**Overhead Slides for**

# Chapter 17

**of**

# Fundamentals of Atmospheric Modeling

by

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# Mass Flux to and From a Single Drop

Rate of change of mass (g) of single pure liquid water drop

$$\frac{dm}{dt} = 4\pi R^2 D_v \frac{d\rho_v}{dR} \qquad (17.1)$$

Integrate from drop surface to infinity

$$\frac{dm}{dt} = 4\pi r D_v \left(\rho_v - \rho_{v,r}\right) \qquad (17.2)$$

Rate of change of heat energy at drop surface due to conduction

$$\frac{dQ_r^*}{dt} = -4\pi R^2 \kappa_d \frac{dT}{dR} \qquad (17.3)$$

Integrate from drop surface to infinity

$$\frac{dQ_r^*}{dt} = 4\pi r \kappa_d \left(T_r - T\right) \qquad (17.4)$$

Relationship between change in mass and heat energy at surface

$$m c_W \frac{dT_r}{dt} = L_e \frac{dm}{dt} - \frac{dQ_r^*}{dt} \qquad (17.5)$$

Combine (17.4) and (17.5) and assume steady state

$$L_e \frac{dm}{dt} = 4\pi r \kappa_d \left(T_r - T\right) \qquad (17.6)$$

# Mass Flux to and From a Single Drop

Combine equation of state at saturation

$$p_{v,s} = \rho_{v,s} R_v T$$

with Clausius Clapeyron equation

$$\frac{\mathrm{d}p_{v,s}}{\mathrm{d}T} = \frac{\rho_{v,s} L_e}{T}$$

to obtain

$$\frac{\mathrm{d}\rho_{v,s}}{\rho_{v,s}} = \frac{L_e}{R_v}\frac{\mathrm{d}T}{T^2} - \frac{\mathrm{d}T}{T} \qquad (17.7)$$

Integrate from infinity to drop surface

$$\ln\frac{\rho_{v,s}(T_r)}{\rho_{v,s}(T)} = \frac{L_e}{R_v}\frac{(T_r - T)}{T T_r} - \ln\frac{T_r}{T} \qquad (17.8)$$

Simplify since $T \approx T_r$

$$\frac{\rho_{v,s}(T_r) - \rho_{v,s}(T)}{\rho_{v,s}(T)} = \frac{L_e}{R_v}\frac{(T_r - T)}{T^2} - \frac{T_r - T}{T} \qquad (17.9)$$

Substitute (17.6) into (17.9)

$$\frac{\rho_{v,s}(T_r) - \rho_{v,s}(T)}{\rho_{v,s}(T)} = \frac{L_e}{4\pi r \kappa_d T}\left(\frac{L_e}{R_v T} - 1\right)\frac{\mathrm{d}m}{\mathrm{d}t} \qquad (17.10)$$

# Mass Flux to and From a Single Drop

Substitute (17.2) into (17.10)

$$\frac{\rho_v - \rho_{v,s}(T)}{\rho_{v,s}(T)} = \left[\frac{L_e}{4\pi r \kappa_d T}\left(\frac{L_e}{R_v T} - 1\right) + \frac{1}{4\pi r D_v \rho_{v,s}(T)}\right]\frac{dm}{dt}$$

(17.11)

Mass-flux form of growth equation

$$\frac{dm}{dt} = \frac{4\pi r D_v\left(p_v - p_{v,s}\right)}{\frac{D_v L_e p_{v,s}}{\kappa_d T}\left(\frac{L_e}{R_v T} - 1\right) + R_v T} \qquad (17.12)$$

Rewrite mass-flux form equation for trace gases and particle sizes

$$\frac{dm_i}{dt} = \frac{4\pi r_i D'_{q,i}\left(p_q - p'_{q,s,i}\right)}{\frac{D'_{q,i} L_{e,q} p'_{q,s,i}}{\kappa'_{d,i} T}\left(\frac{L_{e,q} m_q}{R^* T} - 1\right) + \frac{R^* T}{m_q}} \qquad (17.13)$$

# Fluxes to and From a Single Drop

Change in mass as a function of change in radius

$$\frac{\mathrm{d}m_i}{\mathrm{d}t} = 4\pi r_i^2 \rho_{p,i} \frac{\mathrm{d}r_i}{\mathrm{d}t} \qquad (17.14)$$

Radius-flux form of growth equation

$$r_i \frac{\mathrm{d}r_i}{\mathrm{d}t} = \frac{D'_{q,i}\left(p_q - p'_{q,s,i}\right)}{\frac{D'_{q,i} L_{e,q} \rho_{p,i} p'_{q,s,i}}{\kappa'_{d,i} T}\left(\frac{L_{e,q} m_q}{R^* T} - 1\right) + \frac{R^* T \rho_{p,i}}{m_q}} \qquad (17.15)$$

