Aerosol Dynamics Model

Four Lognormal Modes

- Lognormal distribution and properties
  - e.g. Volume-mean for lognormal distribution
- Four lognormal mode algorithm
  - Coarse mode
  - Accumulation mode
  - Condensation mode
  - Nucleation mode

MATLAB Lognormal Distribution

```
 for dp=1:NUMBERsections     %loop to assign data points to lognormal fit
   Dp(dp)=MINdiameter*(MAXdiameter/MINdiameter)^(dp/NUMBERsections);
   %increments the diameter over the plotted range for the specified number of sections
   %Equation for lognormal distribution, [Eqn. 7.33, Seinfeld and Pandis, 1998]
   dNdlnDp(dp)=(N/(((2*pi)^0.5)*log(sg)))*exp((-(log(Dp(dp))-log(Dpg))^2)/(2*log(sg)^2));
  end
```

- A loop is used to assign each element of the vectors Dp and dNdlnDp to a value

MATLAB Lognormal Mean Volume Diameter

```
 for dp=1:NUMBERsections  %loop to assign data points to lognormal fit
   Dp(dp)=MINdiameter*(MAXdiameter/MINdiameter)^(dp/NUMBERsections);
   %increments the diameter over the plotted range for the specified number of sections
   %Equation for lognormal distribution, [Eqn. 7.33, Seinfeld and Pandis, 1998]
   dNdlnDp(dp)=(N/(((2*pi)^0.5)*log(sg)))*exp((-(log(Dp(dp))-log(Dpg))^2)/(2*log(sg)^2));
   %Equation for volume-mean diameter of lognormal distribution, [Eqn. 7.52, Seinfeld and
Pandis, 1998]
   DpgV=exp(log(Dpg)+3*(log(sg))^2);
  end
```

- Mean volume diameter is needed to get mass
- Mean volume diameter is larger than D_{pg}

MATLAB Critical Cluster Size: Four Lognormal-Mode Approach

```
%Run Conditions -- these vary depending on the time and place you are modeling
NCoars=100; %total particle number concentration of accumulation mode in #/cm^3
DpgCoars=5; %geometric mean particle diameter of accumulation mode in micron
sgCoars=1.5; %"sigma-g" or width of accumulation mode distribution
NAccum=100; %total particle number concentration of accumulation mode in #/cm^3
DpgAccum=0.1; %geometric mean particle diameter of accumulation mode in micron
sgAccum=1.5; %"sigma-g" or width of accumulation mode distribution
NCond=100; %total particle number concentration of condensation mode in #/cm^3
DpgCond=0.1; %geometric mean particle diameter of condensation mode in micron
sgCond=1.5; %"sigma-g" or width of condensation mode distribution
NNucln=1; %total particle number concentration of nucleation mode in #/cm^3
DpgNucln=0.005; %estimated geometric mean particle diameter of nucleation mode including H2SO4, H2O in micron
sgNucln=1.1; %estimated "sigma-g" or width of nucleation mode distribution
…
for dp=1:NUMBERsections  %loop to assign data points to lognormal fit
%Equation for lognormal distribution, [Eqn. 7.33, Seinfeld and Pandis, 1998]
dNdlnDp(t+1,dp)...
   =(NCoars/(((2*pi)^0.5)*log(sgCoars)))*exp((-(log(Dp(dp))-log(DpgCoars))^2)/(2*log(sgCoars)^2))...
   +(NAccum/(((2*pi)^0.5)*log(sgAccum)))*exp((-(log(Dp(dp))-log(DpgAccum))^2)/(2*log(sgAccum)^2))...
   +(NCond/(((2*pi)^0.5)*log(sgCond)))*exp((-(log(Dp(dp))-log(DpgCond))^2)/(2*log(sgCond)^2))...
   +(NNucln/(((2*pi)^0.5)*log(sgNucln)))*exp((-(log(Dp(dp))-log(DpgNucln))^2)/(2*log(sgNucln)^2));
end
```

Deposition

- Deposition rate matlab code
- Settling velocity
- Deposition only size distribution evolution
  - Summary for 96 hr

