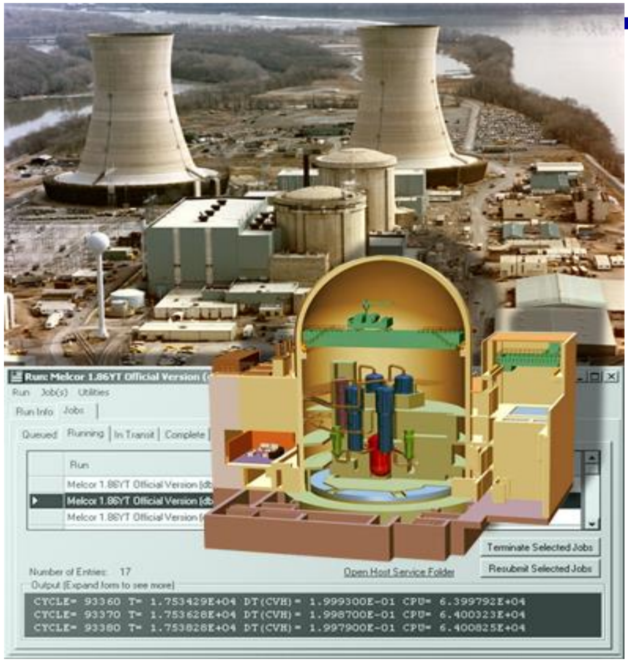

Number of Entries: 17

Output (Expand form to see more)

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CYCLE= 93370 T= 1.753628E+04 DT(CVH)= 1.998700E-01 CPU= 6.400323E+04
CYCLE= 93380 T= 1.753828E+04 DT(CVH)= 1.997900E-01 CPU= 6.400825E+04
```

Aerosol Physics

Presented by

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SAND2018-4218 C

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Aerosol Physics

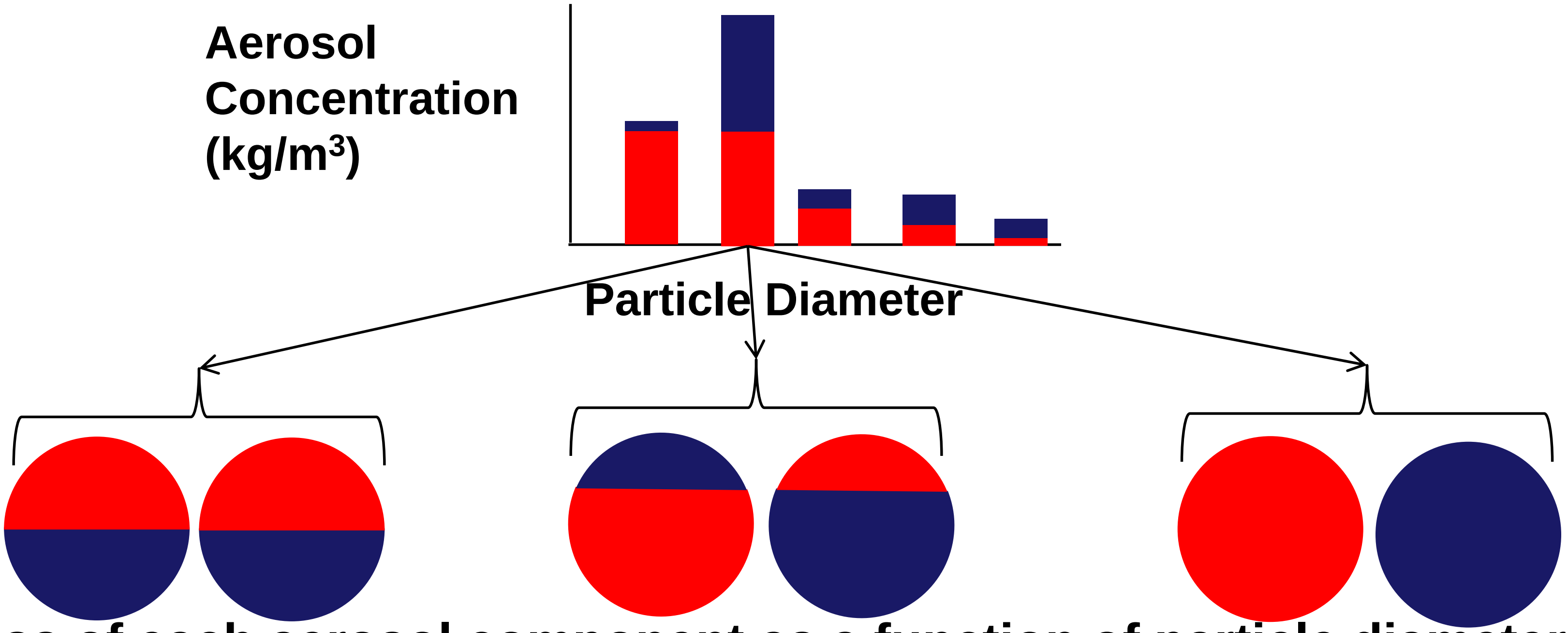
- Agglomeration of aerosols
  - Several mechanisms cause collisions and sticking to produce larger particles
    - Brownian diffusion (random relative motions)
    - Differential gravitational settling (“sweep up”)
    - Turbulent agglomerating by shear and inertial forces
- Hygroscopic models discussed in another presentation

MAERÓS (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.