Change in mass as a function of change in volume

$$\frac{\mathrm{d}m_i}{\mathrm{d}t} = \rho_{p,i} \frac{\mathrm{d}\upsilon_i}{\mathrm{d}t}$$

Volume-flux form of growth equation

$$\frac{\mathrm{d}\upsilon_i}{\mathrm{d}t} = \frac{\left(48\pi^2 \upsilon_i\right)^{1/3} D'_{q,i}\left(p_q - p'_{q,s,i}\right)}{\frac{D'_{q,i} L_{e,q} \rho_{p,i} p'_{q,s,i}}{\kappa'_{d,i} T}\left(\frac{L_{e,q} m_q}{R^* T} - 1\right) + \frac{R^* T \rho_{p,i}}{m_q}} \qquad (17.16)$$

# Gas Diffusion Coefficient

Molecular diffusion

Movement of molecules due to their kinetic energy, followed by collision with other molecules and random redirection.

Uncorrected gas diffusion coefficient ($cm^2\ s^{-1}$)

$$D_q = \frac{3}{8Ad_q^2\rho_a}\sqrt{\frac{R^*Tm_a}{2\pi}\left(\frac{m_q + m_a}{m_q}\right)} \tag{17.17}$$

Example 17.1.

Calculate diffusion coefficient of carbon monoxide

| | |
|---|---|
| $T$ | = 288 K |
| $p_a$ | = 1013 mb |
| $\rho_a$ | = 0.00123 g cm$^{-3}$ |
| $m_q$ | = 28 g mole$^{-1}$ |
| $D_q$ | = 0.12 cm$^2$ s$^{-1}$ |

# Corrected Gas Diffusion Coefficient

Corrected diffusion coefficient

$$D'_{q,i} = D_q \omega_{q,i} F_{q,i} \qquad (17.18)$$

Correction for collision geometry and sticking probability

$$\omega_{q,i} = \left\{ 1 + \left[ \frac{1.33 + 0.71\mathrm{Kn}_{q,i}^{-1}}{1 + \mathrm{Kn}_{q,i}^{-1}} + \frac{4\left(1 - \alpha_{q,i}\right)}{3\alpha_{q,i}} \right] \mathrm{Kn}_{q,i} \right\}^{-1} \qquad (17.19)$$

Knudsen number for condensing vapor

$$\mathrm{Kn}_{q,i} = \frac{\lambda_q}{r_i} \qquad (17.20)$$

$$\omega_{q,i} \rightarrow \begin{cases} 0 & \text{as} \quad \mathrm{Kn}_{q,i} \rightarrow \infty \quad \text{(small particles)} \\ 1 & \text{as} \quad \mathrm{Kn}_{q,i} \rightarrow 0 \quad \text{(large particles)} \end{cases}$$

(17.21)

Mass accommodation (sticking) coefficient, $\alpha_{q,i}$

Fractional number of gas collisions with particles that results in the gas sticking to the surface. From 0.01 - 1.0.

# Corrected Gas Diffusion Coefficient

Mean free path of a gas molecule

$$\lambda_q = \frac{32 D_q}{3\pi \bar{v}_q}\left(\frac{m_a}{m_a + m_q}\right) \approx \frac{3D_q}{\bar{v}_q} \tag{17.23}$$

Ventilation factor

Corrects for increased rate of vapor transfer due to eddies sweeping vapor to the surface of large particles

$$F_{q,i} = \begin{cases} 1 + 0.108 x_{q,i}^2 & x_{q,i} \le 1.4 \\ 0.78 + 0.308 x_{q,i} & x_{q,i} > 1.4 \end{cases} \tag{17.24}$$

$$x_{q,i} = \mathrm{Re}_i^{1/2}\,\mathrm{Sc}_q^{1/3} \tag{17.24}$$

Particle Reynolds number

$$\mathrm{Re}_i = \frac{2 r_i V_{f,i}}{\nu_a}$$

Gas Schmidt number

$$\mathrm{Sc}_q = \frac{\nu_a}{D_q} \tag{17.25}$$

# Corrected Thermal Conductivity

Corrected thermal conductivity of dry air (J cm$^{-1}$ s$^{-1}$ K$^{-1}$)

$$\kappa'_{d,i} = \kappa_d \omega_{h,i} F_{h,i} \, , \tag{17.26}$$

Correction for collision geometry and sticking probability

$$\omega_{h,i} = \left\{ 1 + \left[ \frac{1.33 + 0.71\mathrm{Kn}_{h,i}^{-1}}{1 + \mathrm{Kn}_{h,i}^{-1}} + \frac{4(1 - \alpha_h)}{3\alpha_h} \right] \mathrm{Kn}_{h,i} \right\}^{-1} \tag{17.27}$$

