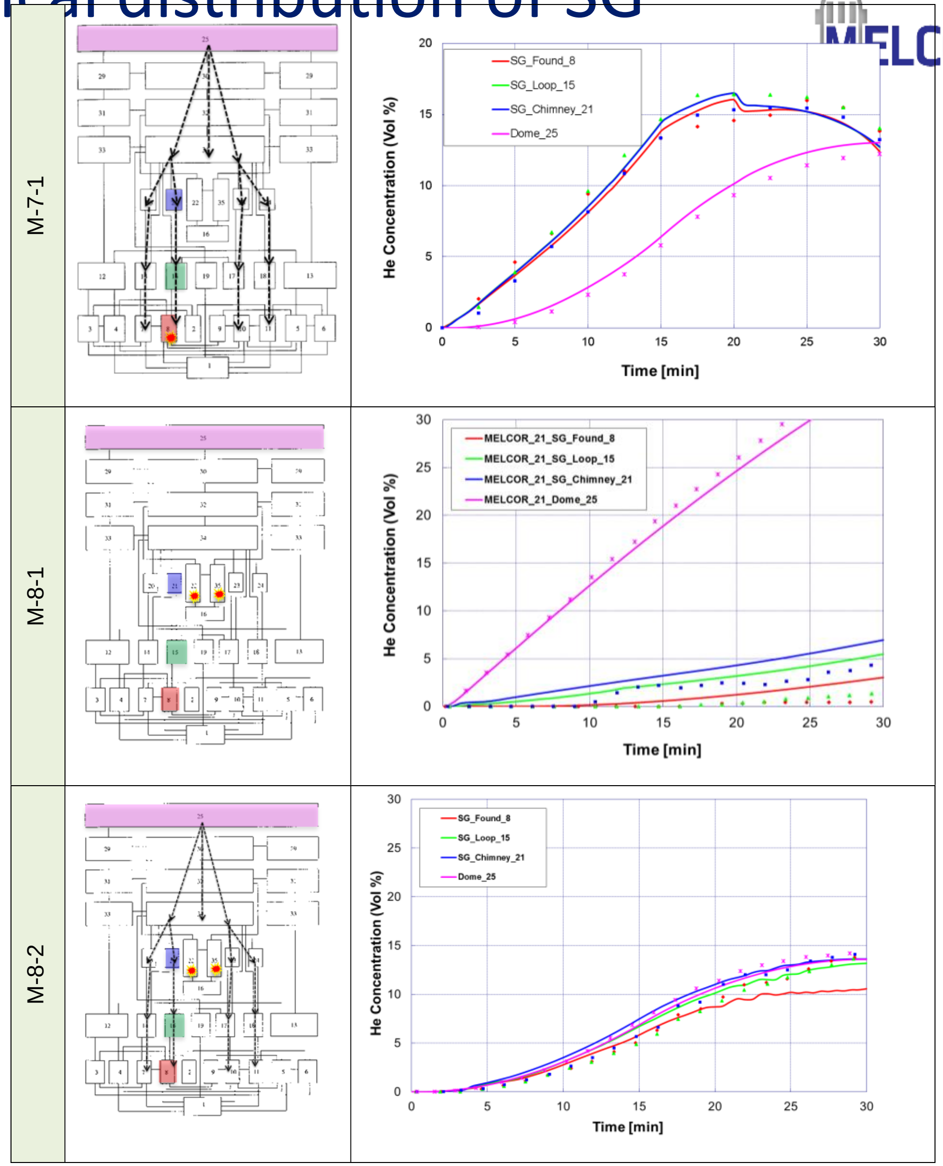


Color indicates CV

# He Concentrations for vertical distribution of SG loop D

Validation

- Concentration in dome is well-predicted for all cases
- M-7-1 shows underprediction of He in mid-level compartments for source in lower level
- Slight under-prediction of concentration for lower compartments in M-8-2 otherwise, well predicted

