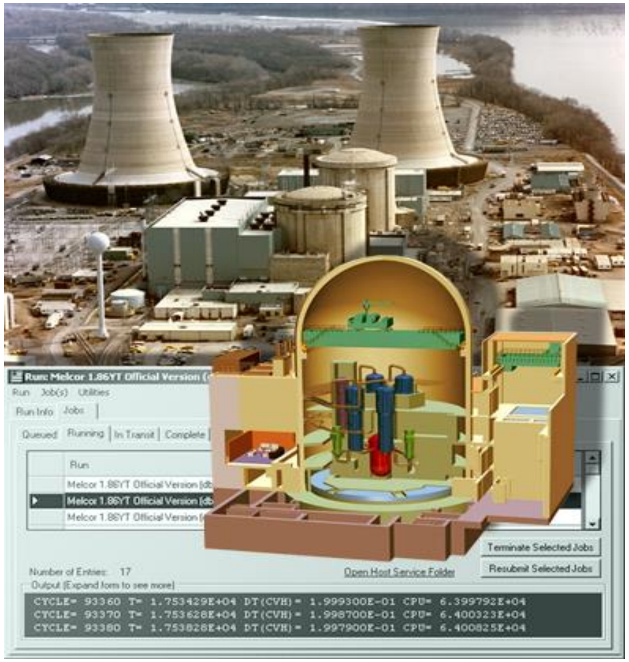

Deposition Modeling

Presented by

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SAND2018-4215 PE

MELCOR Aerosol Deposition

- MELCOR has long had aerosol deposition models for various mechanisms
  - Gravitational settling
  - Brownian diffusion to surfaces
  - Thermophoresis (Brownian process causing migration to lower temperatures)
  - Turbulent Deposition
  - Diffusiophoresis (induced by condensation of water vapor onto surfaces)

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.**

Definitions: Deposition Velocity

Particle deposition is modeled in terms of a deposition velocity V_d, defined as the ratio of the time-averaged particle flux to the surface to the time-averaged airborne particle concentration in the duct. This is then implemented into MELCOR in calculating the rate of deposition on a surface:

$$\frac{1}{A}\frac{dM_C}{dt} = V_d C$$

where

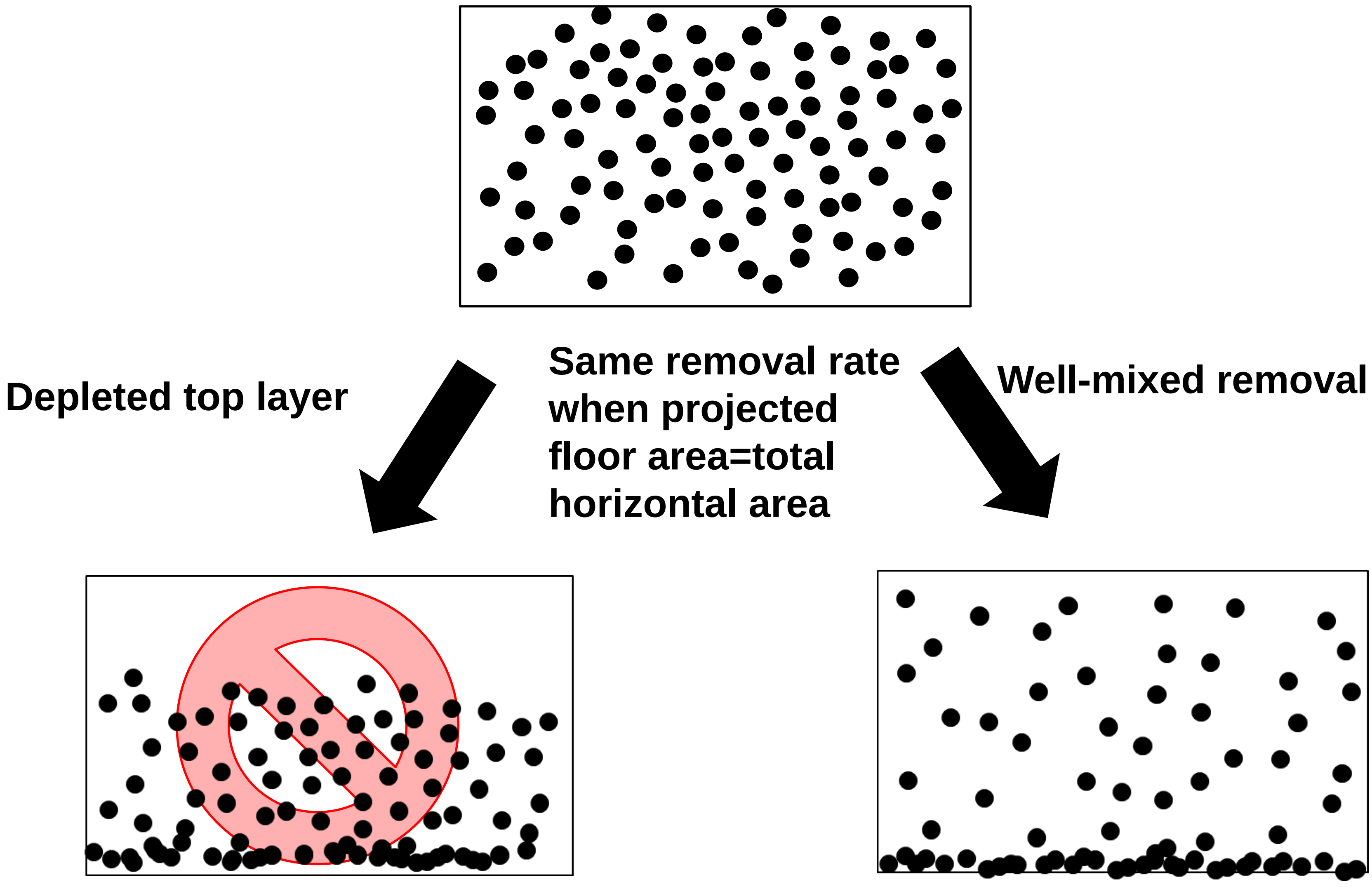
V_d - deposition velocity
C - particle mass concentration
M_C - Mass deposition rate
A - Surface area of deposition surface

