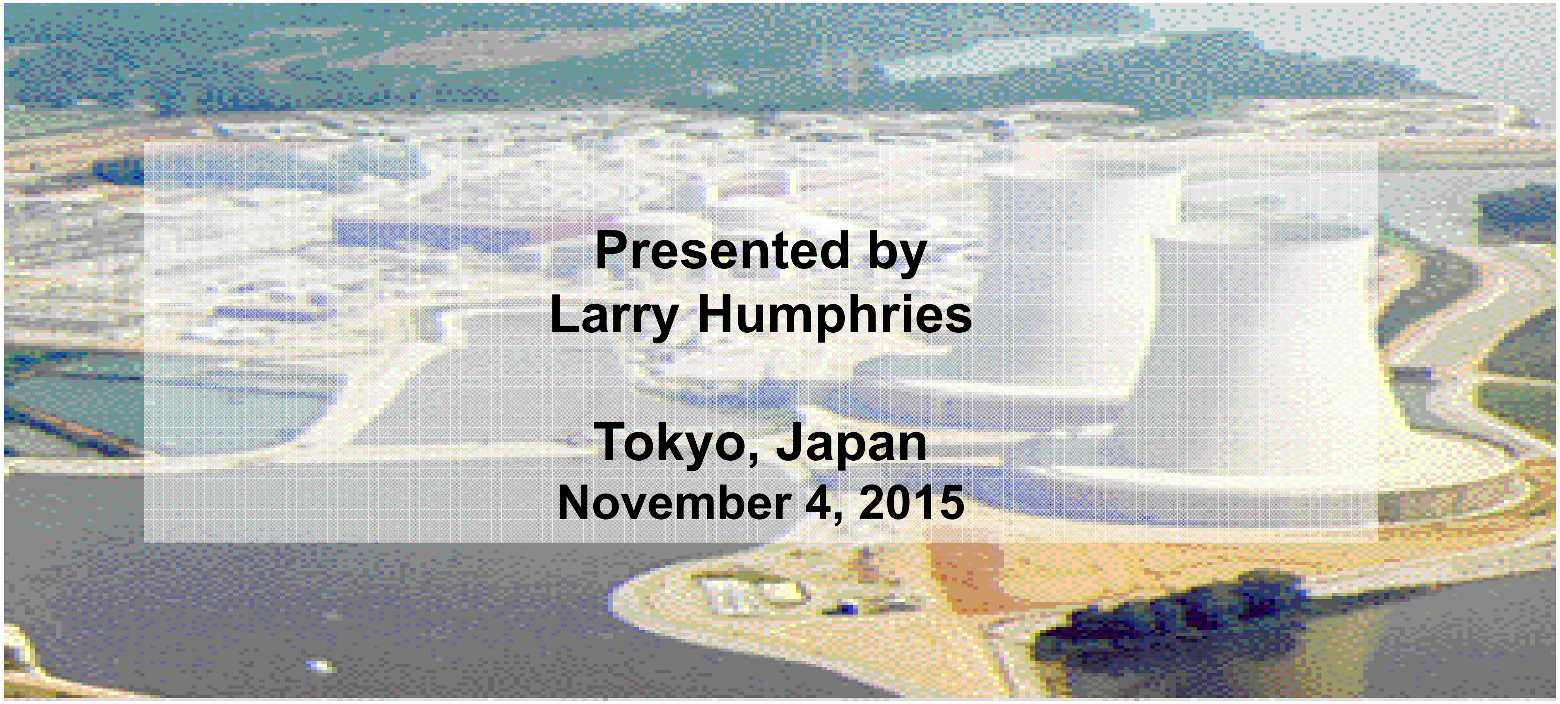
MELCOR RN Package Aerosol and Vapor Physics

SAND2015-10062PE



Presented by
Larry Humphries

Tokyo, Japan
November 4, 2015

What is RN? (1)

- RN is a "Package" (major piece) in MELCOR
  - Originally intended to treat behavior (release, transport, interactions) of RadioNuclides in nuclear reactor accidents
  - Some models (and some coding) are extracted from other codes, but implemented in a more-consistent form
- Basic assumptions
  - RN materials are "traces", hosted by other materials or objects
    - Fuel and/or debris
    - Hydrodynamic materials (pool and atmosphere)
    - Surfaces of heat structures
  - Mass, volume, heat capacity, are negligible
    - Temperature, when needed, taken as that of host
  - RN Package models various properties and interactions, transfer between hosts

What is RN? (2)

- RN is divided into two parts
  - RN1 models mainly within-volume processes, calculated before hydrodynamic advancement
    - Releases, interactions, …
  - RN2 models mainly between-volume processes, calculated during or after hydrodynamic advancement
    - Advection with fluids, removal by filters
- RN in MELCOR can also be used for tracking "trace" materials in non-reactor situations
  - Transport of radiological releases, toxins, and biohazards in buildings, building complexes
  - "Leak-path factor analysis" (Google it)
  - Wikipedia: "[MELCOR] is sometimes, though incorrectly, said to be an acronym of Methods for Estimation of Leakages and Consequences of Releases"

What are RN Classes?

- The RN package distinguishes RN *classes*, groups of materials with properties that are “similar enough” to treat together
  - “Actual” radionuclides (see next slide)
    - Ideal gases (Xe, Kr), alkali metals (Cs, Rb), etc. (default is 17 classes)
    - Important compounds (CsI, Cs_2MoO_4)
  - Boron (from reactor control elements)
  - Concrete (oxides from molten core/concrete interactions)
  - Water (water aerosols that interact with other aerosols)
  - Other trace materials (solid or vapor)
    - Species in Iodine pool model
    - User-defined materials, in reactor or non-reactor calculations

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What are DCH Classes (?)

- Actual radionuclides are sources of decay heat, radiological activity
  - Heat calculated by DCH package in MELCOR
    - (DCH name long preceded Direct Containment Heating)
  - Activity models added by IBRAE
  - Heat and activity sources relocate with radionuclides (in fuel or fluid, on walls, …)
    - MELCOR modeling of feedback was a major advancement in capabilities
- For each class, RN database contains
  - Radioactive masses for which DCH calculates decay heat
    - Heat may be zero
  - Total mass including OH in CsOH, O_4 in Cs_2MoO_4, etc., and possible nonradioactive elements from non-fuel sources
    - Total mass important for aerosol physics

What’s the Difference?

- DCH class generally corresponds to RN class
  - Contains all isotopes of all elements in the class at the time of reactor shutdown, *and all their decay daughters*
  - Non-radionuclide classes included with zero decay heat and activity
- Currently requires redundant input
  - Need for consistency between two packages
    - Input differs between MELCOR 1.8.6 and MELCOR 2.1
      - 2.1 Can’t run RN1 without DCH unless all radioactive masses are zero
      - Most existing output aimed at radioactive masses
- Further confusion from long vs. short names
  - Long names like ‘NOBLE GASES’ and ‘CONCRETE’
  - Short names like ‘XE’ (characteristic element) and ‘CON’
  - Not clear which to use in input
    - Can end up defining unintended new class

Objective of This Presentation

- Give some understanding of a few within-volume models in MELCOR RN1 Package
  - MAEROS
    - Aerosol physics
  - TRAP-MELT
    - Condensation and evaporation involving aerosols and surfaces
  - Water aerosol models
    - CVH “fog”
    - Hygroscopic model

MAEROS (1)
Multicomponent AEROSol model

- Calculates time history of aerosol particle size distribution and <u>CHEMICAL COMPOSITION</u>
  - Calculates changes in masses of each component (material) in each section as a function of time. Prior to this development, material composition of aerosol was unavailable and all particles were assumed to be of the same chemical composition regardless of particle size.
  - Currently limited to requiring that all aerosol components (materials), have the same material density.
  - Solves multi-sectional, multi-component formulation of dynamic equations for deposition and agglomeration.

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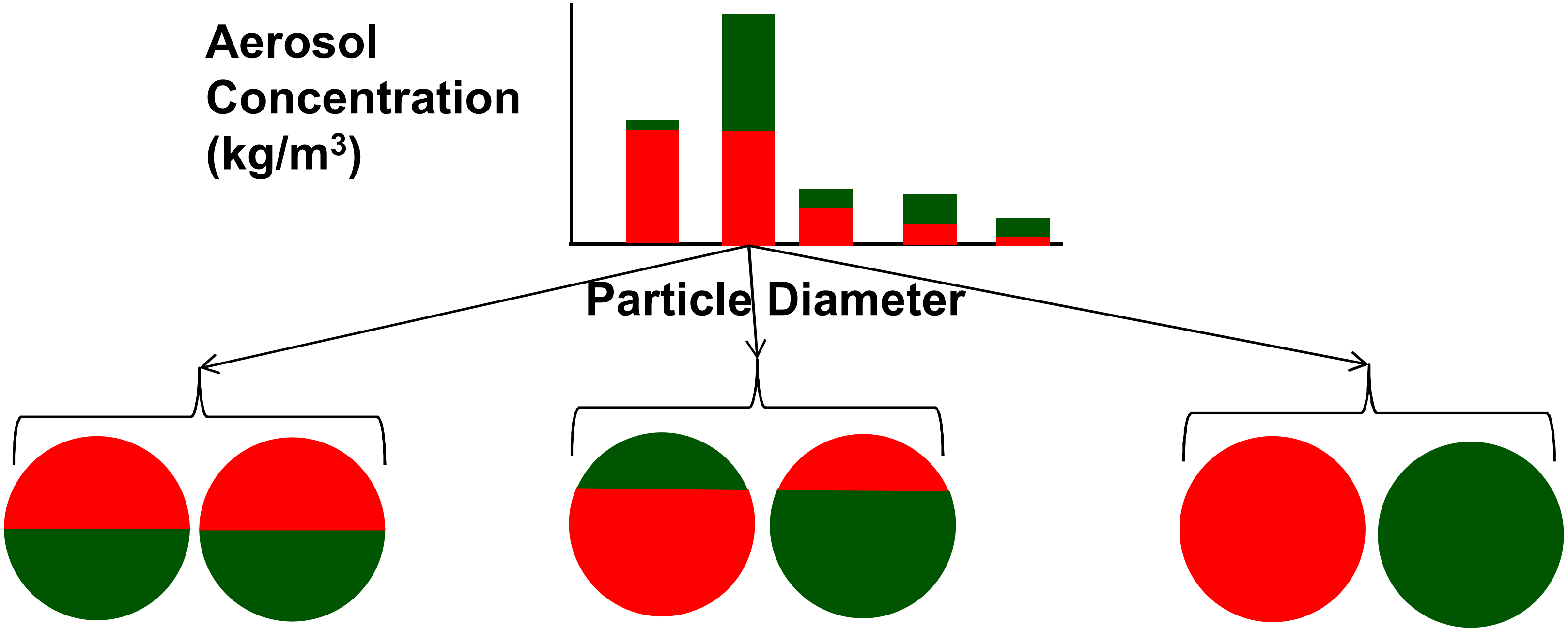
Basic Conceptual MAEROS Model (2)



Mass of each aerosol component as a function of particle diameter is used to determine health effects, but that is not a unique representation.