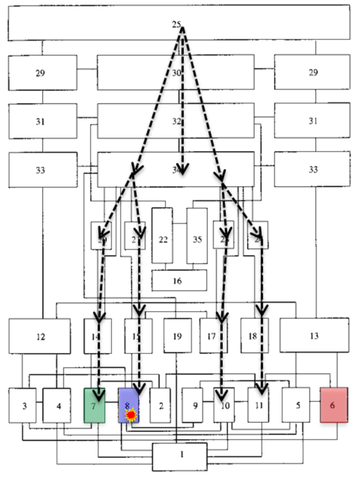
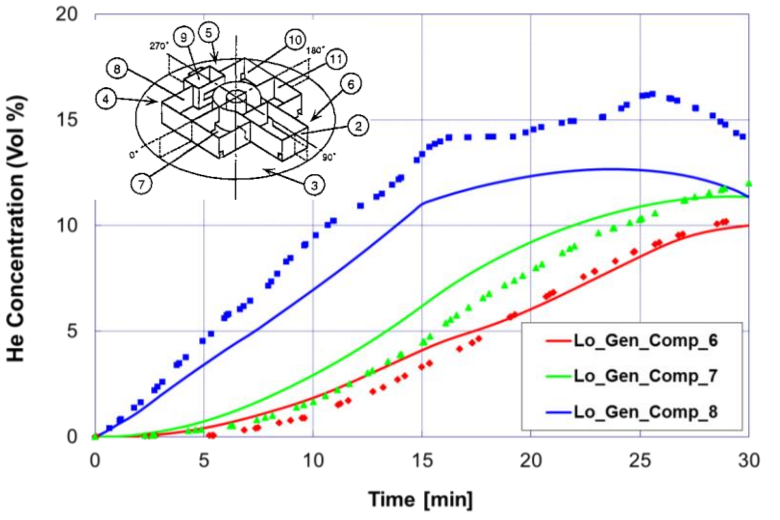


Color indicates CV

# He Concentrations for 1st floor horizontal distribution

- MELCOR predicts concentrations for all lower compartments with reasonable accuracy
- MELCOR predicts concentration in source cell well