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.

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

Aerosol Factors: What to Use

- Chi - Aerosol dynamic shape factor (1.0)
- Gamma - agglomeration shape factor (1.0)
- FSLIP – particle slip coefficient (1.257)
- Stick – particle sticking coefficient (1.0)

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.

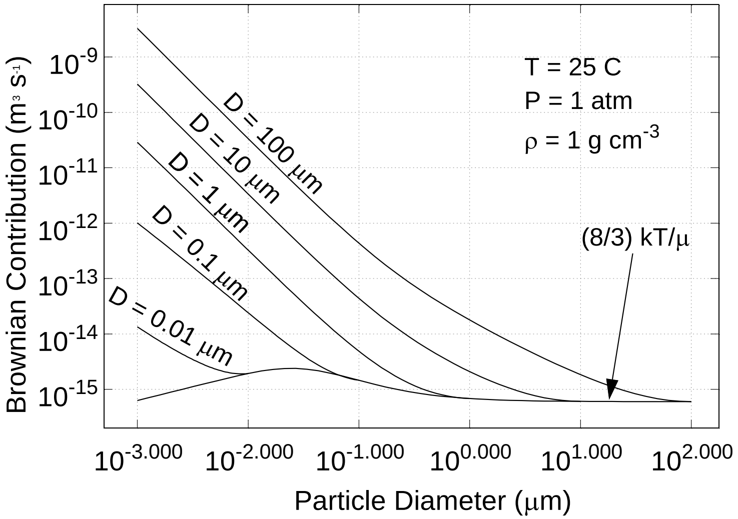
Brownian:	$\beta_B \propto \gamma\, \chi^{-1}\, f(d_i, d_j)$ Stick
Gravitational:	$\beta_{grav} \propto \varepsilon_g\, \gamma^2\, \chi^{-1} (d_i + d_j)^2 (d_i^2 - d_j^2)$ Stick
Turbulent, Shear:	$\beta_{TI} \propto \gamma^3\, \varepsilon^{1/2} (d_i + d_j)^3$ Stick
Turbulent, Inertial:	$\beta_{T2} \propto \gamma^2\, \chi^{-1}\, \varepsilon^{3/4} (d_i + d_j)^2 (d_i^2 - d_j^2)$ Stick

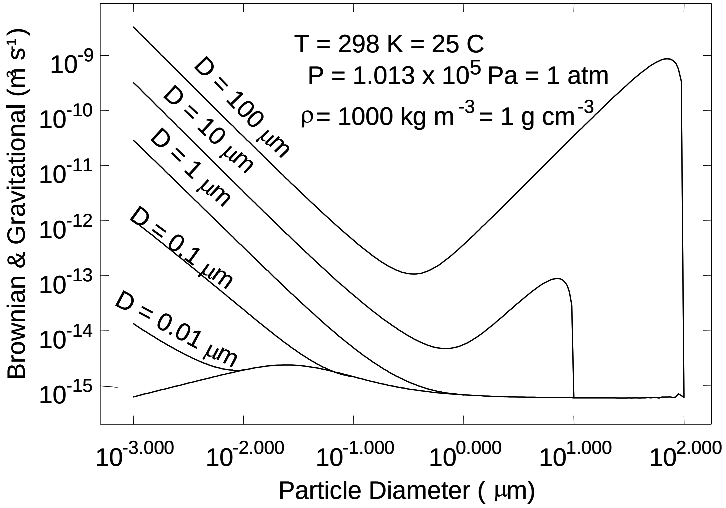
RN1_MS00 chi gamma FSLIP STICK

Recommendation: use default unless data available.

