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MELCOR

MELCOR Workshop – SMR Containment III

Selected Topics in RN Transport

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U.S.NRC

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Overview

High-level description of RN1/RN2 and MAEROS

The MAEROS removal/deposition sectional coefficient and “deposition kernel”

- Gravitational settling
- Brownian diffusion
- Thermophoresis
- Diffusiophoresis
- Turbulent deposition
- Fallout (technically not a component of deposition kernel)

Aerosol growth (shrinkage) by condensation (evaporation) of water

Resuspension

Summary

RN1/MAEROS and RN2

The radionuclide (RN) package generally models behavior (release, transport, and interactions) of radionuclides

- Focused on *release* at EMUG '24 - fission product, structural, and class combination upon release
- Consider aspects of radionuclide *transport* with special attention to LWR SMR phenomena

RN consists of RN1 and RN2, and both have interactions with most every code package

- RN1 concerned mainly with intra-volume processes, generally computed before CVH/FL
  - Release/transport of fission product vapors/aerosols, certain non-radioactive vapors/aerosols, trace materials
  - Aerosol physics
    - Agglomeration/coagulation
    - Deposition
    - Fission product vapor and/or water vapor condensation/evaporation
    - Resuspension
    - Miscellaneous (user sources, fission product chemistry and vapor chemisorption, jet impaction, iodine)
- RN2 concerned mainly with inter-volume processes, generally computed with/after CVH/FL
  - Pool scrubbing, aerosol/vapor filters, spray scrubbing
  - Advection through FL's between CVs
  - Reconcile CVH "fog" to RN "water aerosol" (condensation/evaporation) when hygroscopic model inactive

RN1 entails the Multicomponent AEROSol (MAEROS) model

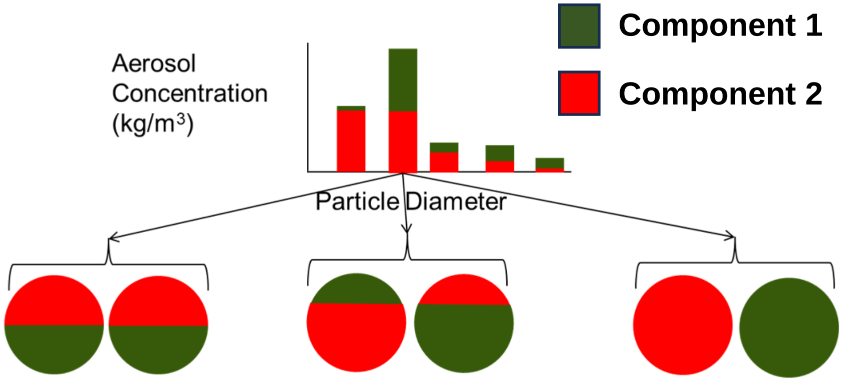
MAEROS

Multi-sectional, multi-component aerosol dynamics model to calculate component-wise aerosol size distribution as a function of time

- A “section” is a particle size bin or an aerosol size group based on particle mass
- A “component” is a “type of aerosol mass” or a “particular type of aerosol material”
- Each component has an independent “size distribution” – component mass distributed by section
  - According to the one size binning scheme defined at the outset of the calculation
    - Default: 10 sections - 0.1 μm and 50 μm - [0.1, 0.186, 0.347, 0.645, 1.20, 2.24, 4.16, 7.75, 14.4, 26.9, 50.0]
    - User definable (RN1_DIM, RN1_ASP)
  - Aerosol “chemical composition” is therefore characterized by section, i.e. the masses of the various components are known in each section, so that aerosol chemical composition varies by section
- All components must currently have the same material density (LWR applications usually 1000 kg/m^3)
- “Classes” represent a way of thinking about materials and map to components for MAEROS purposes
- Component mass comprised of classes mapped to it, and same size distribution in those classes

MAEROS tells:

- Only the mass of each component “in” the aerosol particles of each size bin
- Nothing about composition of any one particle