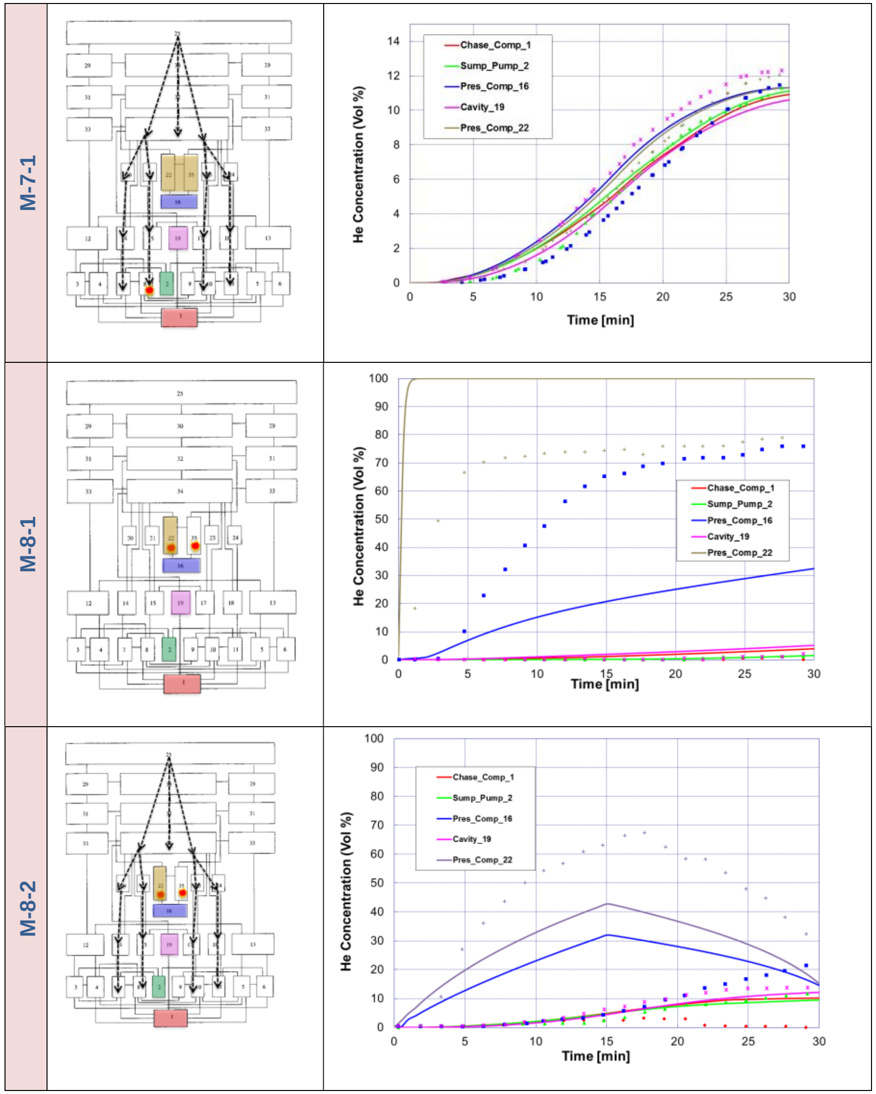
Validation

|  |  |  |
|---|---|---|
| M-7-1 |  |  |

# He Concentrations for vertical distribution of SG loop D

Validation

- Problems in calculating concentration in source volume and dead-end volume adjacent to source volume
- Best agreement in M-7-1 where He source was in a lower CV and sprays were active