It is assumed that each deposition mechanism acts independently and the total deposition velocity can be calculated from the sum of the deposition velocities for each mechanism

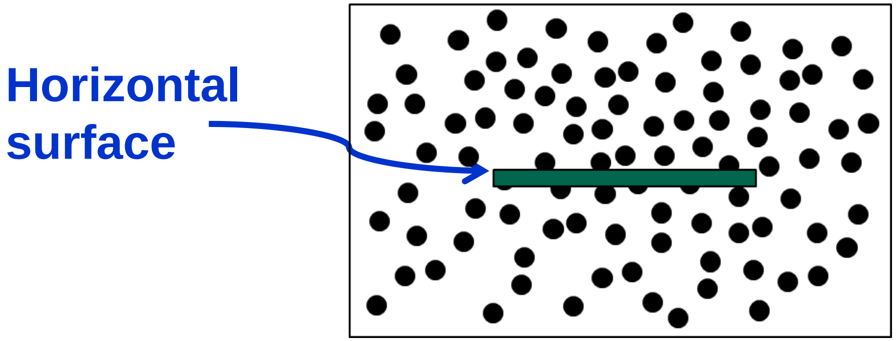
Conceptual Modeling of Settling

- Basic MELCOR approach: All control volumes with aerosol are modeled as spatially well-mixed aerosol within the control volume.
- Settling therefore removes particles homogeneously, and NOT by creating depleted regions within a well-mixed volume.
- Implication: The total horizontal area and NOT just the projected floor area is available for removal by settling.

Conceptual Modeling of Settling (2)

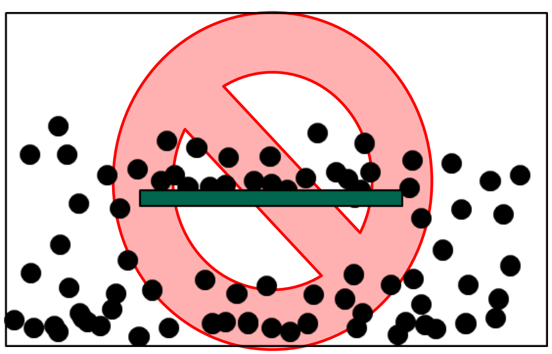


Conceptual Modeling of Settling (3)

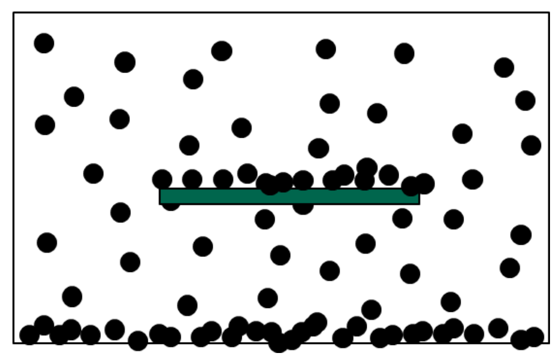


More removal for well-mixed volumes when projected floor area < total horizontal area