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

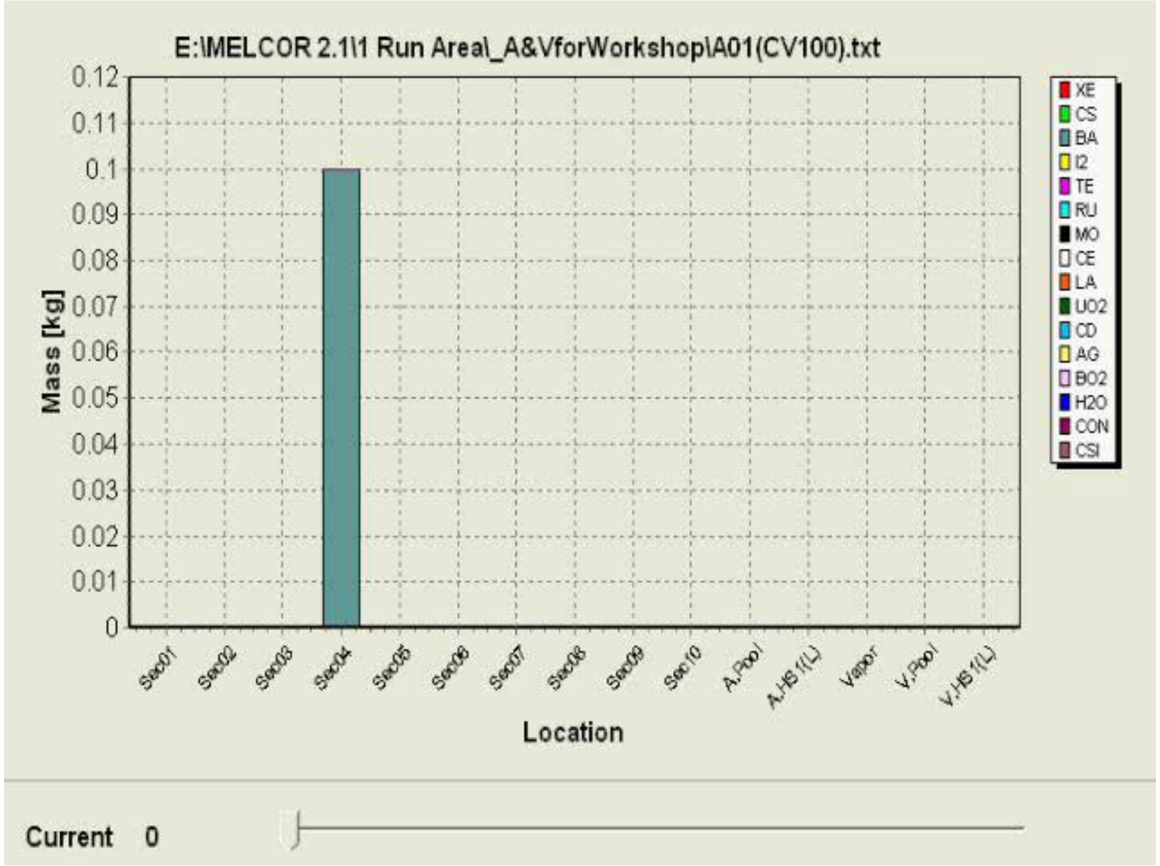
Note on MAEROS Coefficients

- Coefficients used by MAEROS are not typically 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
- Can be re-calculated every time step (RN1_Turb)

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"

Visualization of Results, Case 1

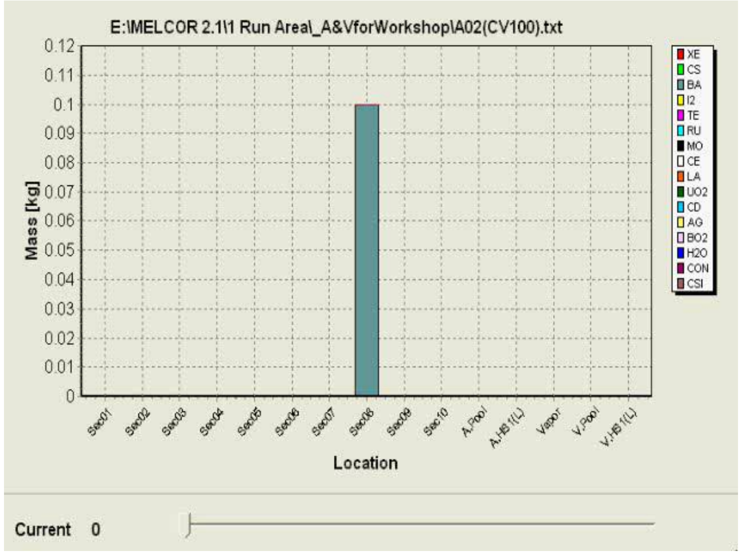


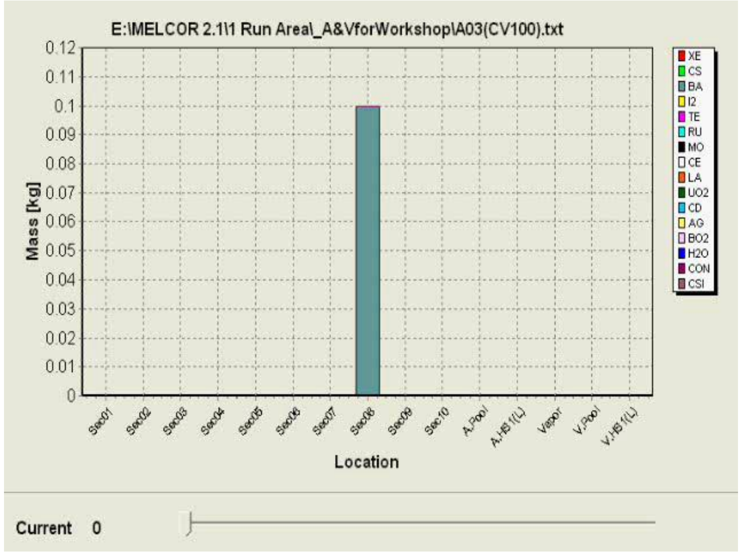
Visualization of Results, Cases 2 and 3

- 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*

Start





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 at least 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

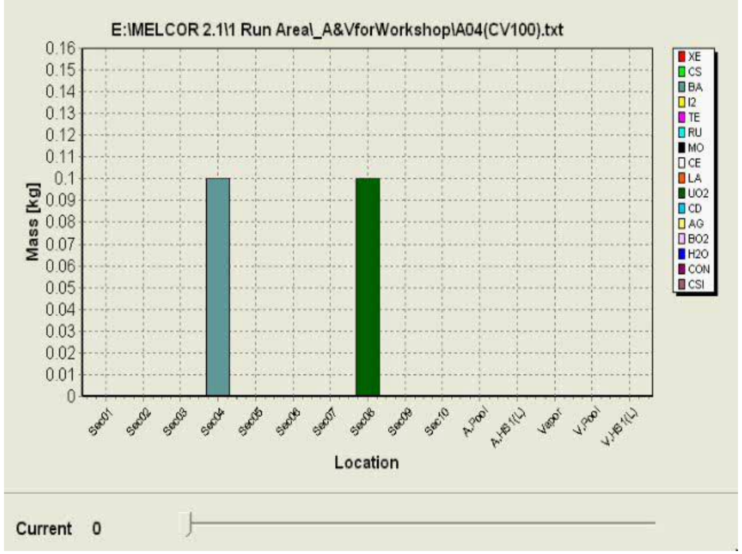
- Ran two versions of a 2 material case
  - –Initial 0.1 kg of Ba aerosol, d_p=0.880μm