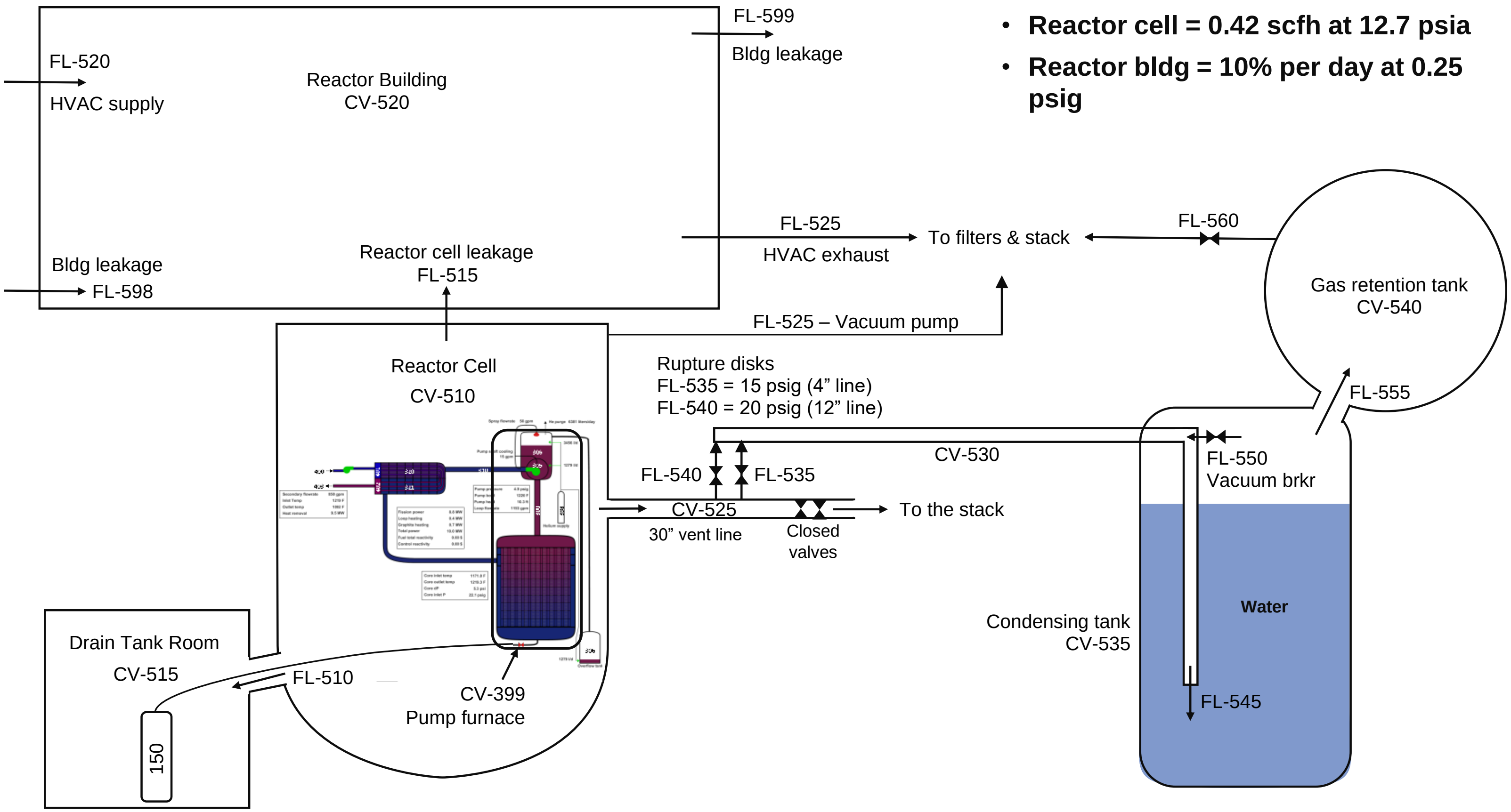


Color indicates CV

# MSRE MELCOR nodalization – reactor cell, condensing tank, and reactor building

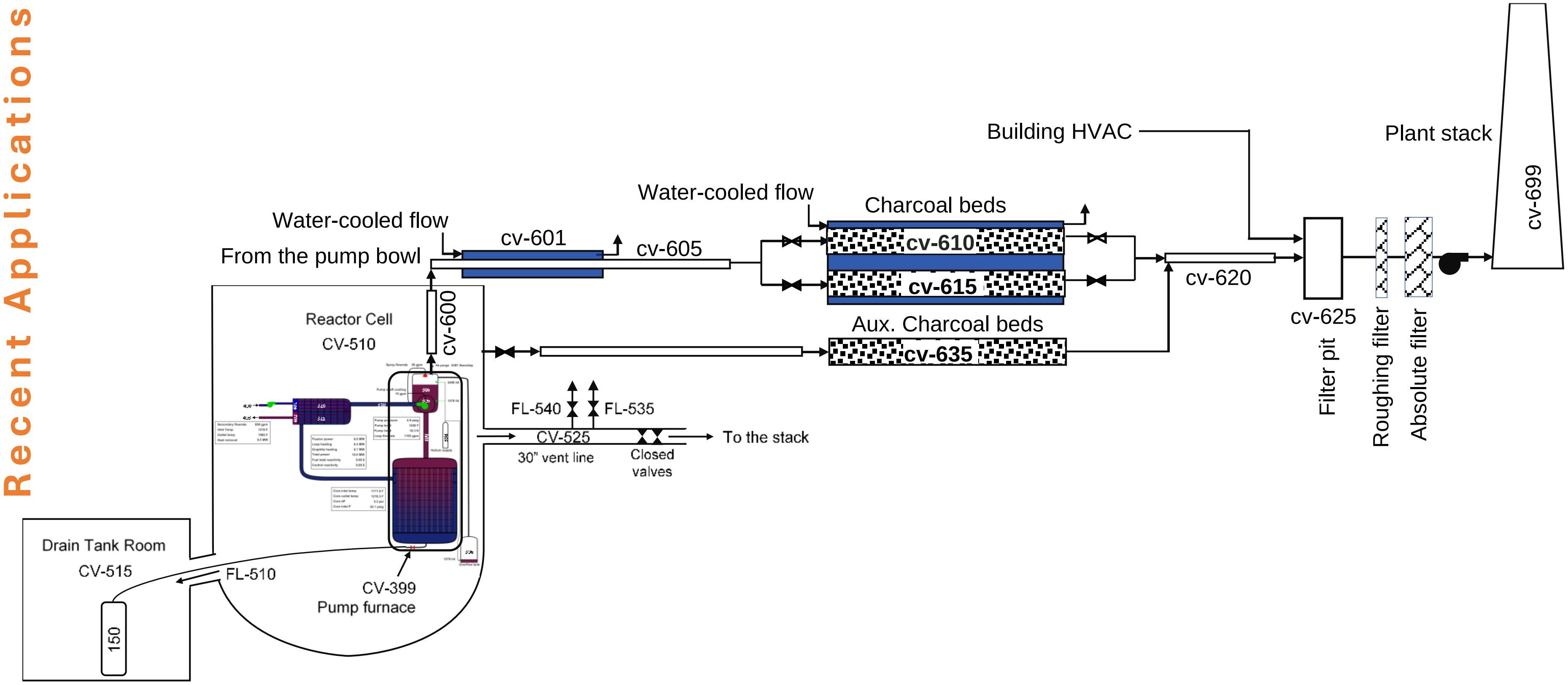
## Leakages

- **Reactor cell = 0.42 scfh at 12.7 psia**
- **Reactor bldg = 10% per day at 0.25 psig**