Depleted layers



Well-mixed removal



Gravitational Deposition

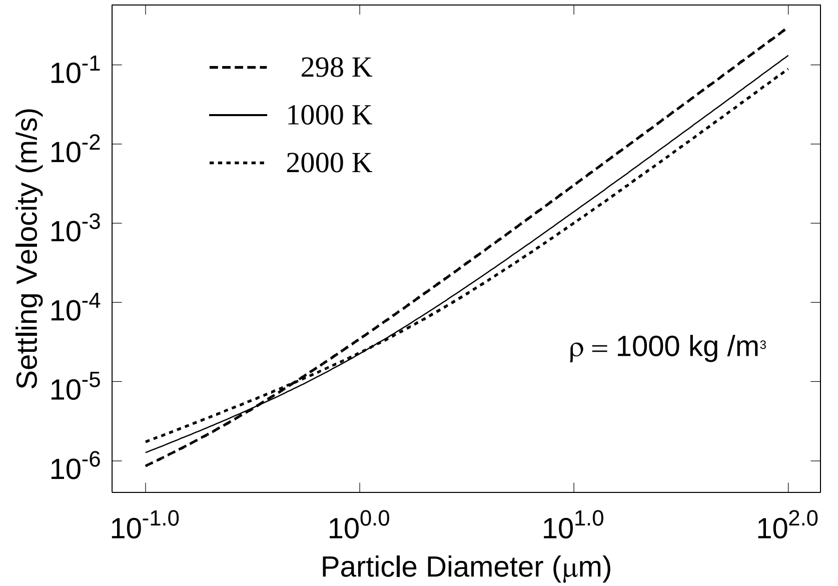
- Gravitational deposition is often the dominant removal process
- Deposition rate is equal to the deposition velocity times the surface area/volume ratio

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

d_p=diameter, ρ= density,

χ=dynamic shape factor (~1)

– Leading size dependence is $\rho\, d_p^2$
  - Note velocity ~3 mm/s for a 10 μm sphere with ρ=1000 kg/m^3



Gravitational Deposition Special Consideration

- Geometry Considerations
  - Rectangular HSs
    - The upper surface of a rectangular heat structure with an angle of inclination less than 45 degrees is considered to be a floor, and the lower surface a ceiling.
      - The orientation parameter ALPHA determines both the inclination and whether the "left" surface is the upper or the lower surface.
    - Both surfaces of a rectangular heat structure with an angle of inclination greater than 45 degrees, and both surfaces of vertical cylinders and spheres are treated as walls.
  - Hemispherical HS
    - The inner (left) surface of a bottom-half hemisphere is treated as a floor and the outer (right) surface as a ceiling. For a top-half hemisphere, the treatment is reversed.
  - Cylindrical HS
    - Surface area for horizontal inside surface reduced by a factor of π to account for downward and side walls (recent change)
  - The user can override these default orientations or deactivate a surface for aerosol deposition through the RN1_DS input records.
- If a control volume contains a water pool, the pool surface is treated as a floor for the purposes of deposition.
  - Area from volume altitude tables
- Fall out
  - Aerosols become larger than the maximum diameter (user-specified)
  - Deposit on pool surfaces, horizontal heat structures, or settle into adjacent CV

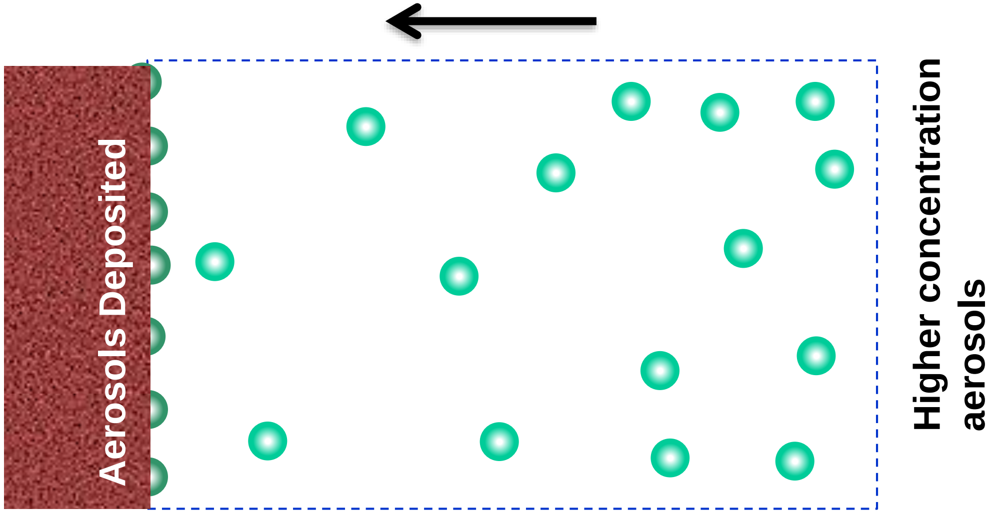
Brownian Diffusion

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

Where

- V_{diff} = diffusion deposition velocity (m/s)
- σ = Boltzman constant (J/s-m^{2}K^4)
- T = atmosphere temperature (K)
- μ = viscosity (N•s/m^2)
- χ = dynamic shape factor
- Δ = user-specified diffusion boundary layer thickness (m)
- C_m =Cunningham slip correction factor (particle mobility