  - –Initial 0.1 kg of UO2 aerosol, d_p=10.57μm
  - □ρ =1000kg/m^3, 10^{-10} m^2 surface
- Case 4: default component assignments
  - –Both Ba and UO2 assigned to component 1
- Case 5: custom component assignments
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

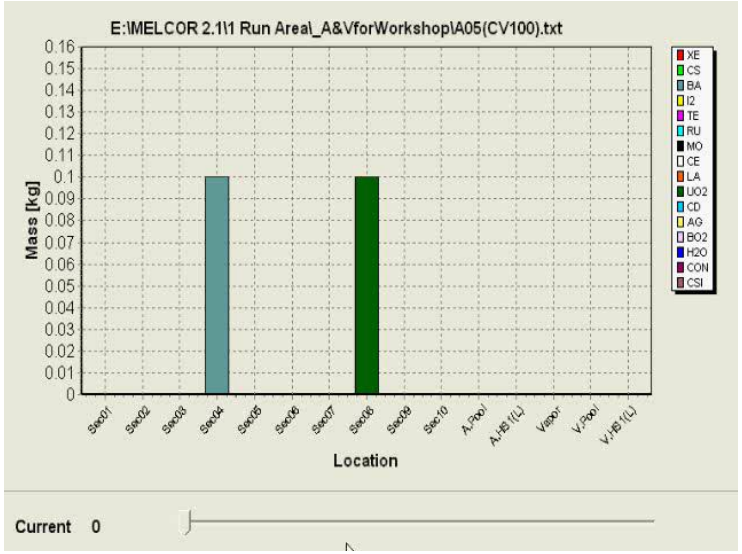
Visualization of Results, Cases 4 and 5

- 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

Start





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 a refers to atmosphere, 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, Δt

$$C_a = M_a/V = \frac{\beta}{\alpha} - \left(\frac{\beta}{\alpha} - C_{a0}\right)e^{-\alpha\Delta t}$$

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

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

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