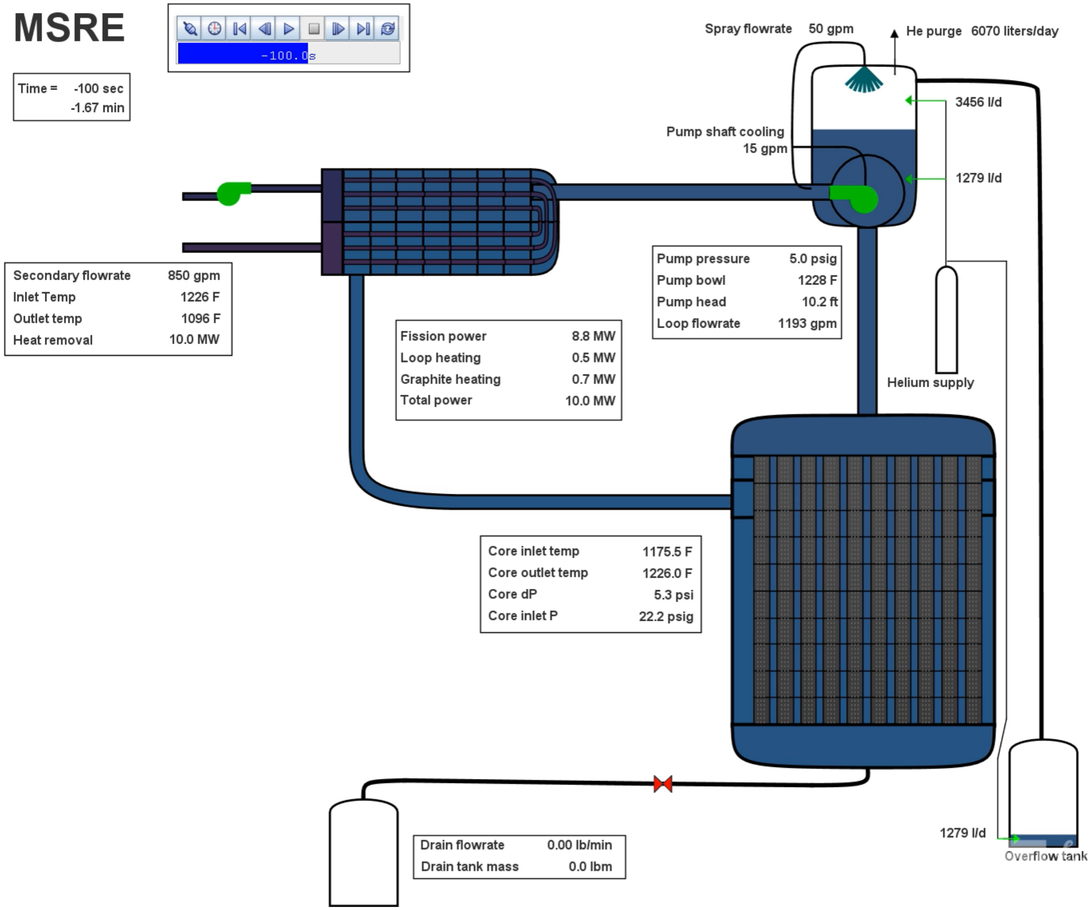


# MELCOR nodalization - offgas system

Recent Applications



# MCA1 salt spill base case – Primary System Response



| | |
|---|---|
| Time = | -100 sec |
| | -1.67 min |

| | |
|---|---|
| Secondary flowrate | 850 gpm |
| Inlet Temp | 1226 F |
| Outlet temp | 1096 F |
| Heat removal | 10.0 MW |

| | |
|---|---|
| Fission power | 8.8 MW |
| Loop heating | 0.5 MW |
| Graphite heating | 0.7 MW |
| Total power | 10.0 MW |