Knudsen number for heat

$$\mathrm{Kn}_{h,i} = \frac{\lambda_h}{r_i} \tag{17.28}$$

Mean free path of heat

$$\lambda_h = \frac{3D_h}{\bar{v}_a} \tag{17.29}$$

# Corrected Thermal Conductivity

Thermal accommodation (sticking) coefficient, $\alpha_t$

Fraction of molecules bouncing off surface of a drop that have acquired temperature of drop ≈ 0.96 for water.

$$\alpha_h = \frac{T_m - T}{T_s - T} \tag{17.30}$$

Ventilation factor

Corrects for increased rate of heat transfer due to eddies

$$F_{h,i} = \begin{cases} 1 + 0.108 x_{h,i}^2 & x_{h,i} \le 1.4 \\ 0.78 + 0.308 x_{h,i} & x_{h,i} > 1.4 \end{cases} \tag{17.31}$$

$$x_{h,i} = \mathrm{Re}_i^{1/2}\,\mathrm{Pr}^{1/3}$$

Prandtl number

$$\mathrm{Pr} = \eta_a c_{p,m} / \kappa_d \tag{17.32}$$

# Corrected Surface Vapor Pressure

Curvature (Kelvin) effect

Increases vapor pressure over small drops

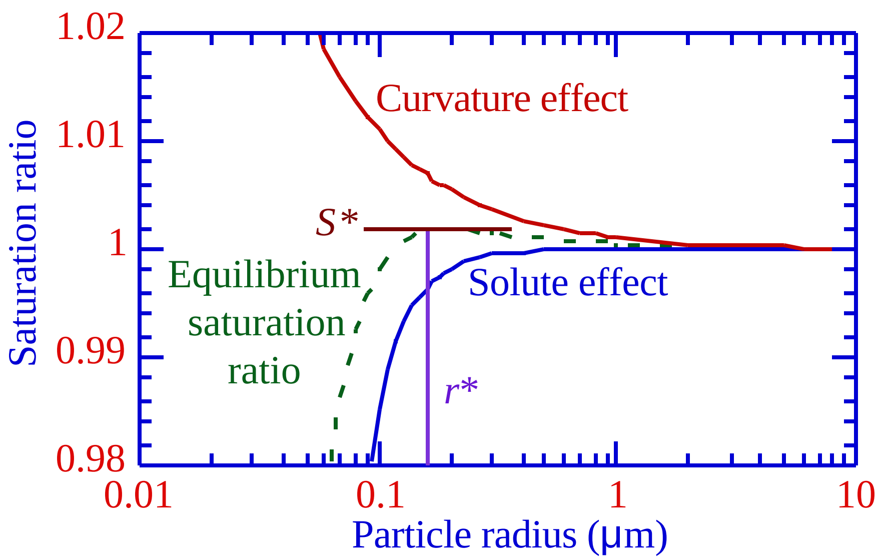
Solute effect

Decreases vapor pressure over small drops

Radiative cooling effect

Decreases vapor pressure over large drops

Fig. 17.1. Curvature and solute effects.



# Curvature Effect

Saturation vapor pressure over curved, dilute surface relative to that over a flat , dilute surface

$$\frac{p'_{q,s,i}}{p_{q,s}} = \exp\left(\frac{2\sigma_p m_p}{r_i R^* T \rho_{p,i}}\right) \approx 1 + \frac{2\sigma_p m_p}{r_i R^* T \rho_{p,i}} \qquad (17.33)$$

Note

$\exp(x) \approx 1 + x$ for small values of $x$

# Solute Effect

Vapor pressure over flat water surface with solute relative to that without solute (Raoult's Law)

$$\frac{p'_{q,s,i}}{p_{q,s}} = \frac{n_w}{n_w + n_s} \qquad (17.34)$$

Relatively dilute solution $n_w >> n_s$

$$\frac{p'_{q,s,i}}{p_{q,s}} \approx 1 - \frac{n_s}{n_w} \qquad (17.35)$$

Number of moles of solute in solution

$$n_s = \frac{i_v M_s}{m_s}$$

Number of moles of liquid water in a drop

$$n_w = \frac{M_w}{m_v} \approx \frac{4\pi r_i^3 \rho_w}{3 m_v} \qquad (17.36)$$

Combine terms --> solute effect

$$\frac{p'_{q,s,i}}{p_{q,s}} \approx 1 - \frac{3 m_v i_v M_s}{4\pi r_i^3 \rho_w m_s} \qquad (17.37)$$