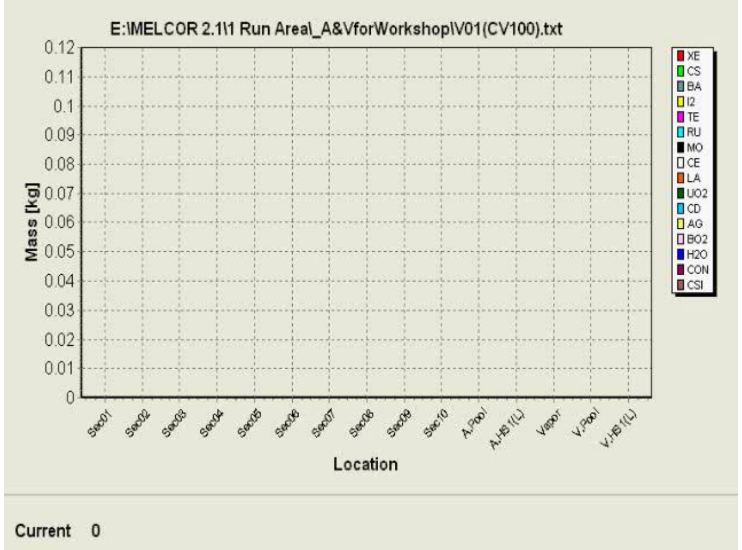
Condensation Aerosols

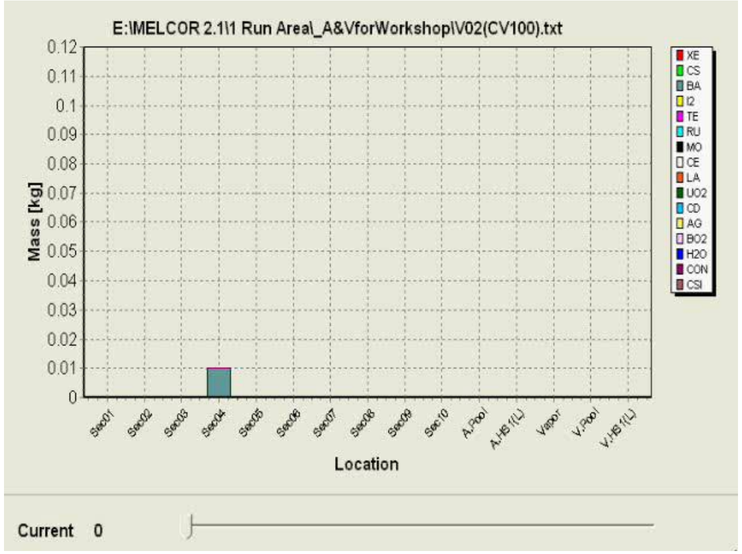
- Ran test cases with the 45 m^3 room and Cs (actually, CsOH) vapor source
  - –Temperature raised to 780 K, where mass corresponding to saturation is 0.00685 kg
  - –Cs-class vapor mass added at 10^{-5} kg/sec
    - Takes 685 s to reach saturation
  - –Chemisorption model turned off
  - –Two cases
    - 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 No vapor, no aerosol
  - Cs concentration rises to saturation
  - First aerosols form in smallest section, then agglomerate rapidly
  - Further condensation on existing aerosols
- Case 2 No vapor, little aerosol
  - Same rise to saturation
  - Most early condensation on existing Ba aerosols

Start





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

Questions