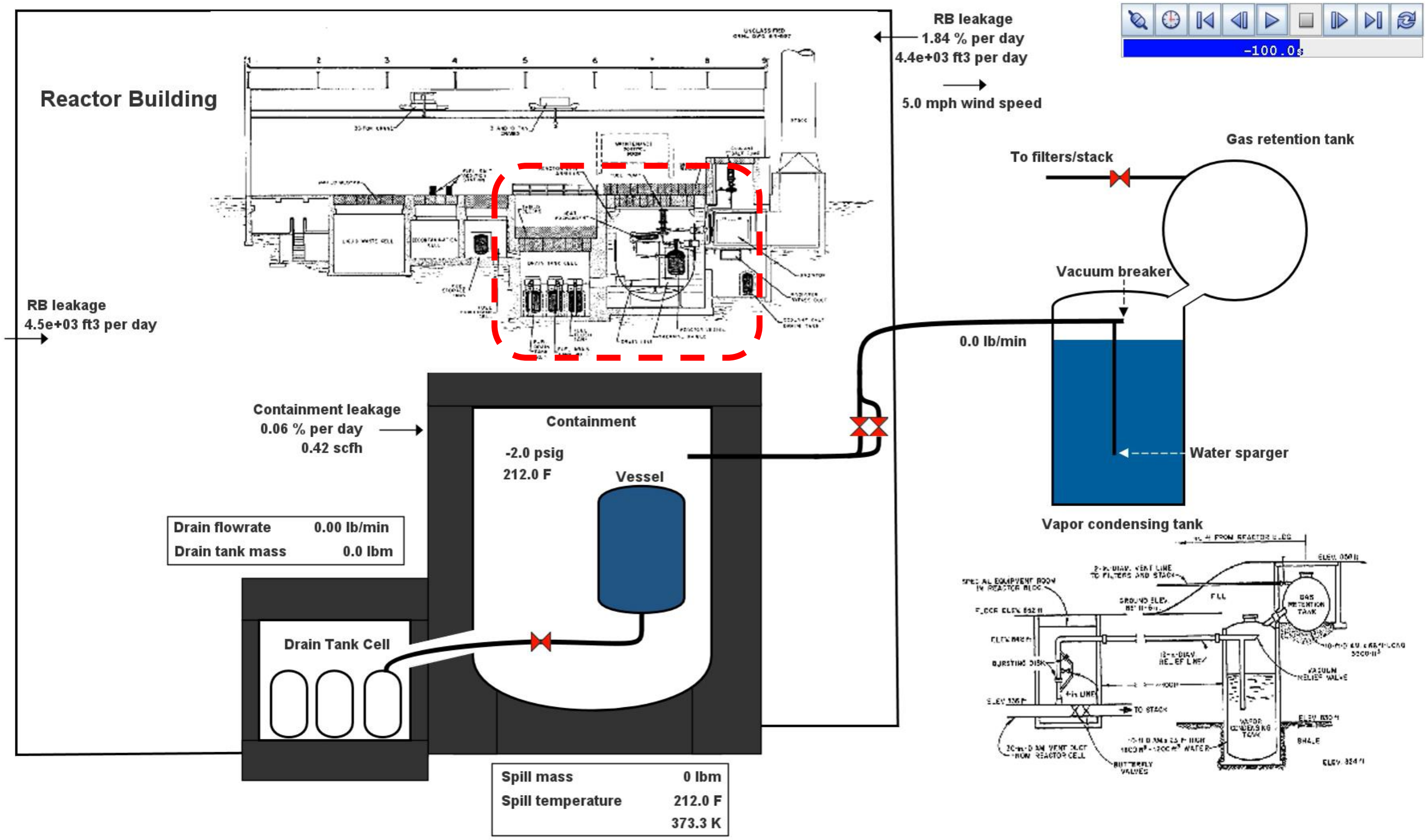
| | |
|---|---|
| Pump pressure | 5.0 psig |
| Pump bowl | 1228 F |
| Pump head | 10.2 ft |
| Loop flowrate | 1193 gpm |

| | |
|---|---|
| Core inlet temp | 1175.5 F |
| Core outlet temp | 1226.0 F |
| Core dP | 5.3 psi |
| Core inlet P | 22.2 psig |