# Köhler Equation

Combine curvature and solute effects --> Sat. ratio at equilibrium

$$S'_{q,i} = \frac{p'_{q,s,i}}{p_{q,s}} \approx 1 + \frac{2\sigma_p m_p}{r_i R^* T \rho_{p,i}} - \frac{3 m_v i_v M_s}{4\pi r_i^3 \rho_w m_s} \qquad (17.38)$$

Simplify Köhler equation

$$S'_{q,i} = 1 + \frac{a}{r_i} - \frac{b}{r_i^3} \qquad (17.40)$$

$$a = \frac{2\sigma_p m_p}{R^* T \rho_{p,i}} \qquad b = \frac{3 m_v i_v M_s}{4\pi \rho_w m_s} \qquad (17.40)$$

Set Köhler equation to zero -->

Critical radius for growth and critical saturation ratio

$$r^* = \sqrt{\frac{3b}{a}} \qquad S^* = 1 + \sqrt{\frac{4a^3}{27b}} \qquad (17.41)$$

Table 17.1. Critical radii / supersaturations for water drops containing sodium chloride or ammonium sulfate at 275 K.

| | Sodium Chloride | | Ammonium Sulfate | |
|---|---|---|---|---|
| Solute Mass (g) | $r^*$ (µm) | $S^*-1$ (%) | $r^*$ (µm) | $S^*-1$ (%) |
| 0 | 0 | ∞ | 0 | ∞ |
| $10^{-18}$ | 0.019 | 4.1 | 0.016 | 5.1 |
| $10^{-16}$ | 0.19 | 0.41 | 0.16 | 0.51 |
| $10^{-14}$ | 1.9 | 0.041 | 1.6 | 0.051 |
| $10^{-12}$ | 19 | 0.0041 | 16 | 0.0051 |

# Radiative Cooling Effect

Surface vapor pressure over curved, dilute surface relative to that over a flat , dilute surface

$$\frac{p'_{q,s,i}}{p_{q,s}} \approx 1 + \frac{L_{e,q} m_q H_{r,i}}{4\pi r_i R^* T^2 \kappa'_{d,i}} \qquad (17.42)$$

Radiative cooling rate (W)

$$H_{r,i} = \left(\pi r_i^2\right) 4\pi \int_0^\infty Q_a\left(m_\lambda, \alpha_{i,\lambda}\right)\left(I_\lambda - B_\lambda\right) d\lambda \qquad (17.43)$$

# Overall Equilibrium Saturation Ratio

Overall equilibrium saturation ratio for liquid water

$$S'_{q,i} = \frac{p'_{q,s,i}}{p_{q,s}} \approx 1 + \frac{2\sigma_p m_p}{r_i R^* T \rho_{p,i}} - \frac{3 m_v i_v M_s}{4\pi r_i^3 \rho_w m_s} + \frac{L_{e,q} m_q H_{r,i}}{4\pi r_i R^* T^2 \kappa'_{d,i}}$$

(17.44)

Equilibrium saturation ratio for gases other than liquid water when surface vapor pressures computed separately

$$S'_{q,i} = \frac{p'_{q,s,i}}{p_{q,s}} \approx 1 + \frac{2\sigma_p m_p}{r_i R^* T \rho_{p,i}} \quad (17.45)$$

# Flux to Drop With Multiple Components

Volume of a single particle in which one species is growing

$$\upsilon_{i,t} = \upsilon_{q,i,t} + \upsilon_{i,t-h} - \upsilon_{q,i,t-h} \tag{17.46}$$

Mass of a single particle in which one species is growing

$$m_{i,t} = \rho_{p,i,t}\upsilon_{i,t} = \rho_{p,q}\upsilon_{q,i,t} + \rho_{p,i,t-h}\upsilon_{i,t-h} - \rho_{p,q}\upsilon_{q,i,t-h} \tag{17.47}$$

Time derivative of (17.47)

$$\frac{dm_{i,t}}{dt} = \rho_{p,i,t}\frac{d\upsilon_{i,t}}{dt} = \rho_{p,q}\frac{d\upsilon_{q,i,t}}{dt} \tag{17.48}$$

since

$$\frac{d\upsilon_{i,t-h}}{dt} = \frac{d\upsilon_{q,i,t-h}}{dt} = 0$$

Combine (17.48) and (17.46) with (17.16)