<u>Basic Approximations</u>

- **The total mass of a particle determines how the particle deposits, agglomerates, and grows.**
- **(Currently) All component material densities are the same.**

MAEROS (3)

- *Sections* are particle size bins based on particle mass.
- Default is 10 sections between 0.1 μm and 50.0 μm in geometric diameter
  - Diameter boundaries: 0.100, 0.186, 0.347, 0.645, 1.20, 2.24, 4.16, 7.75, 14.4, 26.9, 50.0 μm
  - Can change number of sections, limits set through user input
    - To simplify analysis, agglomeration of two particles can't produce mass beyond next-larger section (particle size bin)
    - Requires diameter ratio > $2^{1/3}$ = 1.26
    - For 0.1 to 50 μm diameter, maximum of 26 sections ($2^{n/3} < 50/0.1$), n = 26.
    - Rule of thumb: Up to 9 sections per decade of particle diameter

MAEROS (4)

- ***Components*** **are materials**
  - **Each component has an independent size distribution**
  - **Conventional to take all densities as nominal 1000 kg/m^3**
    - **Particles are rarely single spheres, so aerodynamic diameter is often used instead**
      - **Aerodynamic diameter (d_a) is the diameter of a sphere with a material density of 1000 kg/m^3 with the same settling velocity as the particle**
      - **Dynamic shape factor (χ) and agglomeration shape factor (γ) are included to compensate for nonspherical effects**
      - **$d_a = d_e (\rho/1000)^{0.5}$, d_e = volume equivalent diameter**

Phenomena Treated by MAEROS (1)

- **Deposition on surfaces**
  - Modeled as always sticking to surfaces contacted
  - Several mechanisms drive aerosols to surfaces
    - Gravity ("falling to the floor") usually dominates
    - Brownian diffusion to surfaces
    - Migration to cooler surfaces by thermophoresis
    - Migration to surfaces by diffusiophoresis
    - Turbulent deposition model
- **Resuspension of aerosols**
  - "Liftoff Model for MELCOR," Mike Young
  - SAND2015-6119
- **Agglomeration of aerosols**
  - Several mechanisms cause collisions and sticking to produce larger particles
    - Brownian diffusion (random relative motions)
    - Differential gravitational settling ("sweep up")
    - Turbulent agglomerating by shear and inertial forces

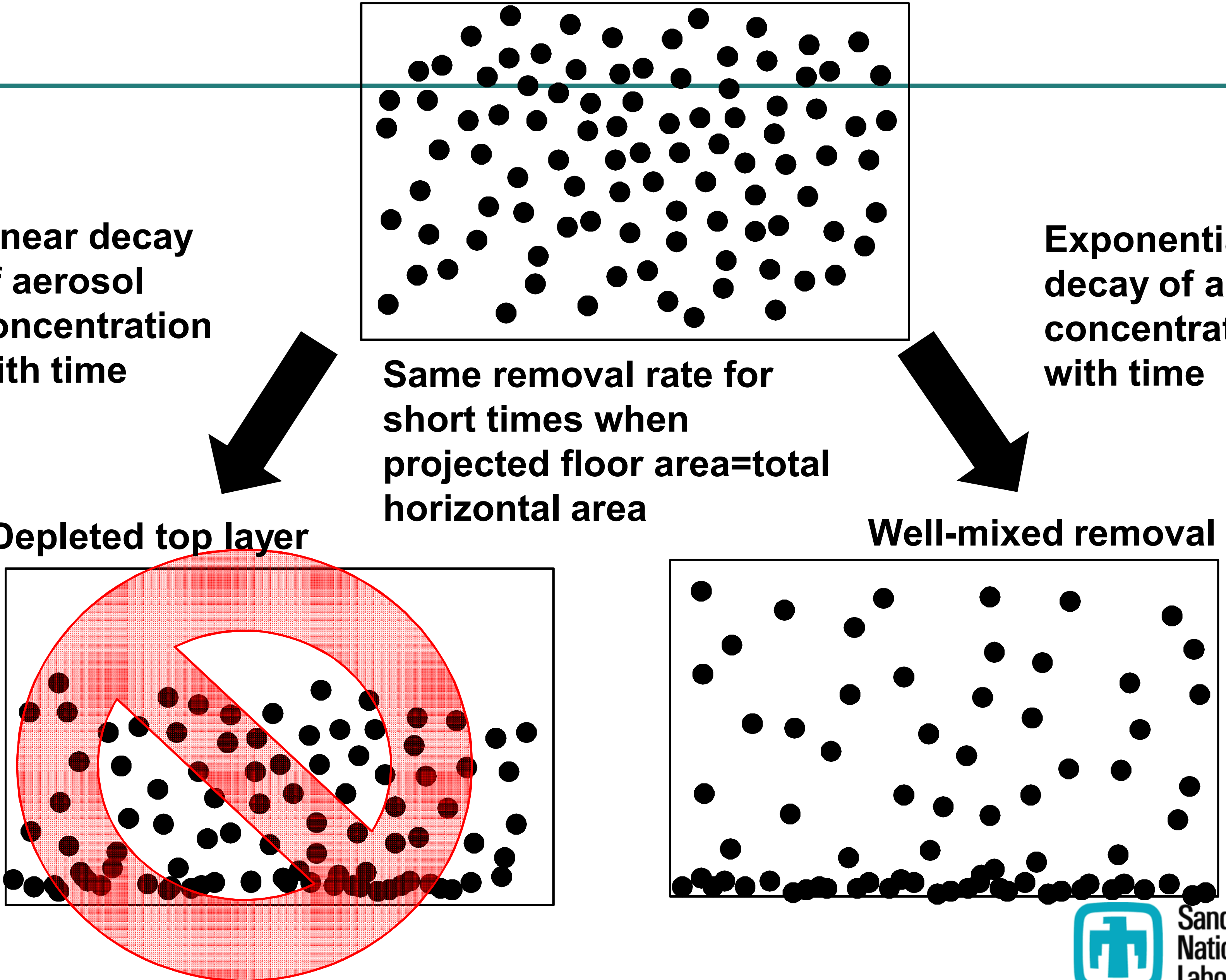
Phenomena Treated by MAEROS (2)

- Condensation and evaporation
  - Disabled in MELCOR in favor of TRAP-MELT
- Disposition of particles that grow larger than computational domain (to conserve mass)
  - Ordinarily "settle" immediately
  - This requires at least one available surface in each volume
    - Ordinarily "floor" or other surface redefined as "floor"
- MELCOR adds additional "settling surfaces" to represent common boundaries of volumes
  - Treated as deposition surfaces
  - Allows aerosols to fall from one volume to another
  - Can also provide destination for oversize particles
    - Settling from a volume to itself is permitted, but considered an "evil practice"

Conceptual Modeling of Settling (1)

- 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)



Linear decay of aerosol concentration with time

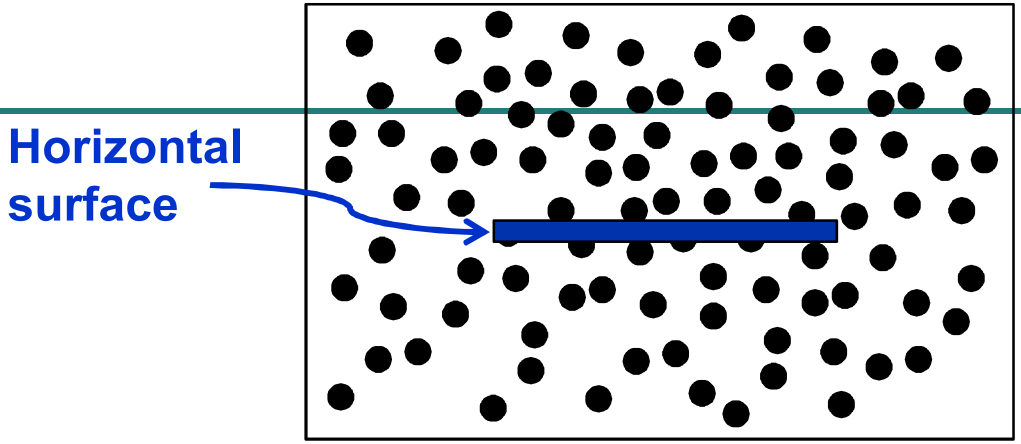
Exponential decay of aerosol concentration with time

Same removal rate for short times when projected floor area=total horizontal area

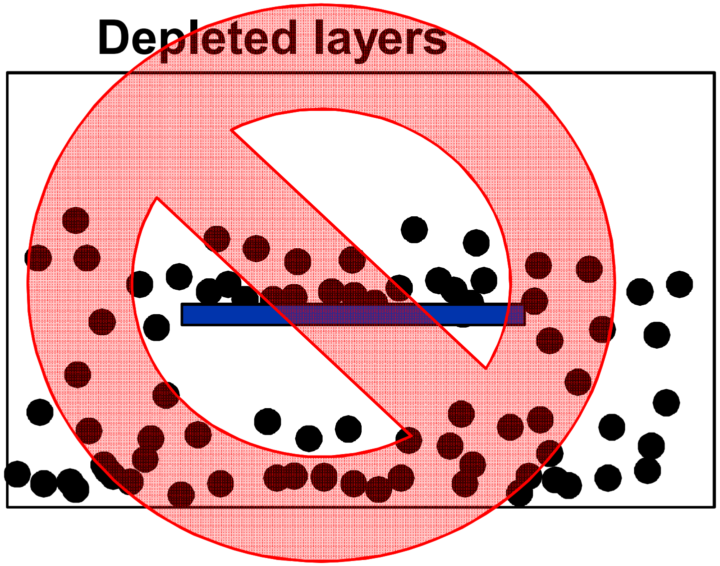
Depleted top layer

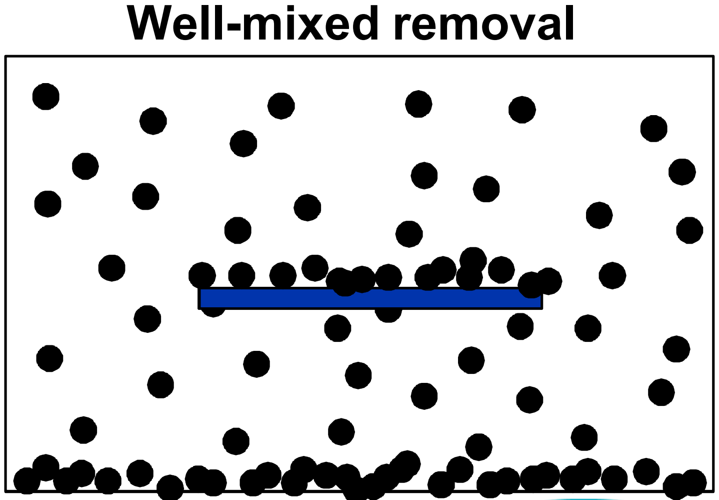
Well-mixed removal

Conceptual Modeling of Settling (3)