| | |
|---|---|
| Drain flowrate | 0.00 lb/min |
| Drain tank mass | 0.0 lbm |

# MCA1 salt spill base case – Reactor Cell Response

Recent Applications



**Reactor Building**

RB leakage
1.84 % per day
4.4e+03 ft3 per day

5.0 mph wind speed

RB leakage
4.5e+03 ft3 per day

Containment leakage
0.06 % per day
0.42 scfh

To filters/stack

Gas retention tank

Vacuum breaker

0.0 lb/min

Water sparger

Vapor condensing tank

Containment

-2.0 psig
212.0 F

Vessel

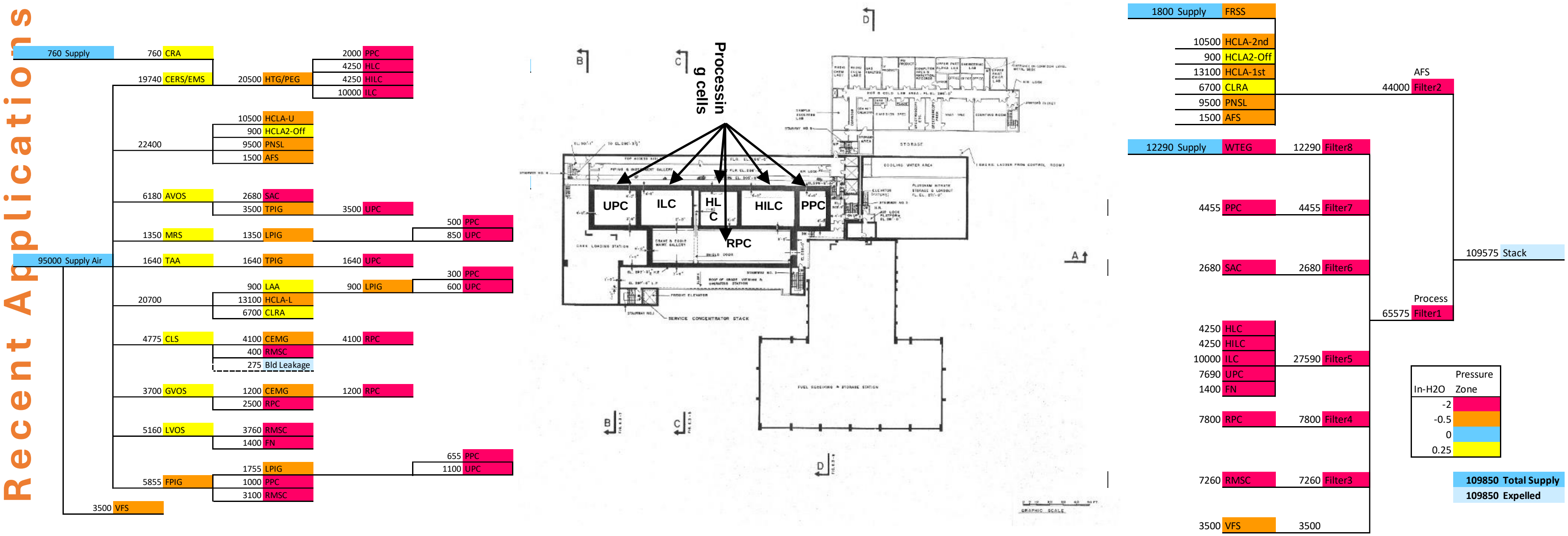
Drain Tank Cell

| | |
|---|---|
| Drain flowrate | 0.00 lb/min |
| Drain tank mass | 0.0 lbm |

| | |
|---|---|
| Spill mass | 0 lbm |
| Spill temperature | 212.0 F<br>373.3 K |

# Reprocessing Facility
# An example on a complex ventilation system

Recent Applications



760 Supply
760 CRA
19740 CERS/EMS
20500 HTG/PEG
2000 PPC
4250 HLC
4250 HILC
10000 ILC
22400
10500 HCLA-U
900 HCLA2-Off
9500 PNSL
1500 AFS
6180 AVOS
2680 SAC
3500 TPIG
3500 UPC
1350 MRS
1350 LPIG
500 PPC
850 UPC
95000 Supply Air
1640 TAA
1640 TPIG
1640 UPC
20700
900 LAA
900 LPIG
300 PPC
600 UPC
13100 HCLA-L
6700 CLRA
4775 CLS
4100 CEMG
4100 RPC
400 RMSC
275 Bld Leakage
3700 GVOS
1200 CEMG
1200 RPC
2500 RPC
5160 LVOS
3760 RMSC
1400 FN
5855 FPIG
1755 LPIG
655 PPC
1100 UPC
1000 PPC
3100 RMSC
3500 VFS

