3.4. Numerical Methods for the Growth of Ice Crystals

The growth of ice particles in clouds is much more complicated than the growth of liquid drops. First, ice particles can grow by acquiring water from all three phases: growth by vapor diffusion, collection of drops and other ice particles. Compared with the growth of droplets, the heat equation for the growth of ice particles requires an extra term to account for the latent heat released during riming. Second, ice particles can have many different shapes, a characteristic that complicates the hydrodynamic behavior and the diffusional growth of ice particles. This section shows some numerical methods that are helpful in solving the growth equations for ice particles.

3.4.1. Quasi-Analytical Solutions for the Growth Equations

The quasi-analytical solution for the growth of ice particles is derived in a somewhat different way from that for liquid drops because of the following two factors: (1) the latent heat release from the freezing of the collected supercooled-drops presents an extra term in the mass and heat transfer equations for the growth of ice particles, (2) the curvature and solute effects are insignificant for the depositional growth of ice. The mass growth and heat transfer equations can be written as:

\[
\frac{dm_i}{dt} = \frac{dm_i}{dt}\bigg|_{\text{acc}} + \frac{dm_i}{dt}\bigg|_{\text{diff}}
\]

\[
\frac{dH_i}{dt} = \frac{dH_i}{dt}\bigg|_{\text{acc}} + \frac{dH_i}{dt}\bigg|_{\text{diff}} + \frac{dH_i}{dt}\bigg|_{\text{cond}}
\]

(3.98)

(3.99)

where the subscripts denote accretion (acc), vapor diffusion (diff), and conduction (cond). For simplicity, let the accretion rates be constant during each time step, so then
\[
\frac{\partial m_i}{\partial t}_{\text{acc}} = \dot{m}_{\text{acc}} = \text{constant, and}
\]
\[
\frac{\partial H_i}{\partial t}_{\text{acc}} = h_w \dot{m}_{\text{acc}} = \dot{H}_{\text{acc}} = \text{constant}.
\]

Other mass-growth and heating rates are expressed as:
\[
\frac{\partial m_i}{\partial t}_{\text{diff}} = \frac{4\pi C D_v f_v (\rho_\infty - \rho_i)}{M_w} = 4\pi C \frac{D_v f_v}{\mathcal{R}} \left[ \frac{e_\infty}{T_\infty} - \frac{e_{sj}(T_i)}{T_i} \right],
\]
(3.100)
\[
\frac{\partial H_i}{\partial t}_{\text{cond}} = 4\pi C \kappa_a f_h (T_\infty - T_i), \text{ and}
\]
(3.101)
\[
\frac{\partial H_i}{\partial t}_{\text{diff}} = h_v \frac{\partial m_i}{\partial t}_{\text{diff}}.
\]
(3.102)

Similar to the procedure used in deriving the analytical solution for drop growth, the total heat change can be approximated as
\[
\frac{\partial H_i}{\partial t} = h_i \frac{\partial m_i}{\partial t} + m_i \frac{\partial h_i}{\partial t} \equiv h_i \frac{\partial m_i}{\partial t} = h_i \left( \frac{\partial m_i}{\partial t}_{\text{diff}} + \frac{\partial m_i}{\partial t}_{\text{acc}} \right).
\]
(3.103)

We can rearrange the heat transfer equation to get
\[
0 = 4\pi C \kappa_a f_h (T_\infty - T_w) + l_s \frac{\partial m_i}{\partial t}_{\text{diff}} + l_f \frac{\partial m_i}{\partial t}_{\text{acc}}
\]
\[
= 4\pi C \left\{ \kappa_a f_h (T_\infty - T_i) + \frac{l_v D_v f_v}{\mathcal{R}} \left[ \frac{e_\infty}{T_\infty} - \frac{e_{sj}(T_i)}{T_i} \right] \right\} + l_f \dot{m}_{\text{acc}}.
\]
(3.104)