Rate of change in volume of one component in one multicomponent particle

$$\frac{d\upsilon_{q,i,t}}{dt} = \frac{\left[48\pi^2\left(\upsilon_{q,i,t} + \upsilon_{i,t-h} - \upsilon_{q,i,t-h}\right)\right]^{1/3} D'_{q,i}\left(p_q - p'_{q,s,i}\right)}{\dfrac{D'_{q,i} L_{e,q}\rho_{p,q} p'_{q,s,i}}{\kappa'_{d,i} T}\left(\dfrac{L_{e,q} m_q}{R^* T} - 1\right) + \dfrac{R^* T \rho_{p,q}}{m_q}} \tag{17.49}$$

# Flux to a Population of Drops

Volume as a function of volume concentration

$$\upsilon_{q,i,t} = \frac{v_{q,i,t}}{n_{i,t-h}}$$

Substitute volumes into (17.49)

$$\frac{\mathrm{d}v_{q,i,t}}{\mathrm{d}t} = \frac{n_{i,t-h}^{2/3}\left[48\pi^2\left(v_{q,i,t} + v_{i,t-h} - v_{q,i,t-h}\right)\right]^{1/3} D'_{q,i}\left(p_q - p'_{q,s,i}\right)}{\dfrac{D'_{q,i} L_{e,q}\rho_{p,q} p'_{q,s,i}}{\kappa'_{d,i}T}\left(\dfrac{L_{e,q} m_q}{R^* T} - 1\right) + \dfrac{R^* T \rho_{p,q}}{m_q}}$$

(17.50)

Partial pressure in terms of mole concentration

$$p_q = C_q R^* T \qquad (17.51)$$

Vapor pressure in terms of mole concentration

$$p'_{q,s,i} = C'_{q,s,i} R^* T \qquad (17.51)$$

# Flux to a Population of Drops

Combine (17.50) with (17.51)

$$\frac{d v_{q,i,t}}{d t} = n_{i,t-h}^{2/3}\left[48\pi^2\left(v_{q,i,t} + v_{i,t-h} - v_{q,i,t-h}\right)\right]^{1/3} D_{q,i,t-h}^{eff} \frac{m_q}{\rho_{p,q}}\left(C_{q,t} - C'_{q,s,i,t-h}\right)$$

(17.52)

Effective diffusion coefficient

$$D_{q,i,t-h}^{eff} = \frac{D'_{q,i}}{\dfrac{m_q D'_{q,i} L_{e,q} C'_{q,s,i,t-h}}{\kappa'_{d,i} T}\left(\dfrac{L_{e,q} m_q}{R^* T} - 1\right) + 1} \qquad (17.53)$$

Simplify effective diffusion coefficient for gases other than water

$$D_{q,i,t-h}^{eff} \approx D'_{q,i} = D_q \omega_{q,i} F_{q,i} = \frac{D_q F_{q,i}}{1 + \left[\dfrac{1.33 + 0.71\mathrm{Kn}_{q,i}^{-1}}{1 + \mathrm{Kn}_{q,i}^{-1}} + \dfrac{4\left(1 - \alpha_{q,i}\right)}{3\alpha_{q,i}}\right]\mathrm{Kn}_{q,i}}$$

(17.54)

Corresponding gas-conservation equation

$$\frac{d C_{q,t}}{d t} = -\frac{\rho_{p,q}}{m_q}\sum_{i=1}^{N_B}\frac{d v_{q,i,t}}{d t} \qquad (17.55)$$

# Integrate Growth Equations

Matrix of partial derivatives (17.73)

$$
\begin{array}{c|c|c|c|c|}
 & v_{q,1,t} & v_{q,2,t} & v_{q,3,t} & C_{q,t} \\
\hline
v_{q,1,t} & 1-h\beta_s\dfrac{\partial^2 v_{q,1,t}}{\partial v_{q,1,t}\partial t} & 0 & 0 & -h\beta_s\dfrac{\partial^2 v_{q,1,t}}{\partial C_{q,t}\partial t} \\
\hline
v_{q,2,t} & 0 & 1-h\beta_s\dfrac{\partial^2 v_{q,2,t}}{\partial v_{q,2,t}\partial t} & 0 & -h\beta_s\dfrac{\partial^2 v_{q,2,t}}{\partial C_{q,t}\partial t} \\
\hline
v_{q,3,t} & 0 & 0 & 1-h\beta_s\dfrac{\partial^2 v_{q,3,t}}{\partial v_{q,3,t}\partial t} & -h\beta_s\dfrac{\partial^2 v_{q,3,t}}{\partial C_{q,t}\partial t} \\
\hline
C_{q,t} & -h\beta_s\dfrac{\partial^2 C_{q,t}}{\partial v_{q,1,t}\partial t} & -h\beta_s\dfrac{\partial^2 C_{q,t}}{\partial v_{q,2,t}\partial t} & -h\beta_s\dfrac{\partial^2 C_{q,t}}{\partial v_{q,3,t}\partial t} & 1-h\beta_s\dfrac{\partial^2 C_{q,t}}{\partial C_{q,t}\partial t} \\
\hline
\end{array}
$$