MATLAB Deposition Rate

```
%Deposition Rate
Kn=2*AirMeanFreePath/(Dpg*CMperMIC); %Knudsen number [Seinfeld and Pandis, Eq. 8.1]
Cc=1+Kn*(1.257+0.4*exp(-1.1/Kn)); %Cunningham correction factor [Seinfeld, 1968, p. 317]
ParticleMass=((DpgV*CMperMIC)^3*pi/6)*ParticleDensity; %mean particle mass in grams
Vt=(ParticleMass/GperKG)*GRAVITY*Cc/(3*pi*AirViscosity*Dpg*CMperMIC);
%terminal velocity [Seinfeld, 1968, p. 317]
DepnRate=(N*Vt/Height)*SECperHR; %deposition rate in terms of particles/cm3/hr

%Calculate mass and number changes here
N=N-DepnRate*1;
%new number after loss of particles due to deposition, assuming 1 hr time step
```

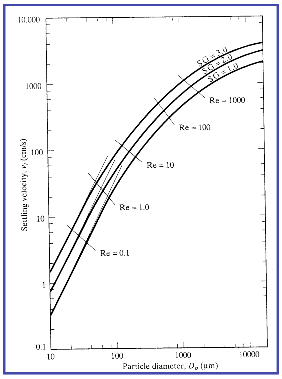
- 1st calculate deposition rate
- 2nd subtract from previous number

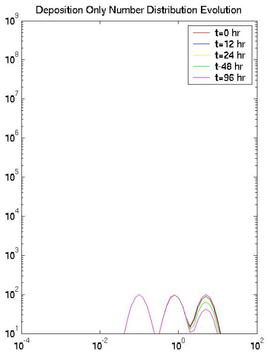
Settling Velocity

- terminal velocity of the particle in this fluid, v_t, where the particle has reached steady state

for unit density spheres in air at 20°C

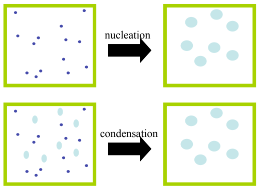
D_p (μm)	τ (sec)	v_t (m sec^{-1})
0.1	9.2×10^{-8}	9.0×10^{-7}
1.0	3.6×10^{-6}	3.5×10^{-5}
10.0	3.1×10^{-4}	3.0×10^{-3}





Condensation

- Condensation rate matlab code
  - Vapor-phase loss
  - Particle-phase growth
- Condensation rates
- Condensation only size distribution evolution
  - Summary for 96 hr



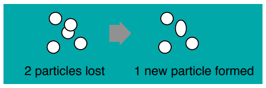
MATLAB Particle and Vapor Changes

```
%Calculate mass and number changes here for each mode
DeltaN=(-DepnRateCoars)*tSTEP;
NCoars=NCoars+DeltaN %new number after deposition loss of particles
DeltaN=(-DepnRateAccum)*tSTEP;
NAccum=NAccum+DeltaN %new number after deposition loss of particles
DeltaN=(-DepnRateCond)*tSTEP;
NCond=NCond+DeltaN %new number after deposition loss of particles
DeltaN=(-DepnRateNucl+NuclRate)*tSTEP;
NNucln=NNucln+DeltaN %new number after deposition loss and nucleation gain of particles
H2SO4(t+2)=H2SO4(t+1)-NuclRate*VaporPerParticle*tSTEP
```

- The sulfuric acid that nucleates new particles is removed from the vapor phase

Coagulation

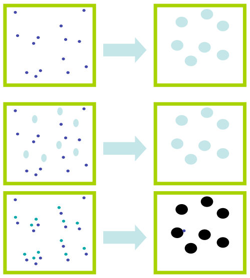
- **Coagulation** is growth by collision of particles
  - decreases particle number
  - increases particle size
  - no net change in particle mass



- the process of coagulation is almost entirely controlled by the physical properties of a particle, namely the particle ambient **diameter**

Nucleation

- Nucleation rate matlab code
- Nucleation rates
- Nucleation only size distribution evolution
  - Initial 0 hr and 12 hr
  - Summary for 96 hr



- Growth of clusters
- **homogeneous**=single phase
- (gas→particles)

