THE DISTRIBUTION OF ATMOSPHERIC ICE PARTICLE SHAPES AND THEIR OBSERVATIONS

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Abstract

This dissertation develops methodological and mathematical techniques for describing the distribution of various ice particle geometries and their 2D observations. It is common for models and observations to integrate both types of distributions when estimating key microphysical properties related to growth and depletion of ice particles. However, much of what is known about the actual 3D ice particle shapes is derived from 2D images or projections of each particle. Ice particle orientations therefore can distort the observed 2D geometry in a way that obscures the underlying 3D structure. A major discovery of this dissertation is that various transformations of ice particle distributions and their projections are represented in closed-form as univariate and bivariate $H$-functions. The properties of $H$-functions are based heavily on the Mellin integral transform. The concepts, notations, and properties of these functions might seem foreign to many in the meteorology and atmospheric science community. Therefore, chapter 2 of this dissertation provides an overview of the relevant math that surrounds $H$-functions as well as their various properties.

Chapter 3 develops an integral transform method for projecting distributions of ice particle habits (approximated as spheroids) onto a 2D plane. This projection process is geometrically analogous to how in situ observations capture ice particle shapes as well as how projected areas are used in microphysical fall speed calculations. Distribution transformations using mapping equations and numerical integration of projection kernels show that both truncation of size distributions and changes in Gaussian dispersion can alter the
modality and shape of projection distributions. As a result, the projection process can more than triple the relative entropy between the spheroidal and projection distributions for commonly assumed model and orientation parameters. This shape uncertainty is maximized for distributions of highly eccentric particles and for particles like aggregates that are thought to fall with large canting-angle deviations. The integral transform methodology is used to propose an in situ approach for estimating model parameters that govern ice particle shape from distribution moments of observed in situ ellipse fit eccentricity or second eccentricity.

Chapter 4 utilizes two separate datasets of best-fit ellipsoid estimates derived from Multi-Angle Snowflake Camera (MASC) observations to construct a bivariate beta distribution for capturing snow aggregate shapes. This mathematical model is used along with Monte Carlo simulated aggregates to study how combinations of monomer properties affect aggregate shape evolution. Plate aggregates of any aspect ratio produce a consistent ellipsoid shape evolution, whereas thin column aggregates evolve to become more spherical. However, thin column aggregates yield fractal dimensions much less than the often assumed value of 2.0. This discovery suggests that aggregates formed in cirrus clouds could exhibit significantly different physical properties than those formed in mixed-phase clouds. Simulated aggregate ellipsoid densities and fractal analogs of density (lacunarity) are much more variable depending on combinations of monomer size and shape. The inconsistent relationship between shape and density suggests that mass-dimensional prefactors should be rescaled in a more physical manner. Both simulations and observations prove aggregates are rarely oblate. These results therefore contradict much of the current literature on snow aggregate shapes, since many models and radar forward simulators assume homogeneous oblate spheroids.

Chapter 5 investigates the effect of convolving particle property distributions when using the bivariate beta distribution from chapter 4. Idealized tests show that the number weighted mean fallspeed for ellipsoidal aggregates is more than 90% less than that of sphere/fractal aggregates, while mass-weighted fallspeeds for ellipsoid aggregates are approximately 60% of sphere/fractal aggregates. The distribution ranges produced by ellipsoidal aggregates is shown to be much more consistent with observed fall speed ranges than using a mass-dimensional relationship alone. This implies that current microphysics
models systematically overestimate mass and number sedimentation fluxes but underestimate size sorting anywhere from 8% to 20%. Properties of the $H$-function are used to develop a spectral bulk modeling methodology that can utilize any number of distribution moments in the estimation of distribution parameters. The use of this spectral bulk microphysics methodology in numerical weather prediction models can therefore provide the computational simplicity of bulk microphysics models while still exhibiting the numerical complexity of bin microphysics models.
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A.2 Ratio of eccentricity moments to uniformly oriented, projected eccentricity moments.
List of Symbols

\( a \)  \( a \)-axis length of spheroidal ice particle
\( a_0 \)  Initial \( a \)-axis length
\( a_n \)  Characteristic \( a \)-axis length for size distribution
\( \alpha \)  First angle rotation for spheroid projection
\( \alpha_{ba} \)  Parameter of bivariate beta distribution \( n(\varphi_{ba}, \varphi_{ca}) \)
\( \alpha_0 \)  \( a_0^{1-\delta_*} \)
\( \alpha_m \)  Coefficient for mass-dimensional relation
\( A_{\text{proj}} \)  Projected area of spheroid
\( b \)  Ellipsoid \( b \)-axis length
\( B(a, b) \)  Beta function
\( \beta \)  Second angle (canting) rotation for spheroid projection
\( \beta_{ba} \)  Parameter of bivariate beta distribution \( n(\varphi_{ba}, \varphi_{ca}) \)
\( \beta_{cb} \)  Parameter of bivariate beta distribution \( n(\varphi_{ba}, \varphi_{ca}) \)
\( \beta_m \)  Exponent for mass-dimensional relation
\( \binom{n}{k} \)  Binomial coefficients
\( c \)  \( c \)-axis length of spheroidal or ellipsoidal ice particle
\( c_0 \)  Initial \( c \)-axis length
\( \delta_* \)  AHAB time-averaged particle growth history
\( D \)  Particle maximum dimension
\( D_0 \)  Initial Maximum Dimension length
\( D_f \)  Fractal dimension

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$D_q$ Generalized fractal dimension