(17.56)

$$\frac{\partial^2 v_{q,i,t}}{\partial v_{q,i,t}\partial t} = -\frac{1}{3}\left(\frac{n_{i,t-h}}{v_{q,i,t}}\right)^{2/3}\left(48\pi^2\right)^{1/3} D^{eff}_{q,i,t-h}\frac{m_q}{\rho_{p,q}}\left(C_{q,t}-C'_{q,s,i,t-h}\right)$$

(17.57)

$$\frac{\partial^2 v_{q,i,t}}{\partial C_{q,t}\partial t} = n_{i,t-h}^{2/3}\left[48\pi^2\left(v_{q,i,t}+v_{i,t-h}-v_{q,i,t-h}\right)\right]^{1/3} D^{eff}_{q,i,t-h}\frac{m_q}{\rho_{p,q}}$$

(17.58)

$$\frac{\partial^2 C_{q,t}}{\partial v_{q,i,t}\partial t} = -\frac{\rho_{p,q}}{m_q}\frac{\partial^2 v_{q,i,t}}{\partial v_{q,i,t}\partial t},$$ (17.59)

$$\frac{\partial^2 C_{q,t}}{\partial C_{q,t}\partial t} = -\frac{\rho_{p,q}}{m_q}\sum_{i=1}^{N_B}\frac{\partial^2 v_{q,i,t}}{\partial C_{q,t}\partial t}$$ (17.60)

# Integrated Solution to Growth Equations

Table 17.2. Reduction in array space and in the number of matrix operations before and after the use of sparse-matrix techniques to solve growth ODEs. $N_B + 1 = 17$.

| | Growth / Evaporation | |
|---|---|---|
| | Initial | After Sparse Matrix Reductions |
| Order of matrix | 17 | 17 |
| No. init. matrix spots filled | 289 | 49 |
| % of initial positions filled | 100 | 17 |
| No. fin. matrix spots filled | 289 | 49 |
| % of final positions filled | 100 | 17 |
| No. operations decomp. 1 | 1496 | 16 |
| No. operations decomp. 2 | 136 | 16 |
| No. operations backsub. 1 | 136 | 16 |
| No. operations backsub. 2 | 136 | 16 |

# Analytical Predictor of Condensation

Assume radius in growth term constant during time step

Change in particle volume concentration

$$\frac{d\,v_{q,i,t}}{d\,t} = n_{i,t-h}^{2/3}\left(48\pi^2 v_{i,t-h}\right)^{1/3} D_{q,i,t-h}^{eff} \frac{m_q}{\rho_{p,q}}\left(C_{q,t} - C'_{q,s,i,t-h}\right)$$

(17.61)

Define mass transfer coefficient

$$k_{q,i,t-h} = n_{i,t-h}^{2/3}\left(48\pi^2 v_{i,t-h}\right)^{1/3} D_{q,i,t-h}^{eff} = n_{i,t-h} 4\pi r_{i,t-h} D_{q,i,t-h}^{eff}$$

(17.62)

Effective surface vapor mole concentration

$$C'_{q,s,i,t-h} = S'_{q,i,t-h} C_{q,s,i,t-h} \quad (17.63)$$

Volume concentration of a component

$$v_{q,i,t} = m_q c_{q,i,t} / \rho_{p,q} \quad (17.64)$$

Uncorrected surface vapor mole concentration

$$C_{q,s,i,t-h} = p_{q,s,t-h} / R^* T$$

# Analytical Predictor of Condensation

Substitute conversions into (17.61) and (17.55)

$$\frac{\mathrm{d}c_{q,i,t}}{\mathrm{d}t} = k_{q,i,t-h}\left(C_{q,t} - S'_{q,i,t-h}C_{q,s,i,t-h}\right) \qquad (17.65)$$

$$\frac{\mathrm{d}C_{q,t}}{\mathrm{d}t} = -\sum_{i=1}^{N_B}\left[k_{q,i,t-h}\left(C_{q,t} - S'_{q,i,t-h}C_{q,s,i,t}\right)\right] \qquad (17.66)$$

Integrate (17.65) for final aerosol concentration

$$c_{q,i,t} = c_{q,i,t-h} + hk_{q,i,t-h}\left(C_{q,t} - S'_{q,i,t-h}C_{q,s,i,t-h}\right) \qquad (17.67)$$