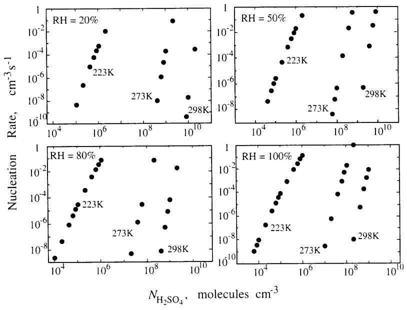
- **heterogeneous**=two phases
- (gas+particles→big particles)

- **heteromolecular**=more than one species of vapors nucleate together
- (two kinds of gases→particles)

MATLAB Nucleation Rate

```
%Run Conditions -- these vary depending on the time and place you are modeling
H2SO4(1)=0.001*2.463e10; %initial mixing ratio of H2SO4 vapor in molec/cm3
VaporPerNuclParticle=(.005/.001)^3*100; %estimated number of molecules H2SO4 vapor in each
particle
…
%Nucleation Rate for nucleation mode
NuclRate=(3.38e6+2.45e8*(H2SO4(t+1)^0.147))*SECperHR
% nucleation rate at 273K and 80%RH in p/cm3/hr from Seinfeld and Pandis, Fig. 10.11
 if ((NuclRate*VaporPerNuclParticle*tSTEP)>H2SO4(t+1))
% check if all vapor nucleates, determine max. possible rate
   NuclRate=(H2SO4(t+1)/VaporPerNuclParticle)/tSTEP
end
```

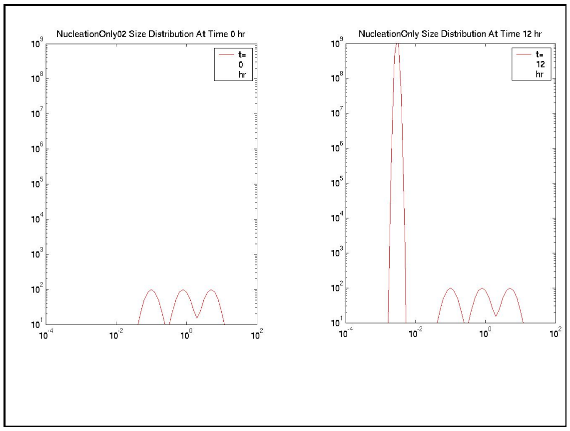
- To evaluate nucleation, the model needs humidity (p_B) and acidity (N_A) plus temperature (T)

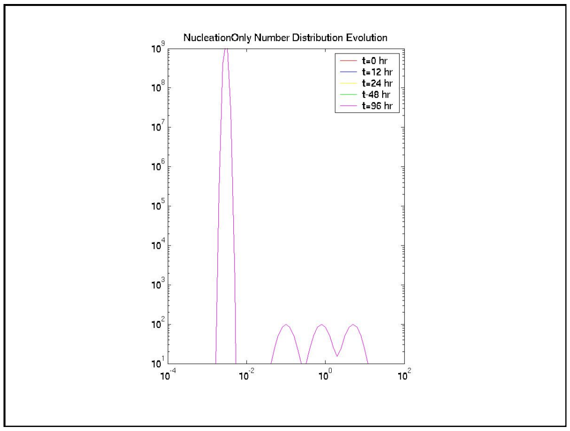


- Rate depends exponentially on temperature
  - Faster at colder temperatures

$$J = \left(4\pi R_p^{*2}\right)\frac{p_B}{\left(2\pi m_B kT\right)^{\frac{1}{2}}} N_A \exp\left(-\frac{\Delta G^*}{kT}\right)$$

Kulmala and Laaksonen, 1990


NucleationOnly02 Size Distribution At Time 0 hr
t=
0
hr
10^9
10^8
10^7
10^6
10^5
10^4
10^3
10^2
10^1
10^-4
10^-2
10^0
10^2
NucleationOnly Size Distribution At Time 12 hr
t=
12
hr
10^9
10^8
10^7
10^6
10^5
10^4
10^3
10^2
10^1
10^-4
10^-2
10^0
10^2


NucleationOnly Number Distribution Evolution
t=0 hr
t=12 hr
t=24 hr
t-48 hr
t=96 hr
10^9
10^8
10^7
10^6
10^5
10^4
10^3
10^2
10^1
10^-4
10^-2
10^0
10^2