MAEROS

MAEROS solves for total aerosol mass per unit fluid (atmosphere) volume in section l at t

$$Q_l(t) = \sum_{k-1}^{s} Q_{l,k}(t)$$

Time-integrating rate equations for aerosol concentrations $Q_{l,k}(t)$ for each component k

- Complicated conservation statement (see RM)
- Every mechanism whereby $Q_{l,k}$ could increase or decrease due to:
  - Agglomeration/coagulation by Brownian diffusion, differential gravitational settling, and turbulence
  - Deposition by gravitational settling, Brownian diffusion, thermophoresis, diffusiophoresis, and turbulence
  - User-defined sources
- So-called sectional coefficients characterize the various agglomeration and deposition mechanisms
- Other phenomena impact aerosol size distribution and dynamics, but not formally integrated into the MAEROS solution framework (handled other ways in MELCOR implementation)
  - Resuspension
  - Fission product vapor and/or water vapor condensation/evaporation including the hygroscopic model
  - Miscellaneous (fission product chemistry and vapor chemisorption, jet impaction, iodine)

For LWR SMR, focus attention on:

- Deposition/removal sectional coefficients - $\overline{\mathfrak{R}}_{l,k}$ in the MAEROS equations for $\dot{Q}_{l,k}(t)$ (see RM)
- Resuspension
- Condensation/evaporation to/from aerosol particle surfaces

Deposition Kernel

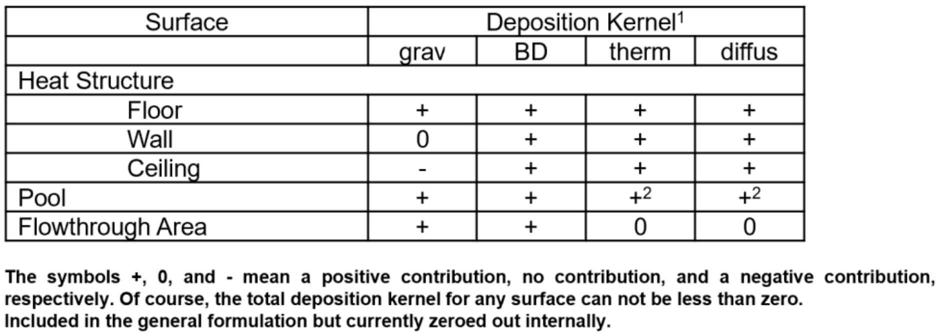
Require $\bar{\Re}_{l,k}$ [kg/m^3/s] i.e. the deposition section l coefficient for component k

Three “types” of surface in a CV for which MAEROS computes a deposition kernel

- Heat structure surface, where three distinct orientations (ceiling, wall, floor) are respected
- Pool surface
- Flow-through area with the open passage area regarded as a surface

Five possible contributors to $\bar{\Re}_{l,k}$, though not all are computed for all surfaces

- Gravitational settling on surface
- Brownian diffusion to surface
- Thermophoretic deposition on surface
- Diffusiophoretic deposition on surface
- Turbulent deposition on surface
  - Not computed unless RN1_TDS says so
  - Only possible for heat structure surfaces
- Fallout to/on surfaces is a related concept



Surface	Deposition Kernel[1]			
	grav	BD	therm	diffus
Heat Structure				
Floor	+	+	+	+
Wall	0	+	+	+
Ceiling	-	+	+	+
Pool	+	+	+[2]	+[2]
Flowthrough Area	+	+	0	0

[1] The symbols +, 0, and - mean a positive contribution, no contribution, and a negative contribution, respectively. Of course, the total deposition kernel for any surface can not be less than zero.

[2] Included in the general formulation but currently zeroed out internally.