Mass balance equation

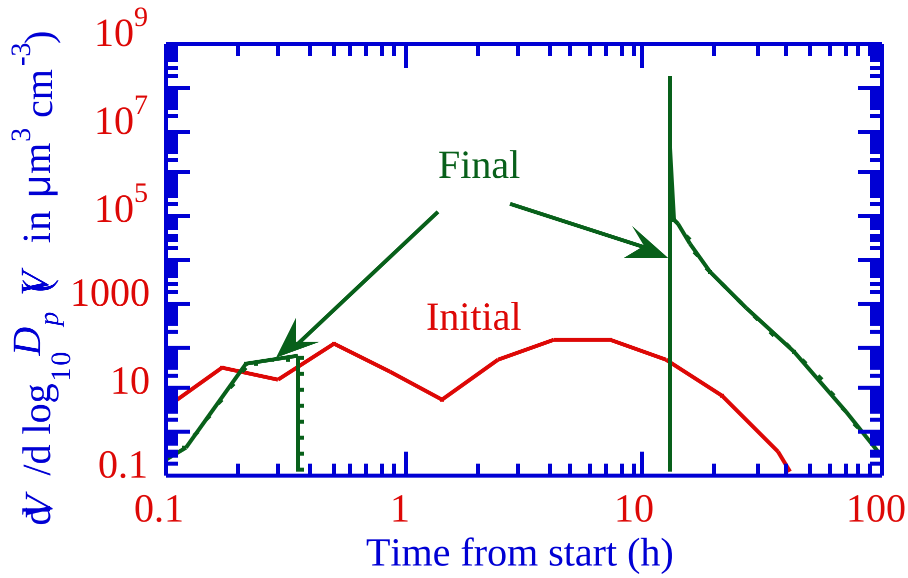
$$C_{q,t} + \sum_{i=1}^{N_B}\left(c_{q,i,t}\right) = C_{q,t-h} + \sum_{i=1}^{N_B}\left(c_{q,i,t-h}\right) = C_{tot} \qquad (17.68)$$

Substitute (17.67) into (17.68)

$$C_{q,t} = \frac{C_{q,t-h} + h\sum_{i=1}^{N_B}\left(k_{q,i,t-h}S'_{q,i,t-h}C_{q,s,i,t-h}\right)}{1 + h\sum_{i=1}^{N_B}k_{q,i,t-h}} \qquad (17.69)$$

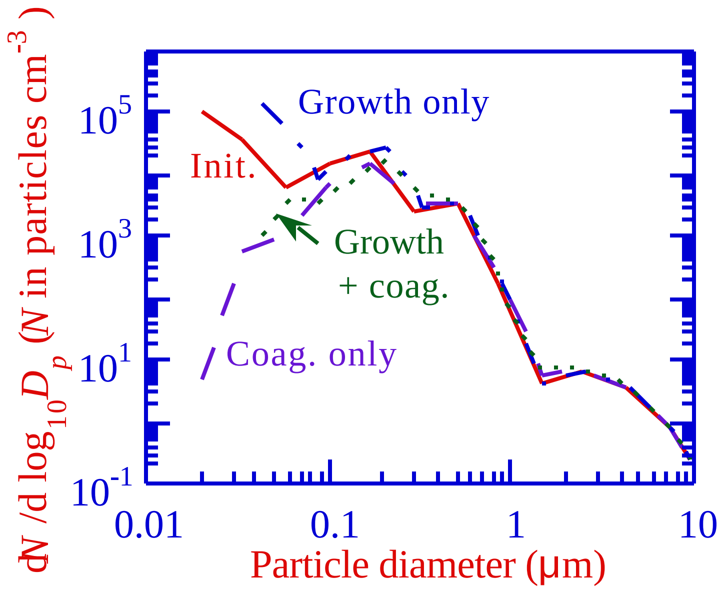
# APC Growth Simulation

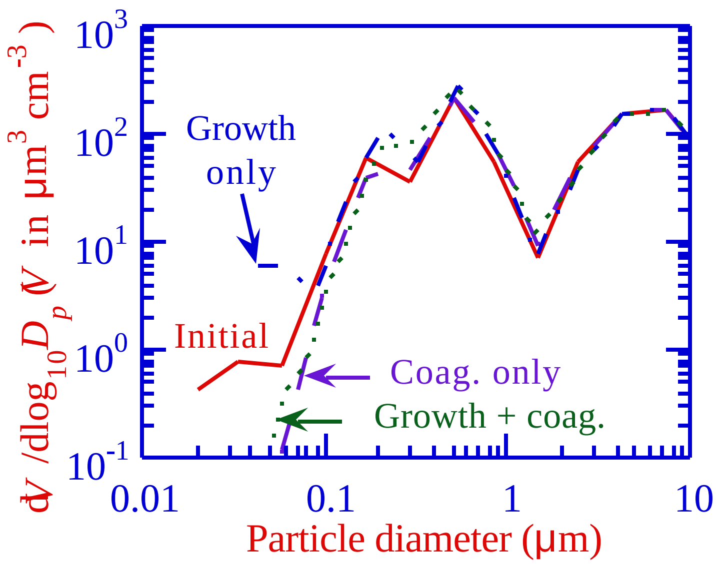
Fig. 17.2. Comparison of APC solution, when $h$ = 10 s, to an exact solution of condensational growth. Both solutions lie almost exactly on top of each other.