Net Direction of motion of aerosols

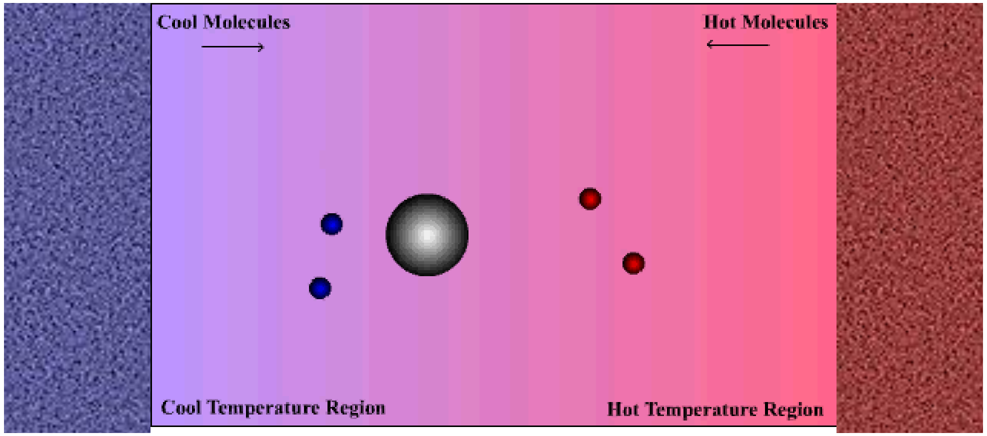


$$C_m = 1 + \frac{2\lambda}{d_p}\left[F_{slip} + 0.4\exp\left(-1.1 d_p / 2\lambda\right)\right]$$

λ = mean free path in air
F_{slip} = slip factor
d_p= particle diameter

- Diffusion of aerosols in a concentration gradient from a higher to a lower concentration region.
  - Assumption that there is no gas velocity perpendicular to the deposition surface
  - This mechanism is most effective for small aerosol particle sizes

Thermophoresis



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

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

where

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

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_MS0'

∇T = structure surface temperature gradient (K/m) $\quad \nabla T = -q''/k_{air}$

ρ_{gas} = gas density (kg/m^3)

T = wall temperature (K)

F_{slip} = slip factor

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

Click HVAC Example

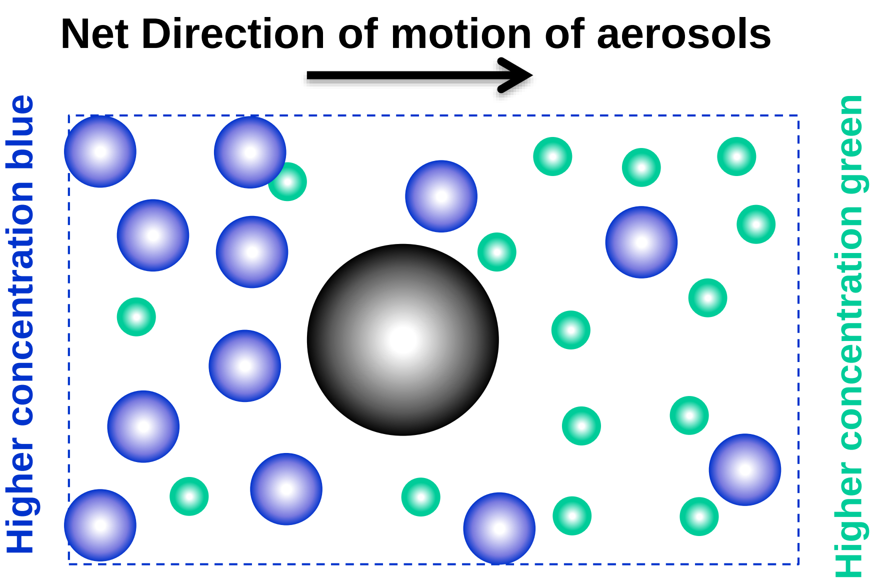
Diffusiophoresis

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

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

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



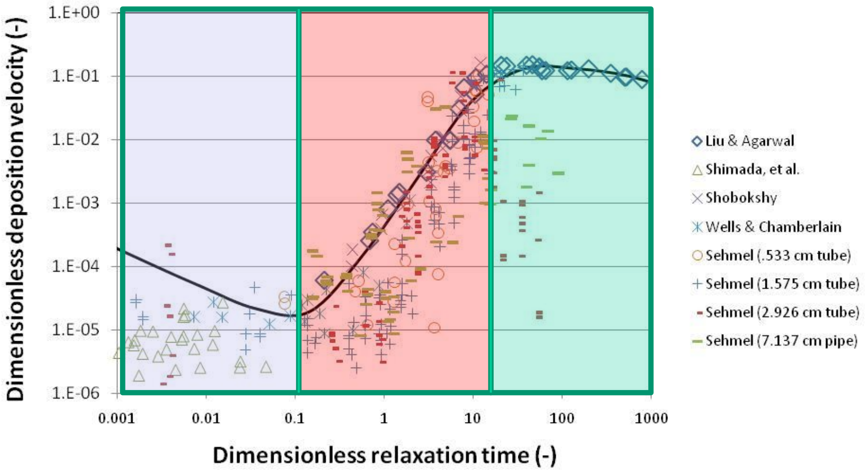
- Net molar flux
  - Gas toward the condensing surface tends to move aerosol particles with it
  - Gas away from an evaporating surface tends to move aerosol particles away
- Differences in the momentum transferred by molecular impacts on opposite sides of the particle tend to drive the particle in the direction of decreasing concentration of the heavier constituent.