Use to <u>total</u> horizontal area to be consistent with well-mixed model of control volume


Depleted layers


Well-mixed removal

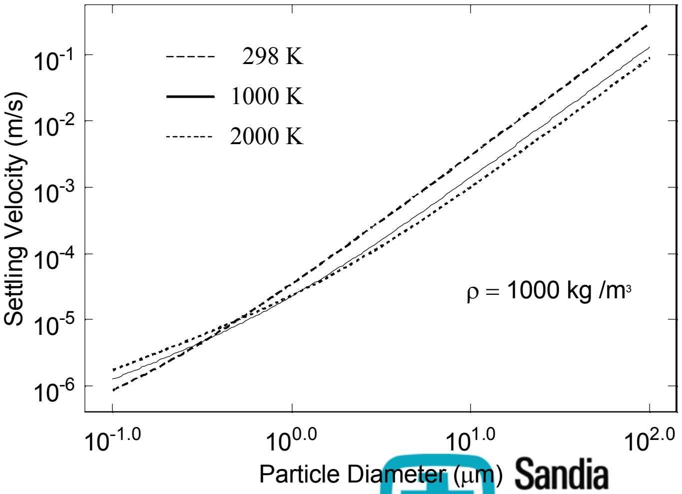
Gravitational Deposition

- 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)

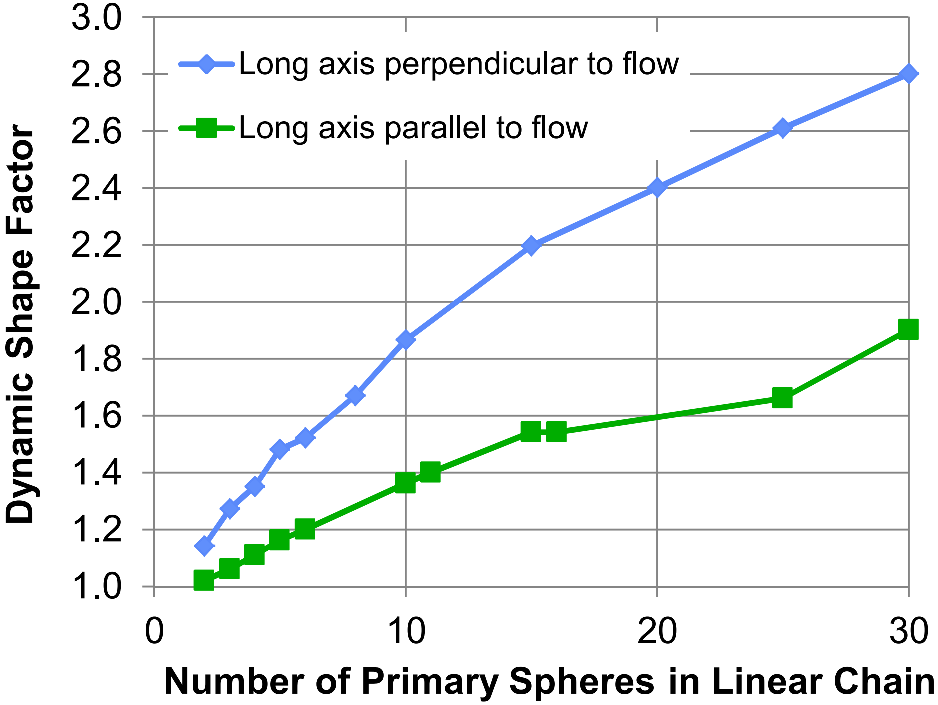
- Leading size dependence is $\rho\, d_p^2$
  - Note velocity ~3 mm/s for a 10 μm sphere with $\rho = 1000\ kg/m^3$



Shape Factors: What to Use and Why

Shapes	χ
Sphere	1.00
Cube	1.08
4 sphere cluster	1.17
Sand	1.57
Talc	2.04

W. C. Hinds, Aerosol Technology, 1982.

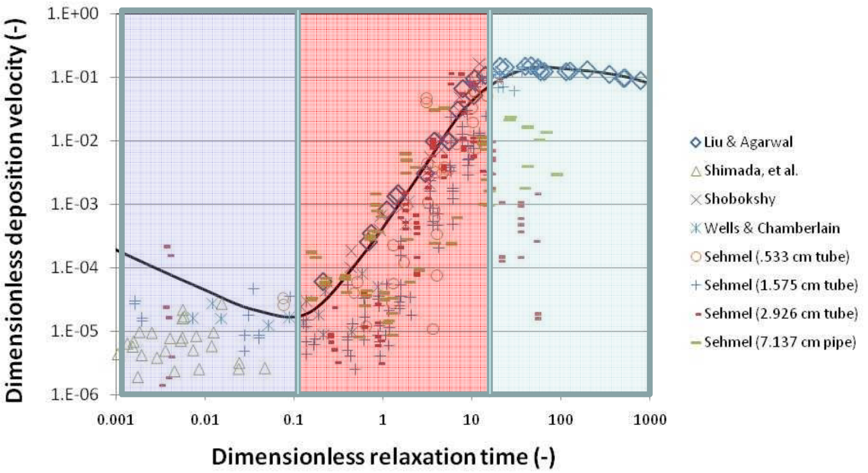


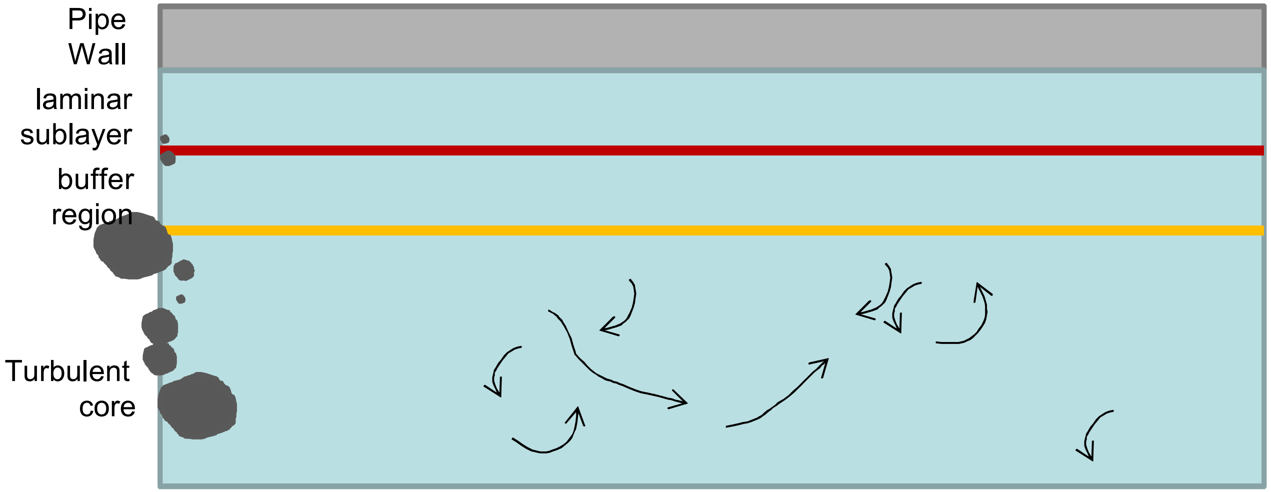
Recommendation: use 1.00 unless data available.

Kasper, G., T. Niida, and M. Yang, "Measurements of viscous drag on cylinders and chains of sphere with aspect ratios between 2 and 50," *J. Aerosol Science*, 16 (6), 535-556, 1985.

Turbulent Deposition Regimes

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





Very small particles where Brownian motion is important to transport particles viscous sub layer.

Larger particles dominated by eddy diffusion where particles are accelerated to the wall due to turbulent eddies in the core and buffer layer and coast across the viscous sub-layer.

Very large particles which are subject to reduced acceleration by the turbulent core and little acceleration to small eddies in the buffer near the wall.