Deposition processes modeled in terms of deposition velocities

- Processes assumed to act independently and sum to total deposition velocity
- Surface areas ascertained from appropriate source (HS and CVH)

Deposition Kernel - Settling

Gravitational settling

- Upward-facing surfaces (HS floors, CV pool surfaces, flow-through areas)
- Often dominant in large CVs
- Atmospheres hosting aerosols are spatially well-mixed
  - Settling removes from airborne inventory homogeneously
  - Total horizontal area of CV available

$$v_{grav} = \frac{d_p^2 \rho_p g C_m}{18 \mu \chi}$$

where

v_{grav} = the downward terminal velocity (m/s)

d_p = the particle diameter (m)

ρ_p = the particle density (kg/m^3)

g = acceleration of gravity = 9.8 m/s^2

C_m = the particle mobility, or Cunningham slip correction factor, which reduces the Stokes drag force to account for noncontinuum effects

$$C_m = 1 + \frac{2\lambda}{d_p}\left[F_{slip} + 0.4 \exp\left(-1.1 d_p / 2\lambda\right)\right] \qquad Kn = \frac{2\lambda}{d_p}$$

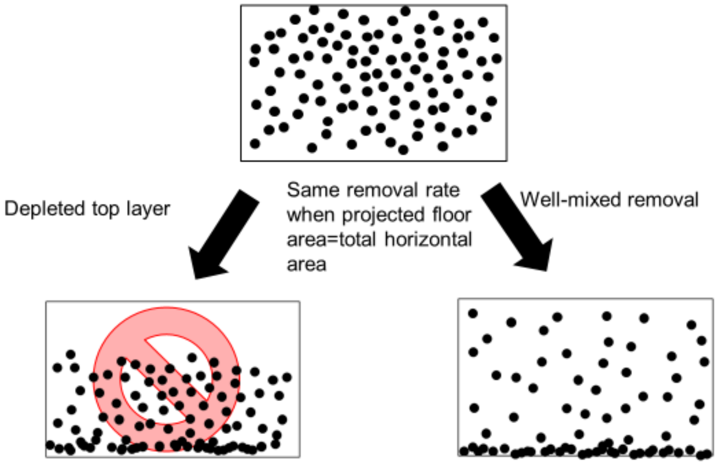
where

λ = mean free path of air at 298 K (~ 0.069 • 10^{-6}m)

F_{slip} = slip factor specified on Input Record RN1_MS00 (default value of 1.257)

μ = viscosity of air at 298 K [~1.8x10^{-5}(N-s/m^2)]

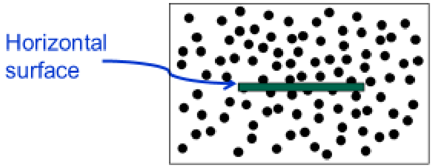
χ = dynamic shape factor



Depleted top layer

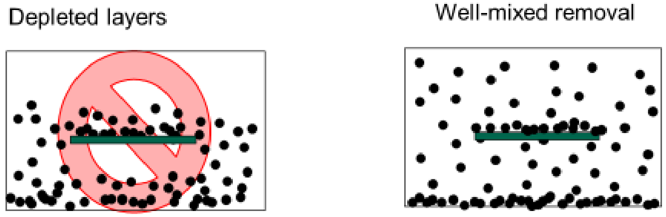
Same removal rate when projected floor area=total horizontal area

Well-mixed removal



Horizontal surface

More removal for well-mixed volumes when projected floor area < total horizontal area



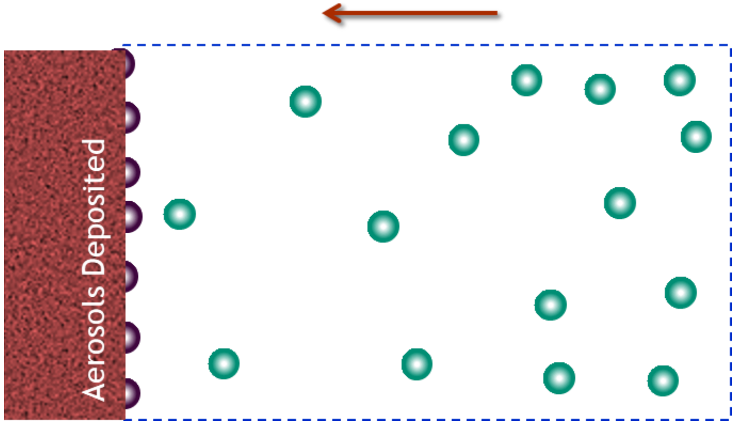
Depleted layers

Well-mixed removal

Deposition Kernel - Brownian

Brownian diffusion

- Computed for all surface types
- Aerosol particle net motion by diffusion in a concentration gradient
- No gas velocity perpendicular to deposition surface
- Note the diffusion boundary layer thickness



$$v_{diff} = \frac{\sigma T C_m}{3\pi \mu \chi d_p \Delta}$$

where

v_{diff} = diffusion deposition velocity (m/s)