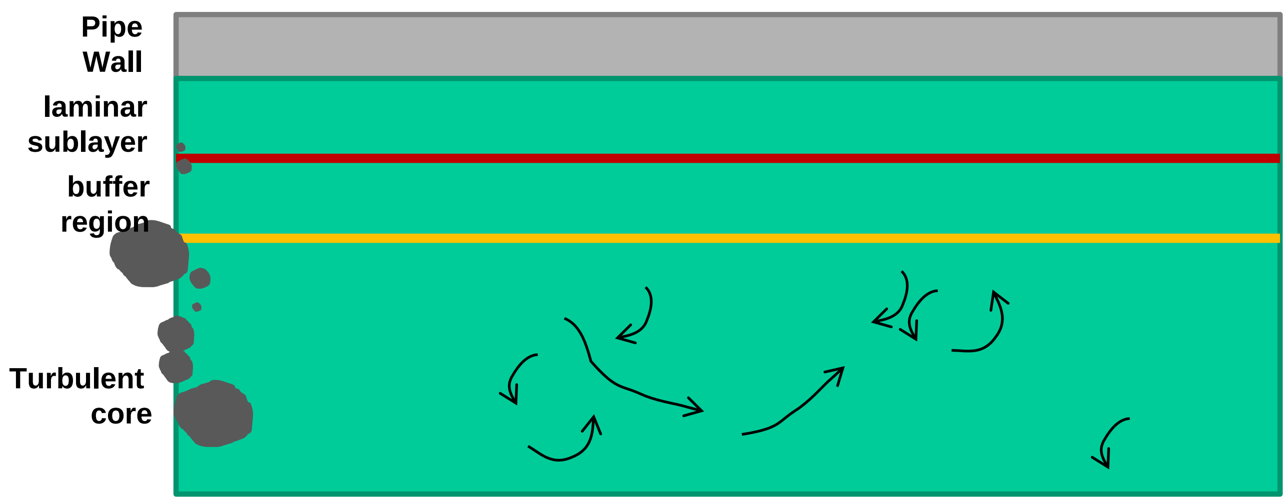
Turbulent Deposition Models

- Turbulent deposition in pipe flow
  - Wood's model for smooth pipes (default)
  - Wood's model for rough pipes
  - Sehmel's model for perfect particle sinks (VICTORIA)
- Bend Impaction Models
  - Pui bend model
  - McFarland bend model
  - Merril bend model

Turbulent Deposition Regimes

- Inertia moderated regime
- Eddy diffusion impaction regime
- Turbulent particle diffusion





Definitions: Particle Relaxation Time, τ

- It is common to correlate the deposition velocity with the particle relaxation time, τ.
- This is the characteristic time for a particle velocity to respond to a change in air velocity.
- For spherical particles of diameter d_p and density r_p in the Stokes flow regime, it is calculated as:

$$\tau = \frac{\rho_m D_p^2 C_{slip}}{18\mu_g}$$

C_{slip} - slip correction factor (-)

- This is nondimensionalized by dividing by the average lifetime of eddies near the walls:

$$\tau^* = \frac{\tau \rho_g \left(u^*\right)^2}{\mu_g}$$

u^* - friction velocity

Turbulent Deposition Model

- Particle Diffusion Regime
  - Davies equation

$$V_d^* = \frac{3\sqrt{3}}{29\pi\tau_*^{1/3}} Sc^{-2/3} \quad \tau_*^{1/3} + K\tau_*^2$$

  - Standard Brownian diffusion model (previous discussion) disabled in favor of turbulent deposition model
- Eddy Diffusion –Impaction Regime

$$V_d^* = \frac{3\sqrt{3}}{29\pi\tau_*^{1/3}} Sc^{-2/3} \quad \tau_*^{1/3} + K\tau_*^2$$

- **K is often determined empirically**

Investigator	k_2
Kneen & Strauss (1969)	3.79×10^{-4}
Liu & Agarwal (1974)	6×10^{-4}
Wood (1981b)	4.5×10^{-4}
Papavergos & Hedley (1984)	3.5×10^{-4}

- **Or calculated from a Fick's law equation (Wood)**

$$N = (D_p + \varepsilon)\frac{dc}{dy}$$

- Inertia Moderated Regime
  - Deposition velocity is either constant

$$V_d^* = \sqrt{\frac{f}{2}} \qquad 10 \le \tau_* < 270$$

  - Or may decrease with increasing dimensionless relaxation time

$$V_d^* = \frac{2.6}{\sqrt{\tau_*}}\left(1 - \frac{50}{\tau_*}\right) \qquad \tau_* \ge 270$$

VICTORIA Modeling

- Three regimes of turbulent deposition as was predicted by Woods model
  - Davies Model is also used for small particles in the turbulent particle diffusion regime
  - Correlation by Sehmel added for particle impaction regime
    - Correlation fit overexperiments for which sticking was promoted (used in VICTORIA).