Turbulent Deposition Model

- Particle Diffusion Regime
  - Davies equation

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

- 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

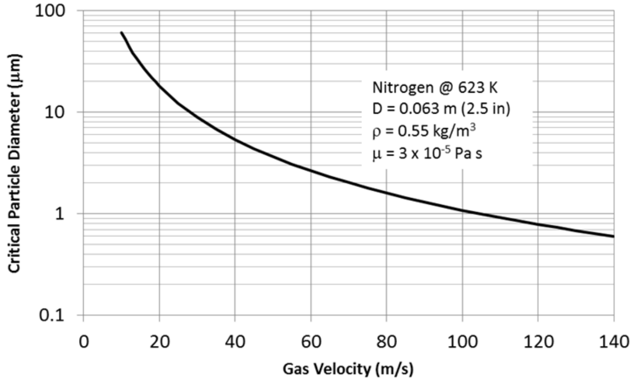
$$V_d^* = \frac{2.6}{\sqrt{\tau_*}}\left(1 - \frac{50}{\tau_*}\right) \qquad \tau_* \ge 270$$

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

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

  - 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



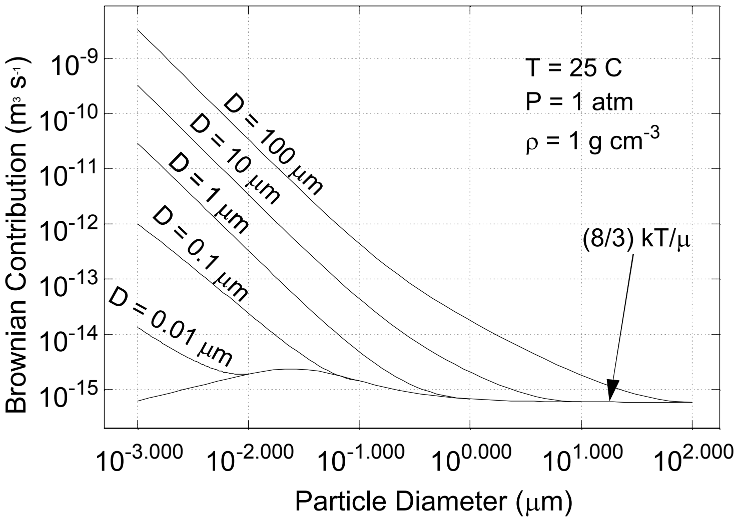
Examples

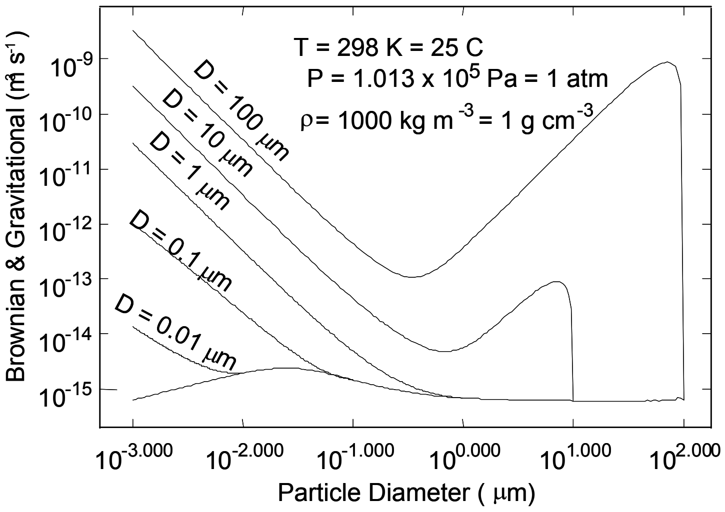
To fully activate resuspension, specify a value of FractResuspend as 1.0, and let MELCOR determine the critical diameter:

HS_LBAR 1. ! Left surface
HS_RBAR 1. ! Right surface

Agglomeration

- **Agglomeration becomes more significant for more concentrated aerosols**
  - **Particles collide, stick, and become larger particles; Rate ~ $\beta N(D_i) N(D_j)$ where N is the number density (m^{-3})**
  - **Brownian mechanism dominates for small particles, differential gravitational for large ones**





Composition of Individual Particles

- MAEROS tells you only the mass of each material in particles in each size bin
  - It *does not* tell you the composition (or distribution of compositions) of any particle
- Deposition and agglomeration depend only on mass, diameter, and shape factors
  - Assume that the densities of the materials are the same and the shape factors depend at most on particle size
  - Then, independent of composition
    - All particles in each section deposit at same rate
      - If fraction x in section ℓ is component n, than fraction x of deposition from this section will be component n
    - *On average*, particle collisions will involve the same masses of each component
      - Section-to-section transfers will carry same mass of each component from section to section

Note on MAEROS Coefficients

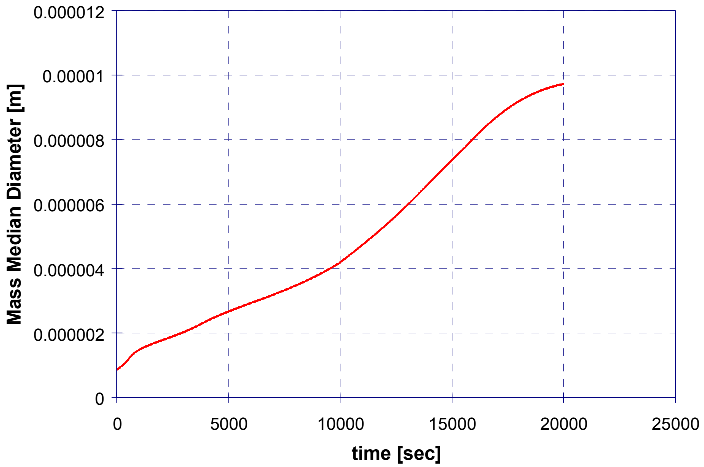
- **Coefficients used by MAEROS are not calculated during transient**
  - **Require integrals over sections for deposition, double integrals for agglomeration**
    - **Calculations are relatively time-consuming**
  - **Values pre-calculated at corners of a finite (*P*,*T*) domain**
    - **Values interpolated for each volume at appropriate (*P*,*T*)**
      - **Recent versions of MELCOR use bilinear interpolation in P^a and T^b,**
    - **Properties of *air* used in pre-calculation**
      - **Should be accurate in normal containment calculations**
      - **May be inaccurate in other cases**

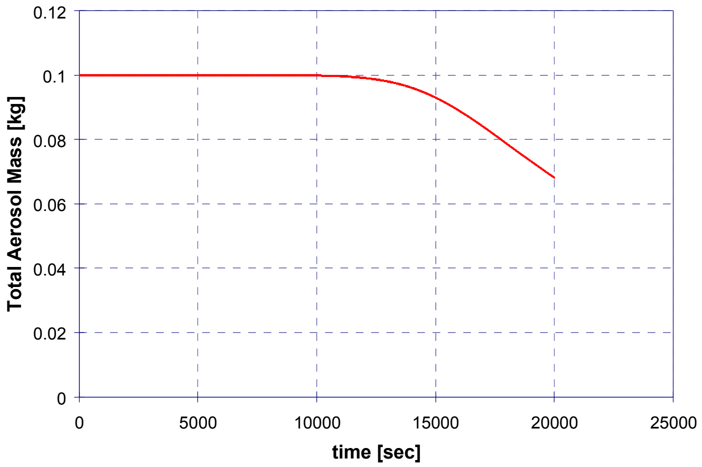
Simple Agglomeration Calculations

- Single material, nominal density = 1000 kg/m^3, tiny surface to effectively eliminate deposition
- Three cases with single d_p ~1μm or ~10μm
  - Case 1: d_p=0.880μm, ρ =1000kg/m^3, 10^{-10} m^2 surface
  - Case 2: d_p=10.57μm, ρ =1000kg/m^3, 10^{-10} m^2 surface
  - Case 3: d_p=10.57μm, ρ =1000kg/m^3, 10^{-10} m^2 surface, settle back to same volume through 15 m^2 "settling surface"

Results of Agglomeration Calculations

- Line graphs don’t provide much insight
- For Case 1

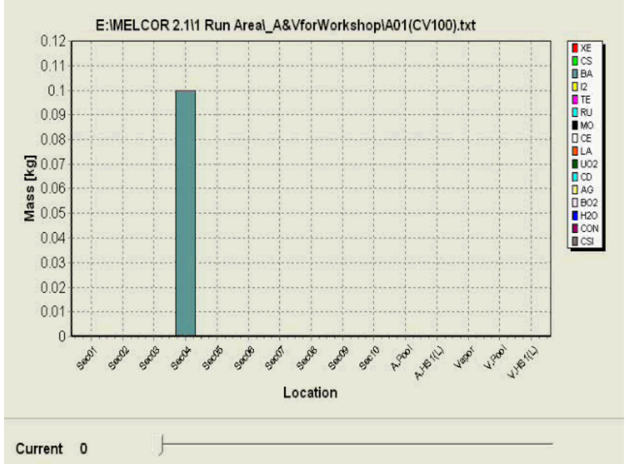




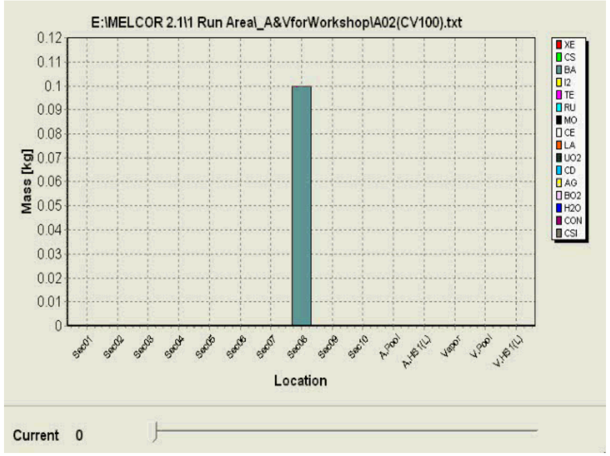
  - Mean diameter increased from ~ 1 μm to almost 10 μm
  - Some mass must have been deposited (or settled)
  - But what *really* happened?
- Other cases are *much* more difficult

Visualization of Results, Case 1

- **Case 1**
  - — Initial ~10 μm (section 8)
  - — Tiny (10^{-10} m^2) deposition area
  - — Rapid growth to section 10 and larger
    - ✶ See creation of larger aerosols, settling of those larger than limit of computational domain

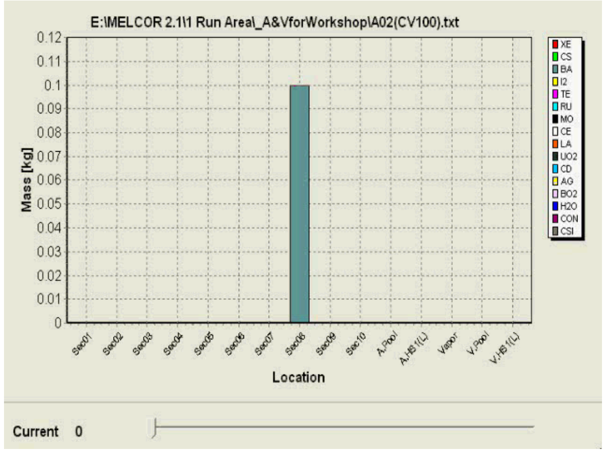


- **Case 2**
  - — Initial ~10 μm (section 8)
  - — Tiny (10^{-10} m^2) deposition area
  - — Rapid growth to section 10 and larger
    - ✶ Mass settles to heat structure surface despite tiny area