σ = Boltzmann constant = $1.38 \bullet 10^{-23}$ (J/s-m^2K^4)

T = atmosphere temperature (K)

μ = viscosity ($N \bullet s/m^2$)

χ = dynamic shape factor

Δ = user-specified diffusion boundary layer thickness specified on input record RN1_MS01 (default value of 10^{-5} m)

Deposition Kernel - Thermophoresis

Thermophoretic deposition

- Not computed for pool surfaces or flow-through areas
- Capture effects of force exerted on aerosol particles by bulk gas temperature gradient
- See RM notes on temperature gradient evaluation

$$v_{therm} = \frac{3\,\mu\,C_m\left(c_t\,Kn + k_{gas}/k_p\right)}{2\;\chi\;\rho_{gas}\,T\left(1+3\,F_{slip}Kn\right)\left(1+2\,c_t\;Kn + k_{gas}/k_p\right)}\,\nabla T$$

where

Kn = $2\lambda / d_p$ (Knudsen number)

ρ_{gas} = gas density (kg/m^3)

T = wall temperature (K)

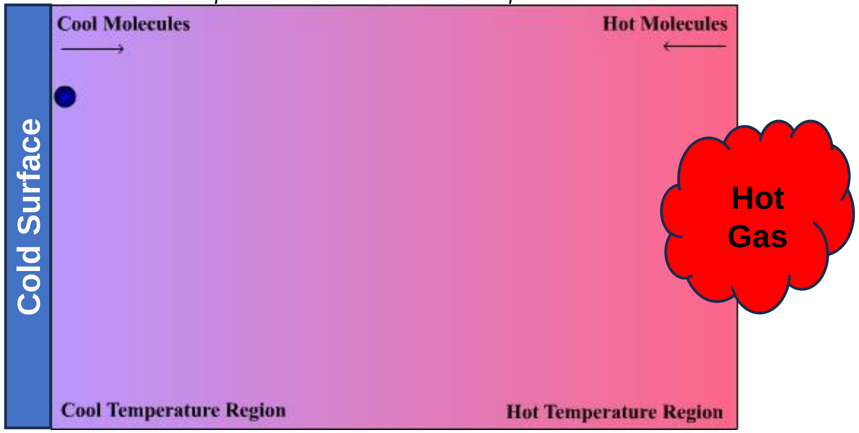
F_{slip} = slip factor

∇T = structure surface temperature gradient (K/m)

k_{gas}/k_p = ratio of thermal conductivity of gas over that for aerosol particle k_p, and is user-specified (on Input Record RN1_MS01)

c_t = constant associated with the thermal accommodation coefficients (specified on Input Record RN1_MS01 with default value of 2.25)

https://aerosol.ees.ufl.edu/thermophoresis/section02.html



Deposition Kernel - Diffusiophoresis

Diffusiophoretic deposition

- Not computed for pool surfaces or flow-through areas
- Related to gaseous component concentration gradients in host gas mix
- Steam condensation/evaporation from/to NCG/steam mix to/from HS surface
  - For example, air/steam mix with condensation/evaporation on/from a deposition surface
  - Local steam depletion in air/steam mix near deposition surface (condensation) drives aerosol deposition
- Two mechanisms
  1. Stefan flow – like a suction effect…net molar flux of gas to/from the surface carries particle
  2. Analogous to thermophoresis…differential momentum to particle by gas mix molecules (heavy vs. light)

$$v_{diffusio} = \left(\frac{\sqrt{M_s}}{X_s \sqrt{M_s} + X_{NC} \sqrt{M_{NC}}} \right) \left(\frac{W_{cond}}{\rho_b} \right) \quad \text{if } W_{cond} \geq 0 \text{ (condensation)}$$

$$v_{diffusio} = W_{cond} / \rho_s \qquad \text{if } W_{cond} < 0 \text{ (evaporation)}$$

where

M_s = molecular weight of water (kg/mole)