# Effect of Coagulation on Condensation

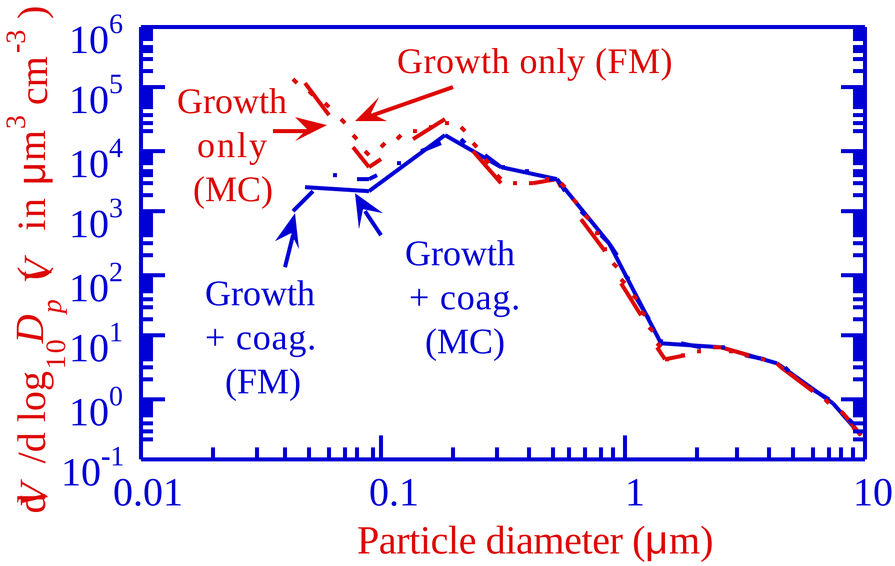
Figs. 17.3 a and b. Growth plus coagulation pushes particles to larger sizes than does growth alone or coagulation alone.



# Moving-Center vs. Full-Moving Size Structure

Fig. 17.4. Comparison of moving-center (MC) particle size structure to full-moving (FM) size structure for the growth / coagulation and growth-only cases shown in fig. (17.3 a).



# Ice Crystal Growth

Rate of mass growth of a single ice crystal

$$\frac{dm_i}{dt} = \frac{4\pi\chi_i D'_{v,i}\left(p_q - p'_{v,I,i}\right)}{\frac{D'_{v,i}L_s p'_{v,I,i}}{\kappa'_{d,i}T}\left(\frac{L_s}{R_v T} - 1\right) + R_v T} \qquad (17.71)$$

Electrical capacitance of crystal (cm)

$$\chi_i = \begin{cases} a_{c,i}/2 & \text{sphere} \\ a_{c,i}e_{c,i}/\ln\left[\left(1+e_{c,i}\right)a_{c,i}/b_{c,i}\right] & \text{prolate spheroid} \\ a_{c,i}e_{c,i}/\sin^{-1}e_{c,i} & \text{oblate spheroid} \\ a_{c,i}/\ln\left(4a_{c,i}^2/b_{c,i}^2\right) & \text{needle} \\ a_{c,i}e_{c,i}/\ln\left[\left(1+e_{c,i}\right)/\left(1-e_{c,i}\right)\right] & \text{column} \\ a_{c,i}e_{c,i}/\left(2\sin^{-1}e_{c,i}\right) & \text{hexagonal plate} \\ a_{c,i}/\pi & \text{thin plate} \end{cases} \qquad (17.72)$$

$a_{c,i}$ = length of the major semi-axis (cm)

$b_{c,i}$ = length of the minor semi-axis (cm)

$$e_{c,i} = \sqrt{1 - b_{c,i}^2/a_{c,i}^2}$$

# Ice Crystal Growth

Effective saturation vapor pressure over ice

$$p'_{v,I,i} = S'_{v,i} p_{v,I}$$

Ventilation factor for falling oblate spheroid crystals

$$F_{q,i}, F_{h,i} = \begin{cases} 1 + 0.14x^2 & x < 1.0 \\ 0.86 + 0.28x & x \geq 1.0 \end{cases} \qquad (17.73)$$

$x = x_{q,i}$ for ventilation of gas

$x = x_{h,i}$ for ventilation of heat