$$u_{t,s} = 1.47 * 10^{-16} \left(\frac{\rho_a}{1000}\right)^{1.01} \left(\frac{2 * 10^4 r_a}{D_H}\right)^{2.1} Re^{3.02} \tilde{v}$$

    - Correlation fit over a more general data set (not used in MELCOR)

$$u_{t,s} = 1.0 * 10^{-16} \left(\frac{\rho_a}{1000}\right)^{1.83} \left(\frac{2 * 10^4 r_a}{D_H}\right)^{2.99} Re^{3.08} \tilde{v}$$

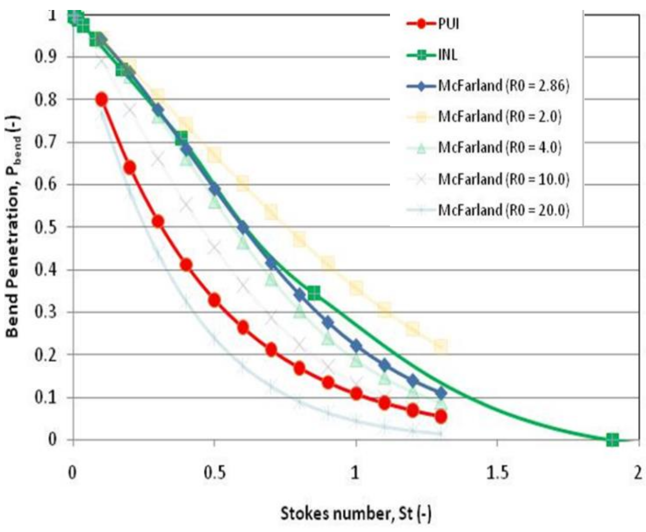
- A maximum is placed on the non-dimensional deposition velocity not to exceed a value of 0.1.

MELCOR Bend Models

- Merril's Bend Model - Theoretic
  - Based on centrifugal force on particle, drift velocity, and geometry
- Pui Bend Model - Empirical
  - Based on experiments by Pui et al. For conditions of $10^2 < Re < 10^4$
  - Correlates the deposition efficiency, η_b due to flow irregularity

$$\eta_b = 1 - 10^{-0.963 St}$$

- McFarland's Bend Model - Empirical
  - Based on fitting an equation to data obtained from physical experiments and Lagrangian simulations.
  - Applicable to arbitrary bend angles and radius of curvature



MELCOR Contraction Models

$$\eta_b = 0 \text{ for } X < 0.213$$

$$\eta_b = \left[1 - \left(\frac{D_o}{D_i}\right)^2\right][1 - \exp(1.721 - 8.557X + 2.227X^2)] \text{ for } 0.213 \le X \le 1.95$$

$$\eta_b = 1 - \left(\frac{D_o}{D_i}\right)^2 \text{ for } 1.95 < X$$

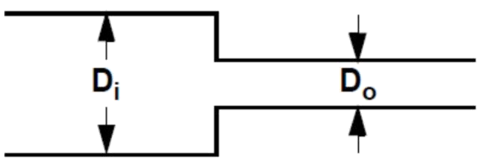
$$X = \sqrt{\mathrm{St}}\left(\frac{D_o}{D_i}\right)^{0.31}$$

where

D_o = pipe diameter at the outlet of the sudden contraction (m)

D_i = pipe diameter at the inlet of the sudden contraction (m)

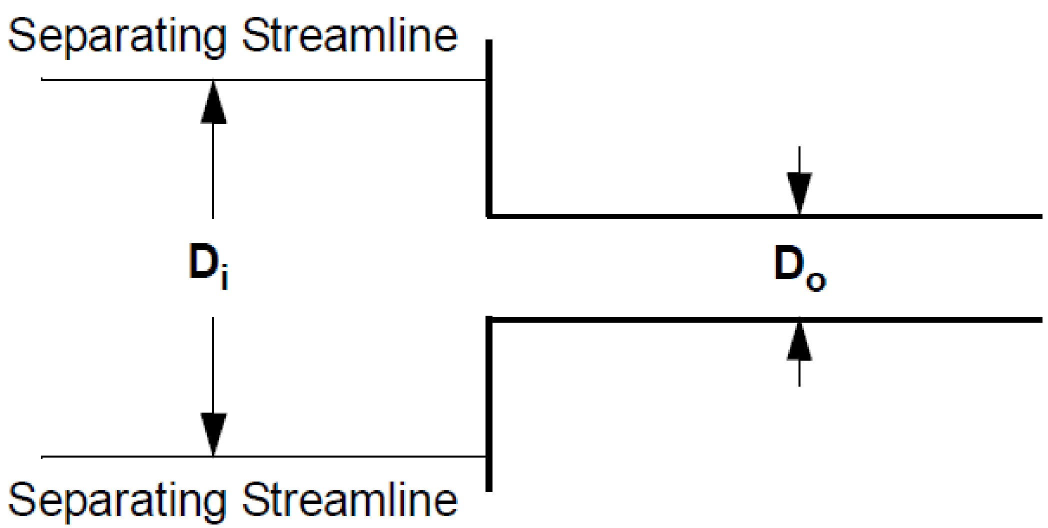
St = particle Stokes number, based on the inlet velocity and the outlet diameter (dimensionless), $\frac{4Cn\rho_a r_a^2 U_i}{9\mu D_o}$