M_{NC} = molecular weight of noncondensible gases (air

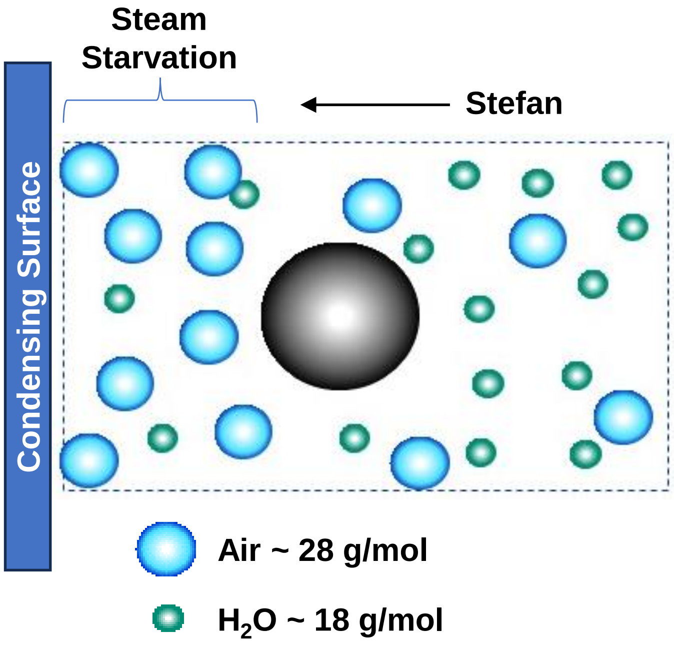
W_{cond} = condensation mass flux to the surface (kg/s-m^2)

ρ_b = density of bulk gas (kg/m^3)

ρ_s = saturation density of water vapor (kg/m^3)

X_s = mole fraction of water vapor in the bulk gas

X_{NC} = mole fraction of noncondensible gases in the bulk gas



Deposition Kernel – Turbulence

Turbulent deposition and impaction

- Only computed for requested surfaces (RN1_TDS) and never for pool surfaces or flow-through area
- Meant to capture deposition effects related to high Reynolds number flow in pipes/bends
- Highly dependent on inertia of aerosol particles and therefore on their size
- Three size regimes
  - Inertia-moderated (largest size)
    - Core turbulence reduces acceleration a little
    - No effect of smaller eddies in buffer or viscous sublayer
  - Eddy diffusion impaction (medium size) - core and buffer eddies move particles to wall past viscous sublayer
  - Turbulent particle diffusion (smallest size)
    - Brownian motion as much or more than turbulent eddy diffusivity
    - Helps transport particles across viscous sublayer

Refer to RN UG/RM and previous RN workshop materials for details of modeling

- Deposition in straight pipes (Woods for smooth, Woods for rough, VICTORIA)
- Impaction in bends (INL/Merrill – theoretical, VICTORIA/Pui & McFarland - empirical)
- Impaction in contractions
- Correlated in terms of deposition velocities
- Notion of “deposition efficiencies” for flow through bends and contractions

Deposition Kernel – Overall with Fallout

Sum up for the final deposition sectional coefficient

- Sum all mechanisms over all surfaces in CV of interest
- Use proper aerosol density for section, $Q_{l,k}$

$$\overline{\Re}_{\ell,k} = \sum_{j=1}^{N_{str}} K_{j,\ell} Q_{\ell,k}$$

$$K_{j,\ell} = \frac{A_j}{V}\left(v_{grav} + v_{diff} + v_{therm} + v_{diffusio} + v_{turbulent}\right)$$