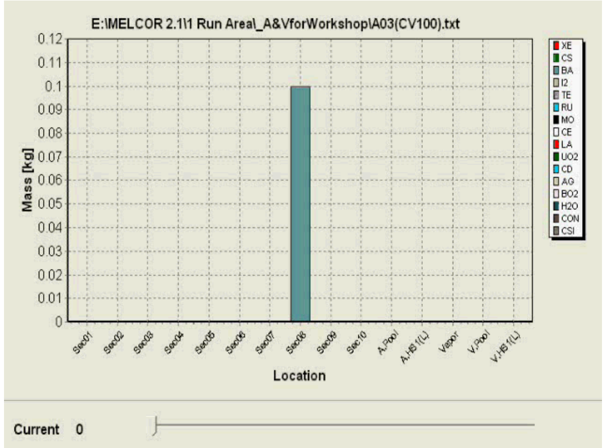


Visualization of Results, Cases 2 and 3

- **Case 2**
  - Initial ~10 μm (section 8)
  - Tiny (10^{-10} m^2) deposition area
  - Rapid growth to section 10 and larger
    - Mass settles to heat structure surface despite tiny area



- **Case 3**
  - Like Case 2 *but* 15 m^2 settling area from volume to itself
  - All mass stays suspended
    - *Huge* population in section 10 sweeps up all smaller aerosols
    - *Not physical*



Multi-Material Aerosols

- **RN Package and MAEROS each treat more than one material, but treatments differ**
  - **Main RN database includes distinct size distribution for each RN class (Cs, Ba, UO2, …)**
  - **MAEROS considers only a limited number of *components***
    - **Each contains one or more RN classes**
      - **Component masses in each section calculated at start of MAEROS advancement as sums of class masses; sub-compositions saved**
      - **Post-advancement component masses are distributed to RN class distributions using sub-compositions**
    - **User can define number of components and the classes assigned to each**
      - **Default is 2, with one component reserved for water and all other classes in the other**
      - **Recommend 3 which (absent further input) will further assign the volatiles (Cs, I2, CsI, CsM) to a separate component**
      - **Can modify these, or add other components to track classes of interest or classes with very different release histories (like CON from ex-vessel core/concrete interactions)**

Two-Material Agglomeration Calculations

- Ran two versions of a 2 material case
  - Initial 0.1 kg of Ba aerosol, d_p=0.880μm
  - Initial 0.1 kg of UO2 aerosol, d_p=10.57μm
  - ρ =1000kg/m^3, 10^{-10} m^2 surface
- Case 4: default component assignments
  - Both Ba and UO2 assigned to component 1
- Case 5: custom component assignments
  - Ba assigned to component 1, UO2 to component 4

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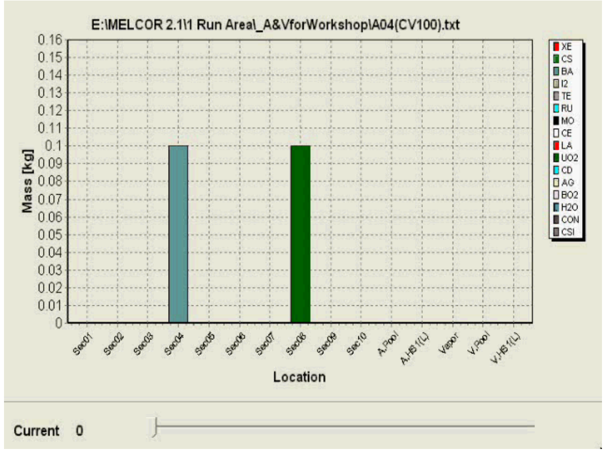
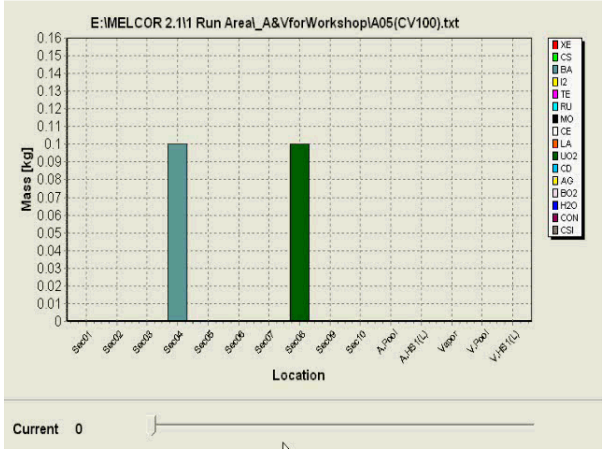
Visualization of Results, Cases 4 and 5

- Case 4 (same component)
  - MAEROS does not maintain distinction
    - Aerosol distribution “homogenized” on first advancement
      - Puts half UO2 mass into smaller section, half Ba mass into larger one



- Case 5 (distinct component)
  - MAEROS maintains distinction
    - Agglomeration of small and large aerosols slowly moves some Ba mass into larger sections



TRAP MELT

- Models condensation and evaporation of RN vapors involving aerosols and surfaces (replaces treatment in stand-alone MAEROS)
- Volatile radionuclides (e.g., CsOH, I_2, CsI, Cs_2MoO_4), have finite vapor pressures that increase with temperature
  - Concentration in atmosphere limited by vapor pressure at T_{atm}
  - Mass can be transported to/from condensed phase on aerosol surfaces and/or structural surfaces
    - Aerosols are at atmosphere temperature
    - Structure surfaces may be hotter or colder
    - Rate limits apply

TRAP MELT Equations

- Conservation of mass, and rate equations are

$$\frac{dM_a}{dt} + \sum_i \frac{dM_i}{dt} = 0 \qquad \frac{dM_i}{dt} = A_i k_i \left(C_a - C_i^s\right)$$

  - *M* is mass, *C=M/V* is concentration, subscript *i* refers to surface, superscript *s* is saturation at surface temperature
    - Surfaces include aerosols, section by section
- Model evaluates closed-form solution for full MELCOR timestep, Δ*t*

$$C_a = M_a / V = \frac{\beta}{\alpha} - \left(\frac{\beta}{\alpha} - C_{a0}\right) e^{-\alpha\Delta t} \qquad M_i = M_{i0} + A_i k_i \left(\frac{\beta}{\alpha} - C_i^s\right) \Delta t - A_i k_i \left(\frac{\beta}{\alpha} - C_{a0}\right) \left(\frac{1 - e^{-\alpha\Delta t}}{\alpha}\right)$$

$$\alpha = \sum_i A_i k_i / V \qquad \frac{\beta}{\alpha} = \frac{\sum_i A_i k_i C_i^s}{\sum_i A_i k_i}$$

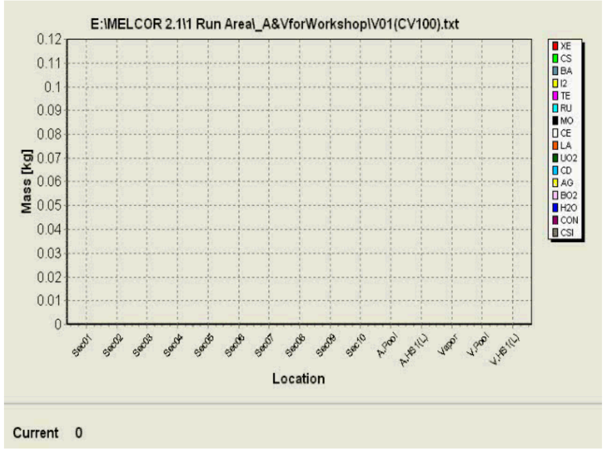
  - Iteration may be needed if any surface mass falls to zero

Condensation Aerosols

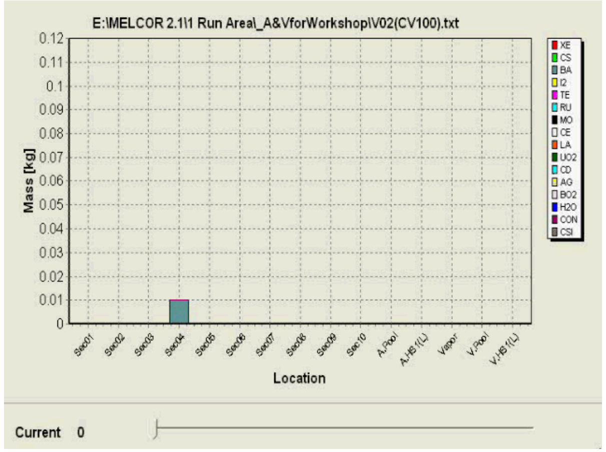
- Ran test cases with the 45 m^3 room and Cs (actually, CsOH) vapor source
  - Temperature raised to 780 K, where mass corresponding to saturation is 0.00685 kg
  - Cs-class vapor mass added at 10^{-5} kg/sec
    - Takes 685 s to reach saturation
  - Chemisorption model turned off
  - Two cases
    - Case 1: no initial vapor or aerosol
    - Case 2: no initial vapor, initial 0.01 kg non-volatile (Ba) aerosol ~0.88 μm

Condensation Aerosol Results

- **Case 1**
  - Cs concentration rises to saturation
  - First aerosols form in smallest section, then agglomerate rapidly
  - Further condensation on existing aerosols



- **Case 2**
  - Same rise to saturation
  - Most early condensation on existing Ba aerosols



Comments on Condensation Calculations

- **See almost no direct condensation on walls**
  - **Wall and aerosol areas comparable (within factor of 10)**
  - **Mass transfer coefficient for wall is *much* smaller**
    - **Characteristic length in Sherwood number (analog of Nusselt number) is much larger, m *vs.* µm**
- **Could construct other cases**
  - **Smaller aerosol concentrations**
  - **Multiple walls**
    - **Different temperatures**
    - **Initial deposited vapors**
  - **Encourage others to try variations**
- **Omitted to allow time for Water Aerosol cases**

Water Aerosols

- Water also forms aerosols, but water vapor is a hydrodynamic material
- Mass, volume, heat capacity of RN vapors and aerosols is ignored by hydrodynamics
- Condensation/evaporation for water aerosols can’t be solved as for other aerosols
  - Interactions too complicated to solve simultaneously

Water Aerosol Models

- MELCOR provides two models
  - Original model
    - Water aerosol identified with CVH "fog" (liquid water in atmosphere)
  - Hygroscopic model
    - RN "takes possession of" all liquid water in atmosphere
      - Necessary to account for hygroscopic and Kelvin effects that modify vapor pressure of water in aerosol form so that it is different from water in the rest of MELCOR (CVH, HS, …)
    - Condensation taken from CVH water vapor, evaporation returned to it
      - Also takes any fog that CVH produced on preceding time step
    - Water aerosols deposited on pool and HS surfaces as ordinary water
    - Mass/energy conservation accounting in CVH and HS adjusted for these transfers