Processing cells
UPC
ILC
HLC
HILC
PPC
RPC

1800 Supply FRSS
10500 HCLA-2nd
900 HCLA2-Off
13100 HCLA-1st
6700 CLRA
9500 PNSL
1500 AFS
AFS
44000 Filter2
12290 Supply WTEG
12290 Filter8
4455 PPC
4455 Filter7
109575 Stack
2680 SAC
2680 Filter6
Process
65575 Filter1
4250 HLC
4250 HILC
10000 ILC
27590 Filter5
7690 UPC
1400 FN
7800 RPC
7800 Filter4
7260 RMSC
7260 Filter3
3500 VFS
3500

| In-H2O | Pressure Zone |
|---|---|
| -2 | 🟥 |
| -0.5 | 🟧 |
| 0 | 🟦 |
| 0.25 | 🟨 |

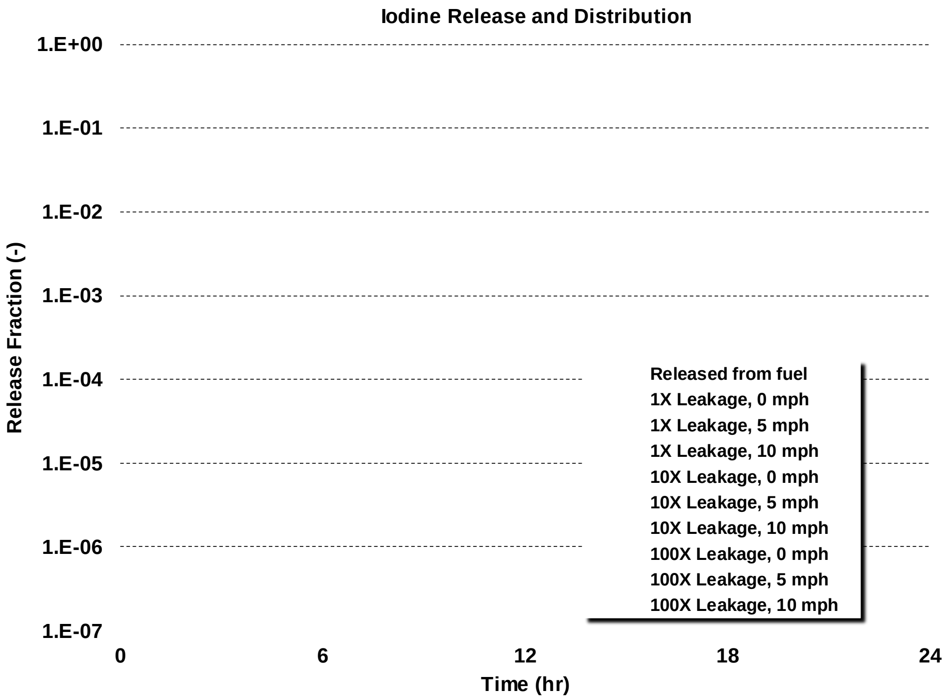
**109850 Total Supply**
**109850 Expelled**

# An example with Wind Effects

Recent Applications

**A series of calculations were performed to investigate the impact of an external wind**

- External wind effects are included in DOE facility safety analysis where there also are not strong driving forces
  - Wind increases building infiltration and exfiltration
  - Upwind and downwind leakage pathways
- Wind effects are modeled as a Bernoulli term
  - $dP = \frac{1}{2}\rho C_p v^2$
  - ASHRAE building wind-pressure coefficients



External wind modeling ref:
"MELCOR Computer Code Application Guidance for Leak Path Factor in Documented Safety Analysis," U.S. DOE, May 2004.
Building wind pressure coefficients.
ASHRAE, 1977, Handbook of Fundamentals, American Society of Heating, Refrigerating and Air-Conditioning Engineers, Inc, 1997.

# End Containment Models