- Based on work by Ye and Pui (1990) and included in Victoria code

MELCOR Vena Contracta

$$\eta_b = \left[1 - \left(\frac{D_o}{D_i}\right)^2\right]\left\{1 - \left[1 + 2\mathrm{St} + 0.617\left(\frac{D_o}{D_i}\right)^2 \mathrm{St}\right]^{-1}\right\}$$



Based on the work of Belyaev and Levin (1972) and encoded in VICTORIA

RN1_TURB - Deposition Modeling Record

Several options for modeling turbulent deposition in pipes are available in MELCOR. Turbulent deposition is only calculated for those heat structure surfaces specified by the user as calculation of turbulent deposition can impact code performance and is only of importance for high Re number flow in pipes and bends. This record specifies the models that will be used in the calculation of turbulent deposition for those heat structures specified in the RN1_TDS table. A description of the models used in MELCOR for predicting turbulent deposition in pipes and bends is provided in the RN reference manual.

(1) TURBMODEL

Deposition Modeling flag for turbulent component

='OFF' or 0, No turbulent deposition modeling

=”VICTORIA' or 1, VICTORIA modeling of deposition in straight pipe sections

='WOODS' or 2, Wood's model for rough pipes

='WOODS_S' or 3, Wood's model for smooth pipes

(type = integer/ character*16, default = 2, units = none)

(2) TRANSMODEL

Deposition Modeling flag for impact deposition in bends and transitions

='OFF' or 0, No deposition modeling in bends

='VICTORIA' or 'PUI' or 1, PUI modeling of deposition in bends

='INL' or 2, INL modeling of deposition in bends

='MCF' or 3, McFarland modeling of deposition in bends.

(type = integer/ character*16, default = 2, units = none)

(3) IMODEL

Deposition Modeling flag

=0, Gravitational, thermophoresis, and diffusiophoresis velocities are calculated at the beginning of the calculation

=1, Gravitational, thermophoresis, and diffusiophoresis velocities are recalculated at each time step. Note that if this option is used, it will affect deposition calculated for all deposition mechanism, regardless of whether turbulent deposition is calculated.

(type = integer/ character*16, default = 0, units = none)

RN_TDS – RN Turbulent Deposition Surfaces

Turbulent deposition may be important for high Re flow in a pipe or in pipe bends and can be activated for each surface. If a surface is not defined in this table, it is assumed that turbulent deposition is not calculated.

(1) NDEP – Number of deposition surfaces associated with turbulent deposition modeling

The following data are input as a table with length NDEP

- (1) NUMTDS - Index for turbulent deposition associated with a particular heat structure surface.
- (2) HS_ID - The heat structure to apply the bend and/or turbulent deposition model.
- (3) ISUR - Surface ('LHS' or 'RHS')to which the deposition modeling is applied.
- (4) CHARL - Characteristic length (i.e., pipe diameter).
- (5) NO_BND - Number of bends associated with the volume.
- (6) ANGLE - Turning angle of the bends.
- (7) RAD_BND - Radius of curvature for bend.
- (8) ROUGH - Surface roughness for the turbulent deposition model (not used in VICTORIA model).
- (9) VelocityFP - The Flow path used to determine flow velocities. This field is optional. If not provided, MELCOR uses the control volume velocity which is calculated from the CV area that is either provided on the CV_ARE record or calculated from the volume divided by the height. If VelocityFP is provided, MELCOR uses the atmosphere velocity for the flow path provided.
- (10) Ncontractions - Number of contraction transitions
- (11) DODIC - Diameter at exit divided by diameter at entrance (<=1)
- (12) FACONT - Multiplier on deposition velocity for contraction
- (13) NVENTUR - Number of venturi transitions
- (14) DODIV - Diameter at venturi restriction divided by diameter at entrance (<=1)
- (15) FAVENT - Mulitiplier on deposition velocity for venturi transitiom

Control Function Arguments

RN1-ADEP(NameHS,s,NameCLS,y)

Aerosol mass of class *NameCLS*, deposited on side *s* (s='LHS' or s='RHS') of heat structure name *NameHS*. The parameter *y* specifies total mass (y='TOT') or radioactive mass only (y='RAD').

(units = kg)

RN1-DEPHS-DIST(NameHS,s,NameCLS,m)

Aerosol mass of class *NameCLS*, deposited on side *s* (s='LHS' or s='RHS') of heat structure name *NameHS in section m*. If m=0 then the total mass deposited is returned.