Original Model for Water Aerosols (1)

- **Hydrodynamic model determines fog mass in each volume using equation of state**
  - **Mass and energy inventories in atmosphere imply mass of liquid water at equilibrium**
- **RN Package accepts new fog mass (after CVH) as new total water aerosol mass, then imposes the change in size distribution**
  - **Uses MAEROS coefficients based on sectional integration of Mason equation (later slide). Equations are**

$$\frac{dQ_{\ell,k}}{dt} = \ldots + {}^{1}\overline{G}_{\ell,k}Q_{\ell} - \sum_{i=1}^{N_a}\left[{}^{2}\overline{G}_{\ell,k}Q_{\ell,k} - {}^{2}\overline{G}_{\ell\pm1,i}Q_{\ell\pm1,k}\right]$$

    - **Terms account for condensation, loss by move to adjacent section, gain by move from adjacent section**

Original Model for Water Aerosols (2)

- Calculate condensation explicitly, normalized so that sum over sections matches net change

$$\Delta m_w = \sum_{\ell} Q_{\ell}\, {}^{1}\overline{G}_{\ell,w}\; X\, \Delta t$$

  - This gives *X*, a measure of the average driving force

- Calculate sectional transfers implicitly, using post-condensation masses $Q^{o+}_{\ell,k}$
  - For condensation, particles grow—only have up-transfers
    - Solve for new mass in smallest section $Q^{n}_{1,k} = \dfrac{Q^{o+}_{1,k}}{1 + X\, \Delta t\; {}^{2}\overline{G}_{1,w}}$
    - Single pass upwards through sections to evaluate others $Q^{n}_{\ell,k} = \dfrac{Q^{o+}_{\ell,k} + X\;\; \Delta t\; {}^{2}\overline{G}_{\ell-1,w} Q^{n}_{\ell-1,k}}{1 + X\, \Delta t\; {}^{2}\overline{G}_{\ell,w}}$
  - For evaporation, particles shrink—only have down-transfers
    - Evaluate mass in largest section, then work downwards

Hygroscopic Model for Water Aerosols

- **Hygroscopic model**
  - **Based on single-step implicit solution of Mason equation, which accounts for conduction of latent heat (a term) and diffusion of water vapor (b term)**

$$\frac{dr}{dt}=\frac{1}{r}\frac{\left(S-S_r\right)}{a+b} \qquad a=\left(\frac{\Delta h_f^2 M_w \rho_w}{RT_\infty k_a^*}\right) \qquad b=\left(\frac{RT_\infty \rho_w}{D_v^* M_v p_{sat}(T_\infty)}\right)$$

  - ***S* is saturation ratio (relative humidity), *S_r* is effective saturation ratio at particle surface**

$$S_r = A_r \cdot \exp\left(\frac{2M_w\sigma}{RT_\infty \rho_w r}\right) \qquad A_r = \exp\left[-\sum_i \frac{\nu_i n_i}{n_w}\right]$$

    - **Activity factor *A_r* accounts for ionization of dissolved soluble aerosols. This *reduces* equilibrium vapor pressure over solution (usually below saturation)**
    - **Exponential multiplier accounts for Kelvin effect, where surface tension effects “resist” condensation. This *increases* equilibrium vapor pressure (can be greater than saturation)**
  - **Solution requires double iteration to determine end-of-step partial pressure and saturation pressure for water**

Full Disclosure (1)

- There are problems with the hygroscopic model, both in MELCOR 2.1 and in 1.8.6
  - The model in MELCOR 1.8.5 “functioned”, but agreement with experiments for validation needed improvement
  - A new formulation was developed that worked much better for strongly hygroscopic cases
  - Realized that it doesn’t work correctly for others
    - Can have *no* water aerosol, significant “fog” mass can appear, and/or water can get “lost” from calculations
- Improvements were made to MELCOR 2.1 Rev.2013-on, were retrofit to 1.8.6
  - Currently make consideration of Kelvin effect optional, default is to neglect
  - Still being tested
    - Much improved results for simple calculations
    - Haven’t fully checked VANAM (ISP37)

Possible Improvements to Implementation

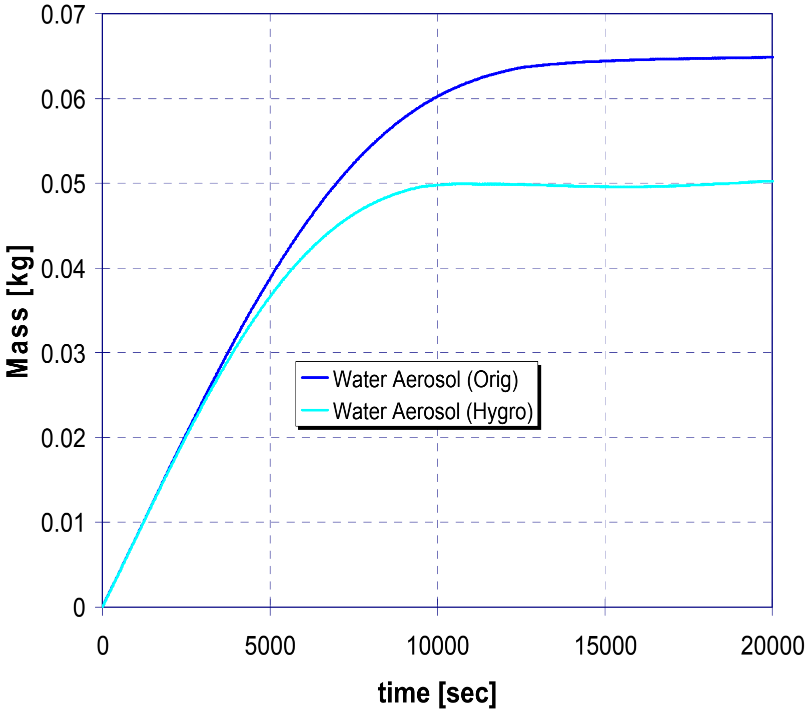
- **Fundamental issue in treating Kelvin effect**
  - **Saturation ratio *S>1* is required for water aerosols in absence of hygroscopic effects**
  - **MELCOR thermodynamics does not include a supersaturated regime**
- **This can probably be dealt with**
  - **Can almost certainly reduce the saturation pressure *used within the model* (with no change to CVH) to allow necessary water to condense**
  - **Would require changes to iteration strategy, untested at this time**

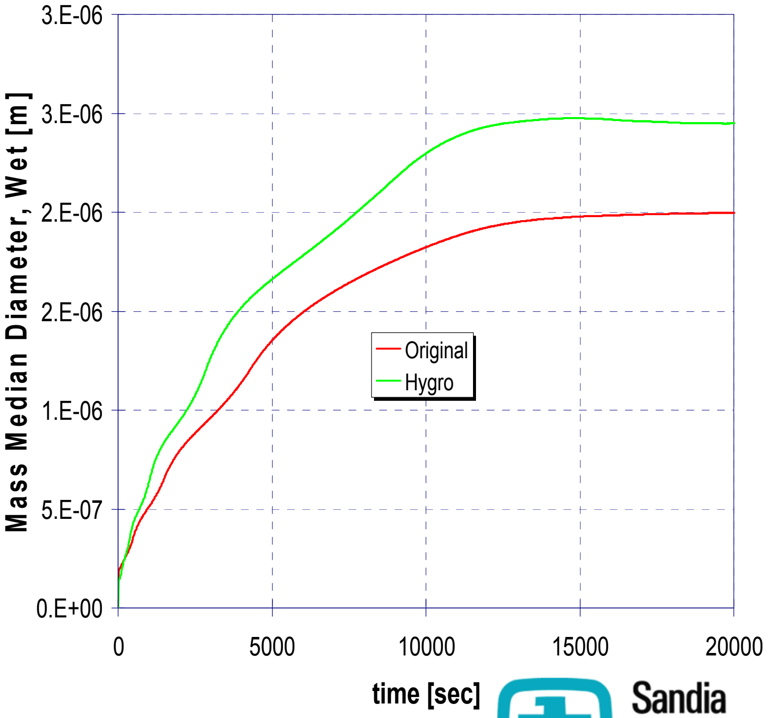
Water Aerosol Calculation

- Ran test cases with the 45 m^3 room, again at 310 K, but now saturated with water vapor
  - Water vapor added (to CVH) at 10^{-5} kg/sec
    - Added with *liquid* enthalpy to avoid heating
  - No initial aerosol
    - Case 1: original model
    - Case 2: hygroscopic model
  - Initial 0.001 kg inert (Ba) aerosol ~0.88 μm
    - Case 3: original model
    - Case 4: hygroscopic model
  - Initial 0.001 kg hygroscopic (Cs) aerosol ~0.88
    - Results using original model look just like inert (Ba) aerosol case (exercise for student)
    - Case 5: hygroscopic model

Results (No Initial Aerosol)

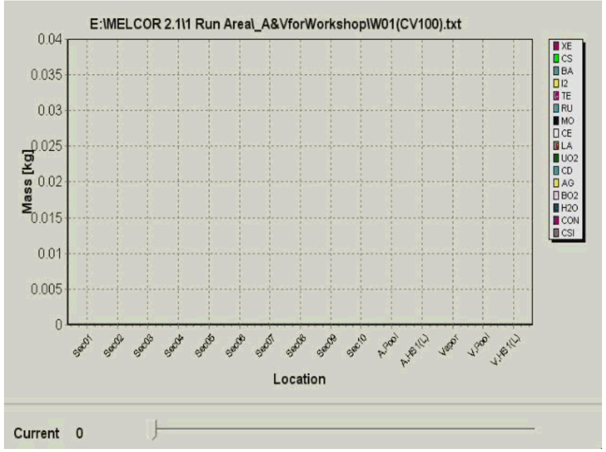
- In a "perfect" world, both models would give the same results
- In current version of MELCOR, results are similar, but not exactly the same



