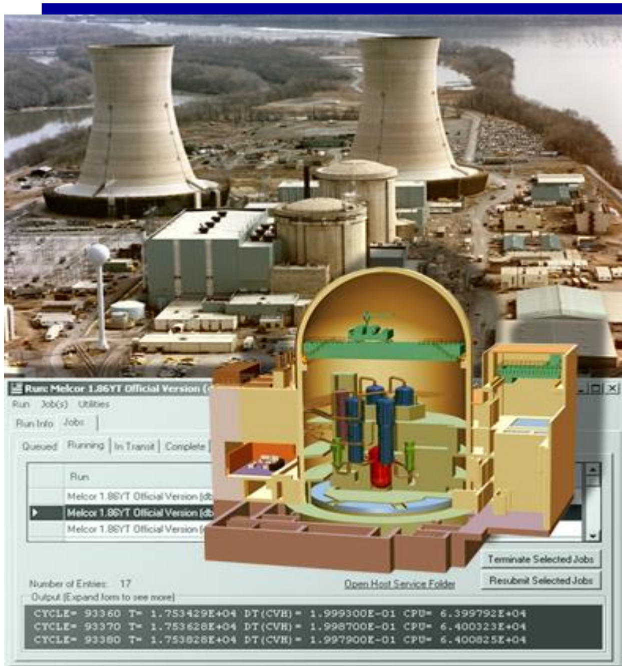

Class Chemistry and Chemisorption in the RN Package

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RN Class Chemistry and Chemisorption

- The following topics are discussed
  - Class Chemistry Model
    - May be used to simulate adsorption, chemisorption, and reactions for **Vapors**
      - Limits classes for consideration (available vapor mass is dominantly Class 2, 4, 16)
    - General class reaction and transfer modeling
    - User may specify reaction rate constant or deposition velocity
  - Chemisorption Model
    - Rate equations for vapor species

Class Chemistry Modeling

- Class reactions
  - First-order reversible reaction
  - Gas-phase in State C to C_1 on a surface (mass transport)

$$\frac{dM_c}{dt} = -\left(\frac{k_m \; A \; / \; V}{k_m A \; / \; V + k_f} \right) \left(k_f M_C - k_r M_{C1} \right)$$

where

k_m	= mass transfer rate constant for the process, based on the mass transfer coefficient calculated by the HS Package, (m/s)
k_f	= forward reaction rate constant from user input, (s^{-1})
k_r	= reverse reaction rate constant from user input, (s^{-1})
A / V	= surface-to-volume ratio, where the surface area is that for the reaction and the volume is that of the control volume (m^{-1}).

  - Deposition velocity

$$\frac{dM_C}{dt} = -V_d (A / V) C = -\frac{dM_{C1}}{dt}$$

Class Chemistry Modeling

- Only function in user-specified control volumes
- Surfaces that may contribute: Heat structures, pools, and aerosols
  - Heat structure may be disabled in case of film through a flag
- Reaction energies may also be specified
  - Energy is deposited to the HS, pool, or atmosphere , i.e., the RN class host

Class Chem. – Class Transfers

- No checks
  - Transfers are arbitrarily imposed by the user
  - Class and locations may be changed for aerosols and/or vapors assuming fast reaction

$$M_{from,\, t+\Delta t} = M_{from,\, t} - \frac{dM}{dt}\Delta t$$

$$M_{to,\; t+\Delta t} = M_{to,\, t} + \frac{dM}{dt}\Delta t$$

  - Example of arbitrary nature:
    - Class A in pool becomes Class B on given HS at a set rate

Input Example

CsI(g) → *CsI(ad)*	rate constant for adsorption is supplied th[illegible] input
CsI(ad) → *CsOH(ad)* + *HI(s)*	instantaneous and complete transfer between classes when water is present. **Note that the water mass is not included in the model; water mass is not explicitly conserved.**
CsOH(g) → *CsOH(ad)*	rate constant for adsorption supplied or condensation limited
CsOH(ad) → *CsOH(g)*	reaction with zero rate constant below T_1
	positive value or instantaneous above T_1
HI(s) ↔ *HI(g)*	controlled by condensation/evaporation

Chemisorption Model

- Only function with Vapors
- 6 chemisorption classes

$$\frac{dM_{ij}}{dt} = A_i k_{ij} C_j \qquad (2.134)$$

M_{ij} = mass of species j chemisorbed on surface i (kg)
A_i = area of surface i (m^2)
k_{ij} = chemisorption coefficient of species j on surface i (m/s)
C_j = concentration of species j in atmosphere (kg/m^3)

The mass chemisorption coefficient k_{ij} is temperature dependent and is given as

$$k_{ij} = a_{ij} e^{-E_{ij}/RT_i} \qquad (2.135)$$

where

a_{ij} = chemisorption coefficient for species j on surface type i (m/s)
E_{ij} = activation energy for species j on surface type i (J/kg)
T_i = temperature of surface i (K)
R = universal gas constant (8314 J/kg-K)

Chemisorption Model - Defaults

Species j	Surface i	A_{ij} (m/s)	E_{ij} (J/kg)	Reference
CsOH	Stainless Steel	0.139	5.96e7	Vine[40]
CsOH	Inconel	0.035	5.95e7	*
CsI	Stainless Steel	2.0e-7	0.0	Sallach[41]
CsI	Inconel	2.0e-6**	0.0	Sallach[41]
HI	Stainless Steel	5.5e-7	2.49e7	Williams[42]
I_2	Stainless Steel	9.0e-10	3.39e7	Williams[42]
Te	Stainless Steel	0.0	-	Sallach[43]
Te	Inconel	0.0	-	Sallach[43]

* Estimated from Sabathier[44] and Elrick[45] data.
** Cesium retained, Iodine released

CA Class	Chemisorption Reaction	Radionuclide Class
1	CsOH on SS	CsOH (2)
2	CsOH on Inconel	
3	CsI on SS	CsI (16)
4	CsI on Inconel	
5	HI on SS	I_2 (4)
6	I_2 on SS	I_2 (4)

Chemisorption Model

- While Inconel is present, a default material must be defined in the material package before it can be used
  - So Inconel is ready, but not available
  - User specified material doesn't function with the chemisorption
    - If user defines a unique stainless steel, they may wish to consider redefining the default stainless steel to maintain chemisorption

CsI Chemisorption

- CsI upon chemisorption is results in CsOH being augmented and iodine mass being released as I_2 (Class 4).
  - –CsI mass will report zero chemisorption mass due to this transfer of mass to CsOH (Class 2).
  - –CsOH must be active to receive mass.

Questions