- Can calculate fraction of mass, section l, deposited on any surface j associated with CV

$$Fr_{j,\ell} = \frac{A_j K_{j,\ell}}{\sum_{j}^{N_{sur}} A_j K_{j,\ell}}$$

Fallout

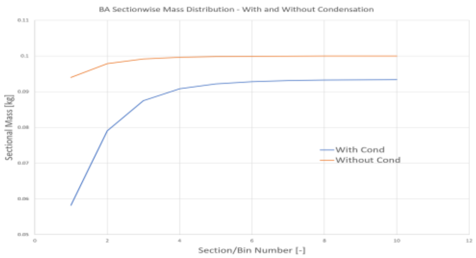
- Agglomeration calculation (not deposition kernel) yields total fallout mass
- Fractionally partition fallout mass over pool surfaces, HS floors, and flow-through areas

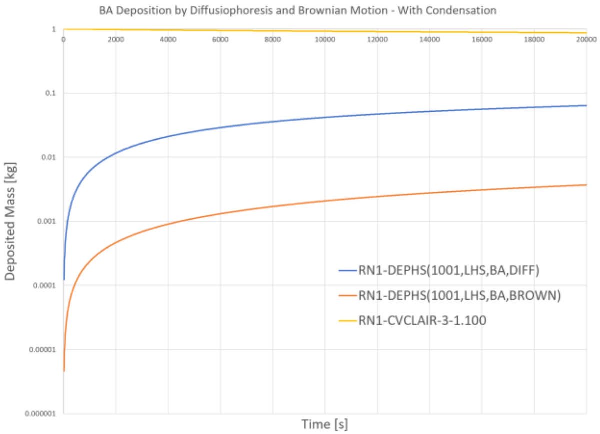
$$Fr_i = A_i \Big/ \sum_{i}^{N_{sur}} A_i$$

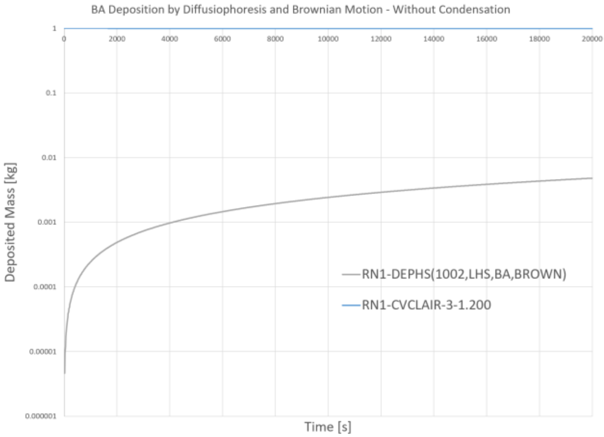
Deposition Kernel Examples

Diffusiophoresis – 2 CVs (45 m^3, 3 m, 330 K, RHUM = 0.9) 3 HSs (2 walls, 1 floor)

- Disable agglomeration, gravitational settling, and thermophoresis
- 1 CV has 1 wall w/ mass transfer:
  - Diffusiophoresis >> Brownian
  - Brownian ~ no condensation
  - Smaller bins more depleted

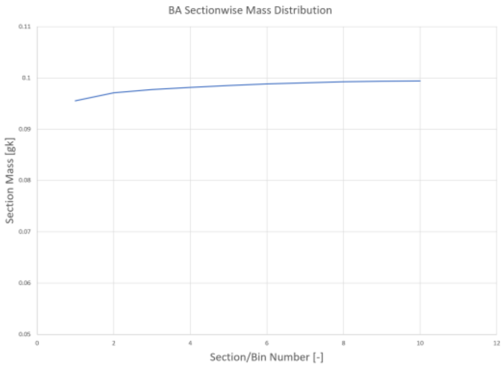


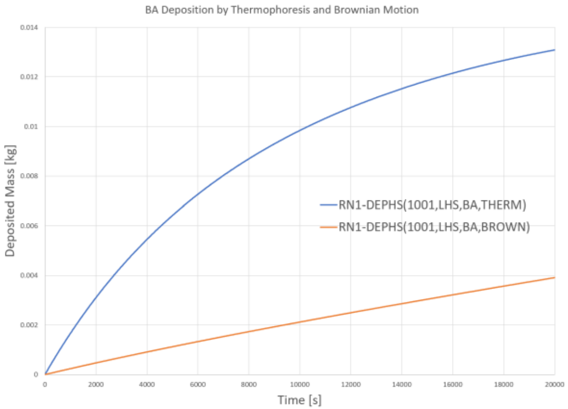




Thermophoresis – 1 CV (45 m3, 3 m, 330 K, RHUM = 0.0) between 2 HSs (hot and cold)