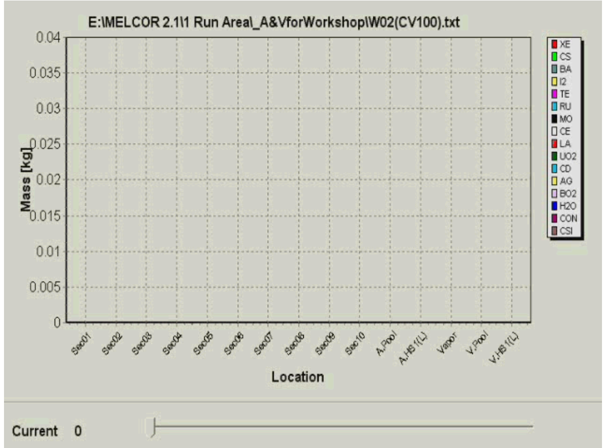


Visualization of Results (No Initial Aerosol)

- Case 1 (Original Model)
  - First aerosols form in smallest section, then agglomerate rapidly
  - Further condensation on existing aerosols

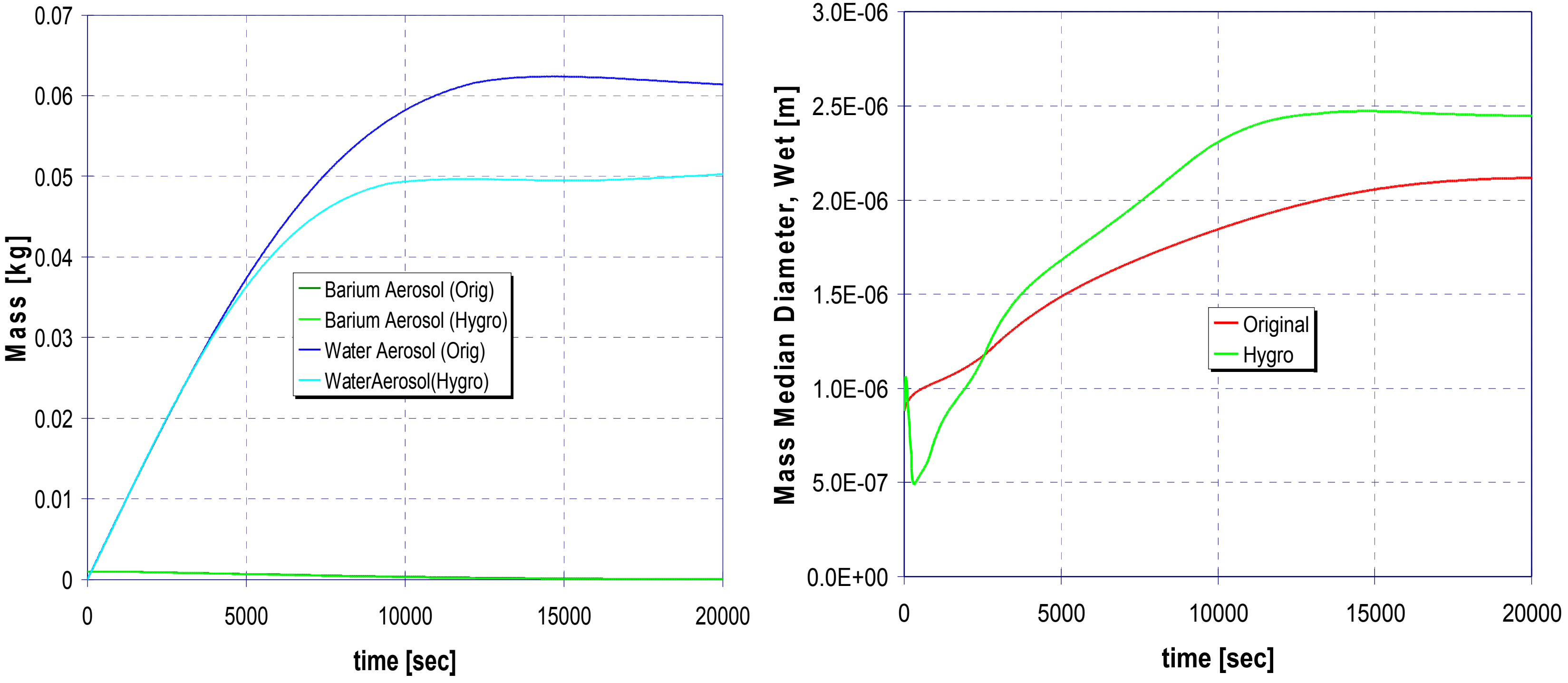


- Case 2 (Hygro. Model)
  - Some differences probably result from different numerical implementation of growth equation
  - Others from addition to smallest aerosol section of condensation in excess of rate based on *end-of-step* conditions



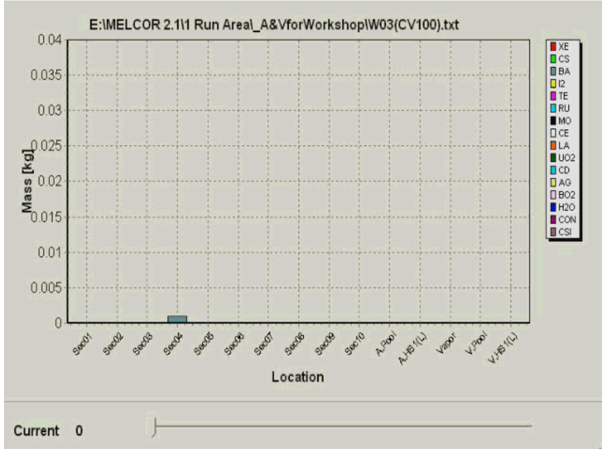
Results (Initial Ba Aerosol)

- **Again, results using the two models are similar, but not exactly the same**

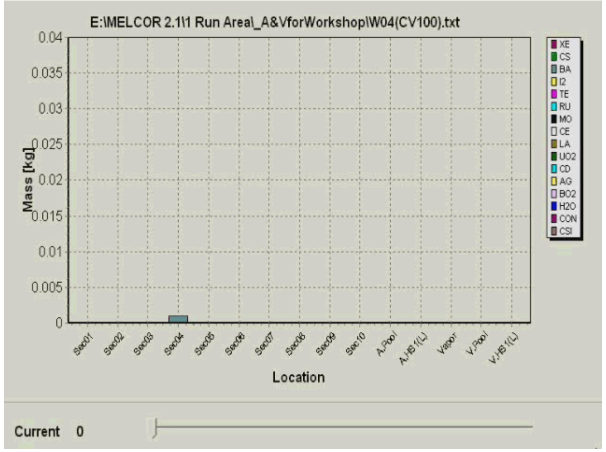


Visualization of Results (Initial Ba Aerosol)

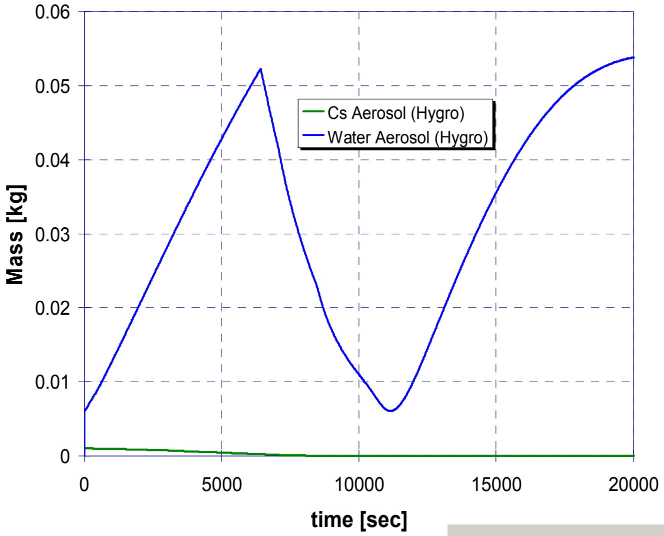
- Case 3 (Original Model)
  - Early condensation on existing Ba aerosols
  - Further condensation on existing Ba and Water aerosols
  - Most Ba deposited relatively quickly

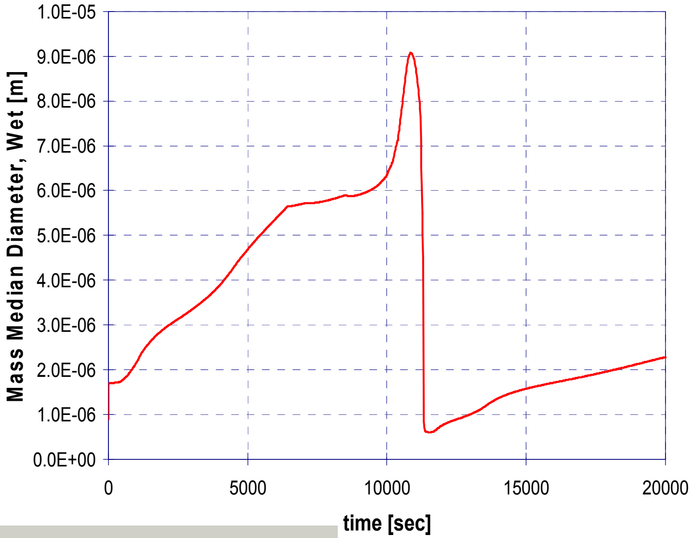


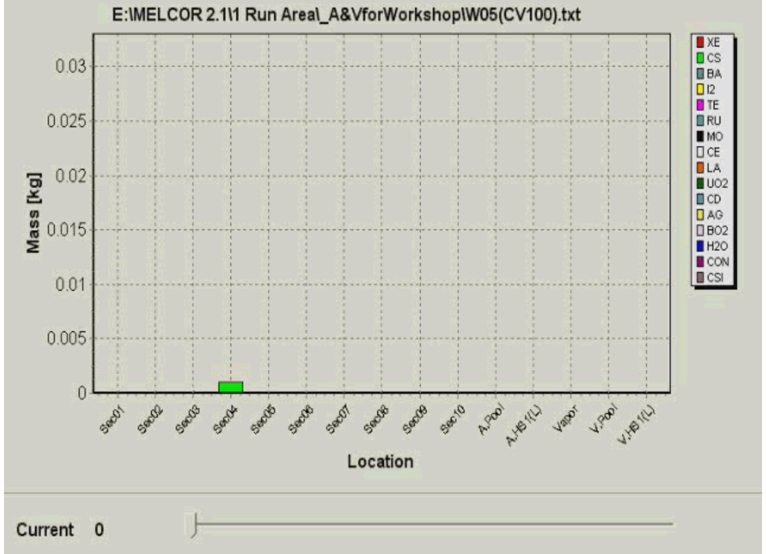
- Case 4 (Hygro. Model)
  - Differences similar to water-only case



Results Case for 5 (Initial Cs Aerosol)