(units = kg)

Control Function Arguments

RN1-DEPHS(NameHS,s,*NameCLS*,p)

Total aerosol mass of class *NameCLS* deposited on side s (s='LHS' or s='RHS') of heat structure HS *NameHS* from deposition physics model p. This is the total mass deposited from each mechanism and does includes mass that may be later resuspended.The deposition models that are tracked are as follows:

p = 'DIFF', Diffusion deposition
p = 'THERM', Thermophoresis
p = 'GRAV', Gravitational settling
p = 'TURB', Turbulent deposition in straight sections
p = 'BEND', Deposition in pipe bends
p = 'VENT', Deposition in venturi transitions
p = 'CONT', Deposition in contraction transitions
(units = kg)

RN1-TOTRES(NameHS,s)

Total radionuclide mass that has been resuspended.

(units = kg)

Condensation/evaporation

- FPs & water can condense/evaporate onto/from
  - Aerosols; heat structure surfaces; and/or water pools
- Aerosol water ≡ fog (CVH pkg)
  - Change in fog mass
    - determined by thermodynamics
    - distributed over aerosol sections
- Water condensation/evaporation for heat structure and water pool surfaces
  - Mason equation
- Calculation of FP vapor condensation/evaporation
  - TRAP-MELT2 rate equations based on
    - surface areas, mass transfer coefficients, atmosphere concentration, and the saturation concentrations corresponding to the temperatures of the surfaces

$$\frac{dM_a}{dt} + \sum_i \frac{dM_i}{dt} = 0$$

$$\frac{dM_i}{dt} = A_i k_i \left(C_a - C_i^s\right)$$

Evaporation of Pools

- Evaporation of RNs from pools is not permitted
- If the pool in a volume completely evaporates, any aerosols in the pool are distributed between the floor heat structures and the flow through areas

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

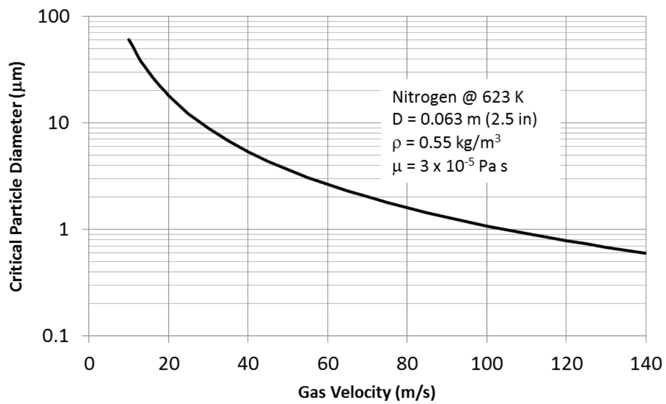
- If the atmosphere in a control volume that is almost completely filled with water completely condenses, all the suspended aerosol mass is added to the aerosol mass in the pool because it is assumed that the pool will then completely fill the control volume.

Re-suspension Model

- Deposited material can be re-suspended
  – All sections for which the lower section boundary particle diameter is greater than a critical diameter
  – Critical diameter is calculated from gas flow conditions

$$D_{crit} = \frac{4 \times 10^{-5}}{\pi \tau_{wall}} \text{ (m)}, \qquad \tau_{wall} = \frac{f \rho v^2}{2} \text{ (N/m}^2\text{)} \qquad f = \frac{0.0791}{Re^{0.25}}$$

  – Does not account for possible changes in size distribution at the surface
  – Assumes continually homogenous distribution of particle sizes
  – Alternatively, critical diameter can be specified by user
    - Control function
    - Constant value
- By default, surfaces do not re-suspend
- Wet surfaces cannot re-suspend.
  – Pools and surfaces with condensed water
- Reference
  – "Liftoff Model for MELCOR," Mike Young
  – SAND2015-6119
- Validation against Tests
  – STORM tests (SR11 and SR12)
  – Validation against LACE tests



Examples

To fully activate resuspension, specify a value of FractResuspend as 1.0, and let MELCOR determine the critical diameter:

HS_LBAR 1. ! Left surface

HS_RBAR 1. ! Right surface

Deposition Special Consideration

- The influence of the aerosol particles on the flow stream is negligible.
  - Not only does this mean that the micro effects on the turbulent flow field, but the macro effects from deposition on surfaces with the subsequent reduction in flow area is not modeled.
- Removal of deposited radionuclides by pools in contact with HS
  - HS package calculates and communicates to the RadioNuclide (RN) package the fraction of liquid (water) mass on each heat structure boundary surface deposited
  - These fractions are used to calculate the relocation of radionuclides from deposition surfaces to the pools of their boundary volumes
- Removal of deposited radionuclides by films
  - Fraction of RNs on a surface relocates in proportion to fraction of film drained
  - Solubility of RN classes in water films can be changed (SC7136)
- Decay heat from deposited radionuclides is treated as a power source at the surface in the equation for the surface temperature.
  - Decay heat from RN deposited on a surface that is absorbed by <u>other</u> surfaces in the same control volume is allocated among the <u>other</u> surfaces in proportion to their areas (excluding the bearing surface).

Decay Heat from Radionuclides on Heat Structure Surfaces	
Current Heat Structure	50%
Atmosphere of current CV	25%
Other surfaces of current CV	25%
Atmosphere of other CVs	0%
Surfaces of other CVs	0%