- Disable agglomeration, gravitational settling, and diffusiophoresis
- 100 K temperature difference b/t HS's
  - Thermophoresis > Brownian
  - Only deposition on cold HS surface





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1 rn1-dephs(1001,LHS,BA,DIFF)
2 rn1-dephs(1001,LHS,BA,THERM)
3 rn1-dephs(1001,LHS,BA,GRAV)
4 rn1-dephs(1001,LHS,BA,TURB)
5 rn1-dephs(1001,LHS,BA,BEND)
6 rn1-dephs(1001,LHS,BA,VENT)
7 rn1-dephs(1001,LHS,BA,CONT)
8 rn1-dephs(1001,LHS,BA,BROWN)
9 rn1-dephs(1001,LHS,BA,FALL)

Water Condensation/Evaporation

Aerosol depletion by growth/fallout due to water condensation in LWR SMR containment

- Phenomenological models not integrated into MAEROS solve
- Effects of condensation/evaporation calculated outside MAEROS aerosol dynamics on any given Δt
- Two ways to model water condensation/evaporation to/from aerosol particle surfaces:
  1. Neglecting hygroscopic effects, surface tension effects, and effects related to molecular mean free path
  2. Accounting for aerosol solubility, Kelvin effect, and non-continuum (free-molecular) effects

Method (1) is the default model

- Essentially an equilibrium thermodynamics approach
- CVH/CVT computes any changes in “fog” (aerosolized water) mass
- Simply distribute the change in fog mass over aerosol sections

Method (2) is the hygroscopic model (see RM)

$$\frac{dr}{dt} = \frac{1}{r}\frac{(S - S_r)}{a + b}$$

- Mason equation describing particle growth
  - Driving force for condensation/evaporation $S - S_r$
  - Kelvin effect restraining particle growth at small radii
  - Chemical activity
  - Conduction of released latent heat of vaporization away from particle surface
  - Diffusion of water vapor to particle surface from atmosphere
  - Free molecular regime corrections when aerosol particle sufficiently small

TRAP-MELT2 and condensation/evaporation of fission product vapors not mentioned here

Resuspension

Allows deposited aerosol resuspension off HS surfaces when model activated (HS_[L|R]BAR)

- Any deposited aerosol belonging to sections with lower size boundary > some D_{crit} resuspend
- Computed outside the MAEROS solve
- Options for critical diameter:
  - User-specified (real value or control function)
  - Default model, calculated according to wall shear which depends on gas flow past deposition surface

$$D_{\mathrm{crit}} = \frac{4 \times 10^{-5}}{\pi \tau_{\mathrm{wall}}}$$

$$\tau_w = \frac{1}{2} f \rho U^2 \qquad f = \frac{0.0791}{\mathrm{Re}^{0.25}} \qquad \mathrm{Re} = \frac{\rho D U}{\mu}$$

where

f = friction factor,

ρ = gas density (kg/m^3), and

U = gas velocity along the surface (m/s)

- Wet surfaces (with surface films) cannot resuspend
- Once aerosol deposition occurs:
  - Cumulative particle size distribution information is stored by section,
  - Size distribution of deposited aerosols does not change thereafter, and
  - Resuspension can potentially occur as above

Summary

Quickly reviewed RN (RN1/RN2) and MAEROS for aerosol dynamics

- Important and sometimes tricky concepts of what MAEROS actually solves
- RN1 for inter-volume processes
- RN2 for intra-volume processes

Focused on the MAEROS deposition kernel

Looked at options for modeling aerosol particle depletion due to condensation/evaporation

Looked at options for modeling resuspension