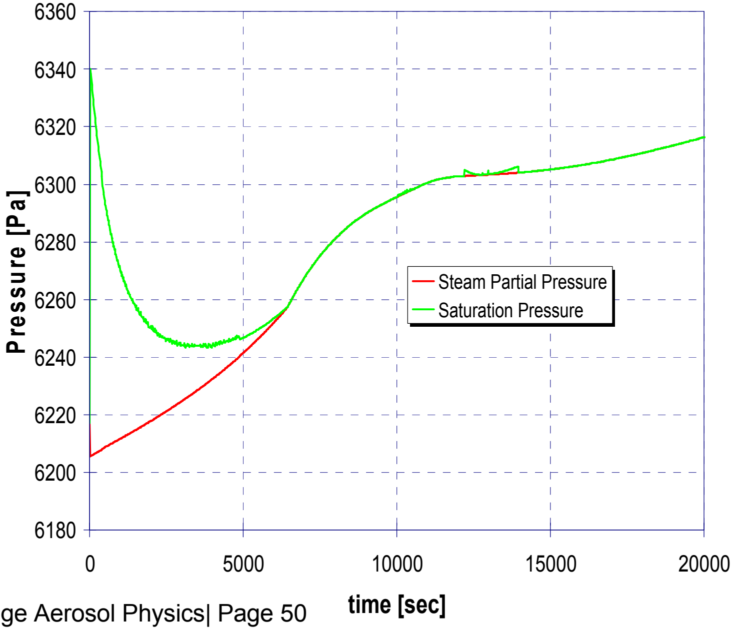


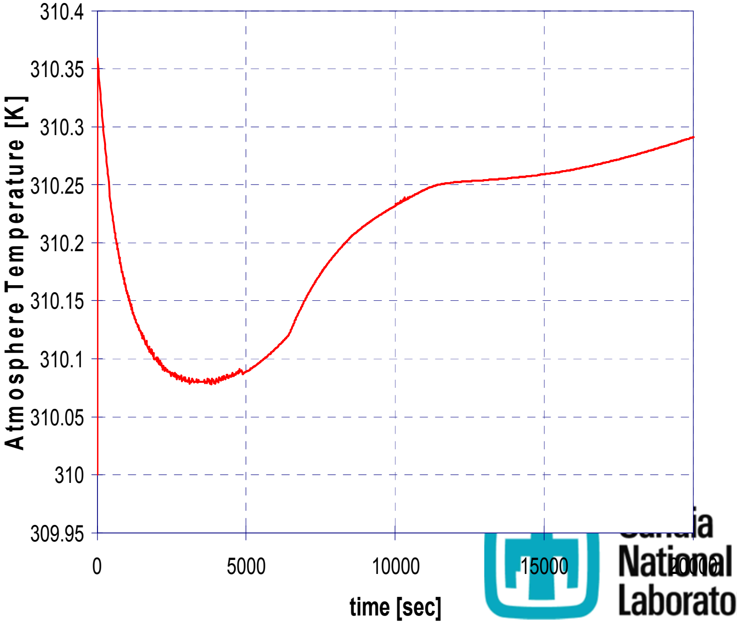


Current 0

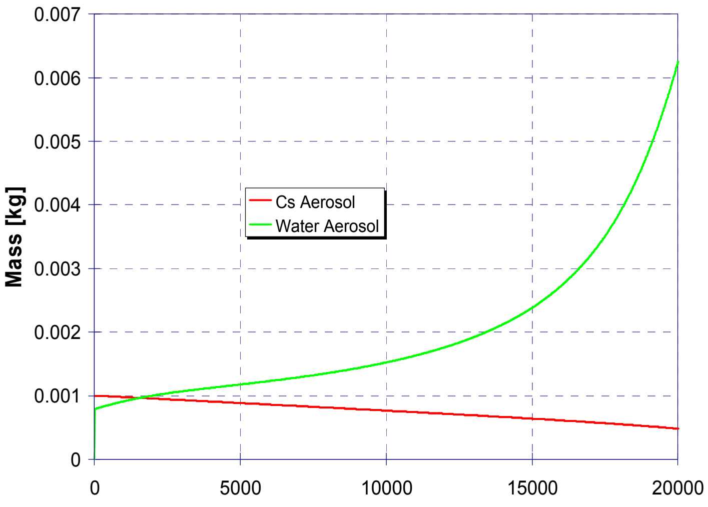
That's Weird - What's Happening?

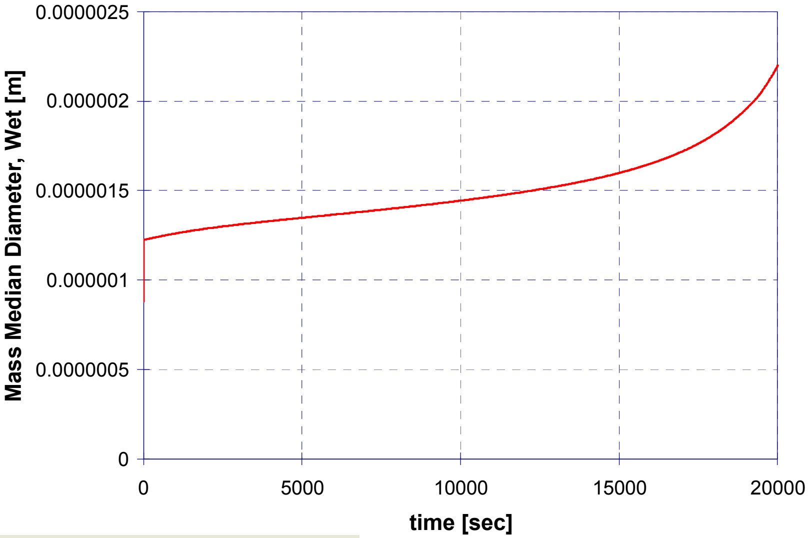
- Initial state is *far* from equilibrium
  - Pure CsOH extremely hygroscopic
  - Initial interaction condenses a lot of water
    - Condensation reduces partial pressure of water vapor; latent heat raises atmosphere temp., saturation press.
  - Most of Cs-containing aerosol deposited by ~6000 s
  - Total surface area too small to support condensation rate at ~11000 s, start forming new crop of tiny aerosols

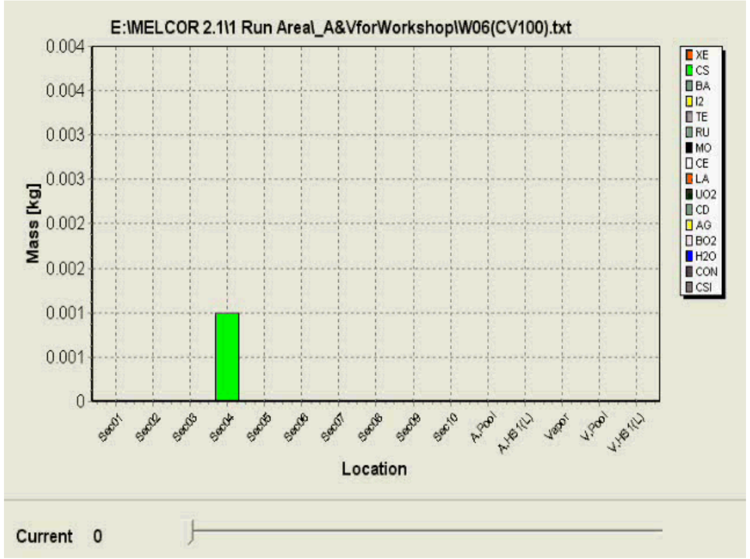




Cs Aerosol, Reduced Initial RH, 85% (1)

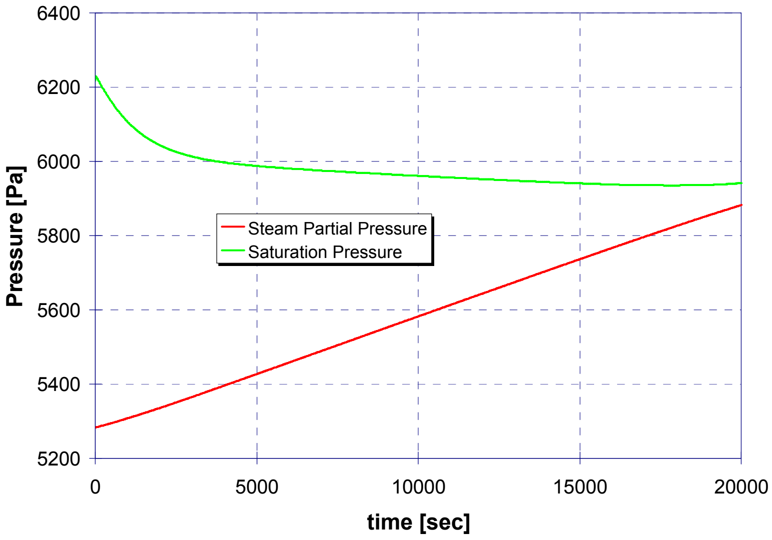


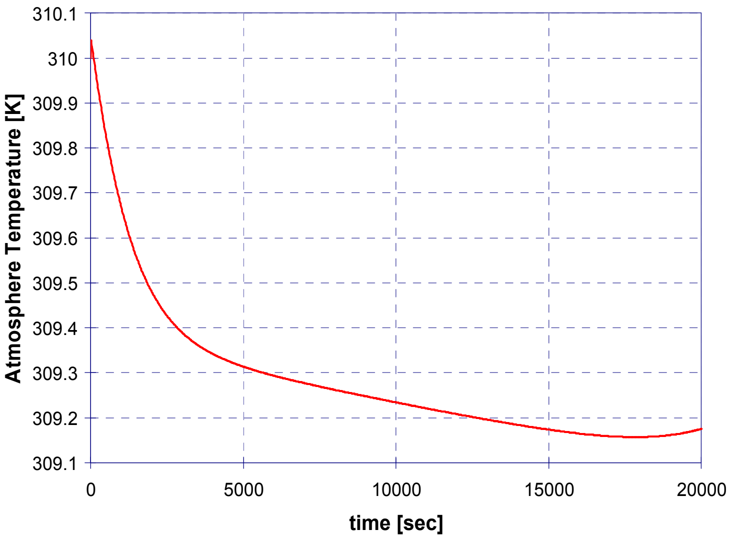




Cs Aerosol, Reduced Initial RH, 85% (2)

- Results look more reasonable
  - Would still see odd behavior if run to later times





Thank You

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