As before, \( l_s = h_v - h_i \) is the molar latent heat of sublimation and \( l_f = h_w - h_i \) is the molar latent heat of freezing. Let us define the temperature difference between the ice particle and air as \( \Delta T \) so that \( T_i = T_\infty + \Delta T = T_\infty (1+\delta) \), where \( \delta = \frac{\Delta T}{T_\infty} \) is normally much less than
unity. The saturation vapor pressure over ice, \( e_{s,i}(T) \), can be obtained by applying the Clausius-Clapeyron equation

\[
e_{s,i}(T_i) = e_{s,i}(T_\infty) \exp\left(\frac{l_s T_i - T_\infty}{\mathcal{R} T_i T_\infty}\right) = e_{s,i}(T_\infty) \exp\left(\frac{l_s \delta}{\mathcal{R} T_\infty (1 + \delta)}\right).
\]  

(3.105)

The exponential can be approximated by the first two terms of its Taylor's series expansion (\( e^x \approx 1 + x \)) such that

\[
-k_a f \frac{f}{T_\infty} \delta + \alpha \left\{ S_{\infty,i} - \frac{1}{1 + \delta} \left[ 1 + \frac{l_s \delta}{\mathcal{R} T_\infty (1 + \delta)} \right] \right\} + \frac{l_t \dot{m}_{\text{acc}}}{4 \pi C} = 0,
\]

(3.106)

where \( \alpha = l_s D_v f_v e_{s,i}(T_\infty) / (\mathcal{R} T_\infty) \) and \( S_{\infty,i} = e_{\infty} / e_{s,i}(T_\infty) \), which is the ice-saturation ratio in the air. Since \( \frac{l_s \delta}{1 + \delta} \approx 1 - \delta \) for \( \delta \ll 1 \), we get

\[
-k_a f \frac{f}{T_\infty} \delta + \alpha \left\{ S_{\infty,i} - (1 - \delta) \left[ 1 + \frac{l_s \delta (1-\delta)}{\mathcal{R} T_\infty} \right] \right\} + \frac{l_t \dot{m}_{\text{acc}}}{4 \pi C} = 0.
\]

(3.107)

The above equation is a cubic function of \( \delta \), and has analytical solutions. However, it is permissible to ignore the third-order term to get the simpler solution:

\[
\delta \approx -a_1 - \sqrt{a_1^2 - a_2}
\]

(3.108)

where

\[
a_1 = \frac{1}{4} \left[ \frac{T_\infty}{l_s} \left( 1 - \frac{k_a f}{\alpha} \frac{f}{T_\infty} \right) - 1 \right], \quad \text{and}
\]

\[
a_2 = \frac{T_\infty}{2 l_s} \left[ (S_{\infty,i} - 1) + \frac{l_t \dot{m}_{\text{acc}}}{4 \pi C \alpha} \right].
\]

We thus derived an analytical solution, \( T_i = T_\infty (1 + \delta) \), for the temperature of ice particle growing by both vapor diffusion and accretion. Under slow growing conditions, we can even ignore the second order terms so that \( \delta \approx -a_2 / (2 a_1) \). Since the solute and curvature...
effects are negligible for ice-phase particles, we can directly apply $\delta$ to the diffusional growth equation:

$$\rightarrow \left. \frac{dm_i}{dt} \right|_{\text{diff}} \approx \frac{4 \pi C D_v f_v e_{s,i}(T_{\infty})}{R T_{\infty}} \left\{ S_{\infty,i} - (1 - \delta) \left[ 1 + \frac{l_0 \delta (1 - \delta)}{R T_{\infty}} \right] \right\}$$

(3.109)

**Linearized capacitance**

The above equation is still nonlinear because of the size and shape dependence of the capacitance $C$. Nevertheless, it can be shown that the ratio of the capacitance $C$ to the spherical-equivalent radius $r_i$ of the ice particle ($q \equiv C / r_i$) is a slowly varying parameter and can be regarded as constant during a typical time-step. The analytical equation of the mass growth rate can thus be linearized by letting $C = q r_i$. Recall that the capacitance of the ice particles can be expressed as:

- **prolate spheroid**: $C = \frac{c \varepsilon}{\ln[(1+\varepsilon)\frac{c}{a}]}$, \[ \varepsilon = (1 - \frac{a^2}{c^2})^{1/2}; \]

(3.110)

- **oblate spheroid**: $C = \frac{a \varepsilon}{\sin^{-1}\varepsilon}$, \[ \varepsilon = (1 - \frac{c^2}{a^2})^{1/2}. \]

For a spherical particle, the aspect ratio $\phi = 1$ and eccentricity $\varepsilon = 0$, the capacitance is the same as the radius of the particle $r_i$. Therefore, we will examine the variation of $C$ only for the two extreme values of the aspect ratio. At the two extremes, where the eccentricity $\varepsilon \to 1$, we have
prolate spheroid: \( C = \frac{c}{\ln \left( \frac{2c}{a} \right)} \),

(3.111)

oblate spheroid: \( C = \frac{2a}{\pi} \).

Invoke the expression for the volume of a spheroid:

\[
V = \frac{4}{3} \pi r_i^3 = \frac{4}{3} \pi a^3 \phi \left( \phi = \frac{4}{3} \pi c^3 / \phi^2 \right),
\]

(3.112)

and the relationship between the change of aspect ratio and volume (see Section 2.3.2.1):

\[
\frac{d \ln \phi}{d \ln V} = \frac{\Gamma - 1}{\Gamma + 2},
\]

(3.113)

where \( \Gamma \) is the inherent growth habit. Thus, we can derive the expression for \( q \) at the extreme values of \( \phi \):

prolate spheroid: \( q = \frac{C}{r_i} = \frac{\phi^{2/3}}{\ln(2\phi)} \equiv \frac{4}{3} \phi^{2/3} (\phi \to \infty) \)

oblate spheroid: \( q = \frac{C}{r_i} = \frac{2}{\pi \phi^{1/3}} \).

(3.114)

The change of \( q \) expressed in terms of the volume change is thus:

prolate spheroid: \( d \ln q = \frac{2}{3} d \ln \phi = \frac{2}{3} \frac{\Gamma - 1}{\Gamma + 2} d \ln V, \)

oblate spheroid: \( d \ln q = -\frac{1}{3} d \ln \phi = -\frac{1}{3} \frac{\Gamma - 1}{\Gamma + 2} d \ln V. \)

(3.115)

We can think of \( d \ln q (=dq/q) \) and \( d \ln V (=dV/V) \) as the fractional change of \( q \) and \( V \).

Since \( \frac{\Gamma - 1}{\Gamma + 2} \) is always less than unity, the magnitude of the change of \( q \) is always less than that of the volume changes. Thus, we can assume that \( q \) is constant during a time step whenever the relative change of \( V \) is small. The relative change of volume can be large only when the ice particles are quite small. But in this situation, the aspect ratio would be quite close to unity and the change of \( q \) would then still be quite small.
Square-root solution

From above analyses, the diffusional growth equation can be simplified as a first-order differential equation

\[ \frac{dm_i}{dt} \bigg|_{\text{diff}} = 4 \pi r_i^2 \rho_i \frac{dr_i}{dt} = \frac{4 \pi r q D_v f_v e_{s,i}(T_\infty)}{R T_\infty} \left\{ S_{\infty,i} - (1 - \delta) \left[ 1 + \frac{l \delta(1 - \delta)}{R T_\infty} \right] \right\} \]

where \( \rho_i \) is the ice density during deposition. This equation can be rearranged to give

\[ \frac{d(r_i)^2}{dt} = \frac{2 q D_v f_v e_{s,i}(T_\infty)}{\rho_i R T_\infty} \left\{ S_{\infty,i} - (1 - \delta) \left[ 1 + \frac{l \delta(1 - \delta)}{R T_\infty} \right] \right\} \equiv A \tag{3.117} \]

where \( A \) is independent of \( r_i \). We thus derived the square-root analytical solution for the equivalent radius of ice particles:

\[ r_i = \left[ r_{i,o}^2 + A \delta t \right]^{1/2} \tag{3.118} \]

Here, \( r_{i,o} \) is the initial equivalent radius and \( r_i \) is the radius after a time \( \delta t \).