$D_{\text{min}}$ Smallest maximum dimension for truncated distribution

$D_{\text{max}}$ Largest maximum dimension for truncated distribution

$D_n$ Characteristic particle maximum dimension for size distribution

$D_{\text{KL}}$ Kullback-Leibler Divergence or relative entropy

$\text{erf}(x)$ Error function

$E(x)$ Complete elliptic integral of the second kind

$E(x^n)$ $n$th moment of distribution $n(x)$

$\epsilon_{\text{ob}}$ Eccentricity (or first eccentricity) of an oblate spheroid

$\epsilon'_{\text{pro}}$ Second eccentricity of a prolate spheroid

$\epsilon_{\text{proj}}$ Eccentricity of 2D ellipse projection

$\epsilon'_{\text{proj}}$ Second eccentricity of 2D ellipse projection

$H(z)$ Fox’s H-function

$H(x,y)$ Bivariate H-function

$\gamma$ Third angle rotation for spheroid projection

$\Gamma(z)$ Gamma function

$\Gamma(z,x)$ Upper incomplete gamma function

$\Gamma(z,x_1,x_2)$ Generalized incomplete gamma function

$\, _1F_1 (a; b; x)$ Kummer’s confluent hypergeometric function

$\, _2F_1 (a, b; c; x)$ Gauss’ hypergeometric function

$pF_q(a_1, \ldots, a_p; b_1, \ldots, b_q; z)$ Generalized hypergeometric function

$I_{\nu}(x)$ Modified Bessel function of first kind with order $\nu$

$K_{\nu}(x)$ Modified Bessel function of second kind with order $\nu$
\( J \)  Jacobian matrix

\( \kappa \frac{1}{2\sigma^2} \)

\( K(x) \)  Complete elliptic integral of the first kind

\( l \)  A length scale associated with fractal particles

\( \lambda_l \)  Lacunarity of particle at grid length, \( l \)

\( \Lambda \)  Orientation and scale averaged lacunarity

\( L \)  Projected length of 2D ellipse

\( l_{ob} \)  Linear eccentricity for oblate spheroid

\( l_{pro} \)  Linear eccentricity for prolate spheroid

\( l_{proj} \)  Linear eccentricity of 2D ellipse projection

\( m_i \)  Ice particle mass

\( M_r \)  \( r \)th distribution moment of number distribution function

\( N \)  Number of boxcounting grid boxes that hold at least one aggregate dipole

\( N_{grid} \)  Number of grid boxes used for fractal calculations

\( N_i \)  Ice number concentration

\( N_{mon} \)  Number of aggregate monomers

\( G_{m,n}^{p,q}(z) \)  Meijer G-Function

\( n(x) \)  Number density function of variable \( x \)

\( \tilde{n}(x) \)  Probability density function of variable \( x \)

\( P_{i,l} \)  Aggregate dipole probabilities within \( l \) sized grid box with index \( i \)

\( \varphi \)  Spheroid aspect ratio \( \frac{c}{a} \)

\( \varphi_n \)  Characteristic aspect ratio

\( \varphi_{ba} \)  Ellipsoid aggregate aspect ratio \( \frac{b}{a} \)
\( \varphi_{ca} \) Ellipsoid aggregate aspect ratio \( \xi_a \)

\( \varphi_{cb} \) Ellipsoid aggregate aspect ratio \( \xi_b \)

\( \varphi_{\text{mon}} \) Aspect ratio of aggregate monomer

\( \varphi_{\text{proj}} \) Projected ellipse aspect ratio

\( \varphi_{\text{int}} \) Intercept spheroid aspect ratio where

\[
\frac{\delta \varphi_{\text{proj}}}{\varphi_{\text{proj}}} = \frac{\delta \varphi_{\text{proj}}}{\varphi_{\text{proj}}}
\]

\( \Phi \) Second definition of aspect ratio, \( \min (\varphi, \varphi^{-1}) \)

\( \Phi_1 (a, b; c; x, y) \) Humbert’s function

\( q \) Multifractal partition moment

\( q_i \) Ice mass mixing ratio

\( \rho_i \) effective ice particle density

\( \bar{\rho}_i \) Average effective ice particle density

\( \sigma \) Gaussian orientation standard deviation

\( \nu \) Size distribution shape parameter

\( V_i \) Ice particle ellipsoid volume

\( V_{i0} \) Ice particle sphere volume with radius, \( a \)

\( \chi_n \) Moment ratio of projected and spheroid (second) eccentricity distributions

\( \xi \) A particular microphysical quantity

\( \xi_n \) A characteristic microphysical quantity

\( \zeta_a \) A general exponent that scales an aggregate’s \( a \) axis

\( \zeta_{ba} \) A general exponent that scales an aggregate’s ellipsoid aspect ratio \( \varphi_{ba} \)

\( \zeta_{ca} \) A general exponent that scales an aggregate’s ellipsoid aspect ratio \( \varphi_{ca} \)

\( Z(q, l) \) Generalized multifractal partition function
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for my father . . . who happens to be an actual meteorologist . . .
Chapter 1

Introduction

1.1 Background and motivation

Scale invariance is an apparent quirk of nature. Stare at any particular region of the troposphere and you’ll perhaps see eddies of various sizes and intensities. Zoom into any one particular eddy and you’ll see even smaller ones that look very much like their parent. The cascade of kinetic energy from the larger parent eddies to their children leads to the observation of an “inertial subrange.” In this regime, eddy kinetic energy is transferred from parents to children without loss of energy to friction. Plotting the turbulent kinetic energy as a function of eddy wavenumber on a log-log scale within the inertial subrange yields a nearly straight line with slope $-5/3$. When eddy energy is expressed as a function of wavenumber, the equation is a simple power-law function. Therefore, inside this regime exists a simple relationship that couples two important properties: energy and size (or wavenumber). Outside this regime, however, lies much more complicated behavior that requires a more sophisticated model.

Knowledge of the natural occurrence of scale-invariant regimes in physical processes and their underlying power-law relationships is nothing new. Despite this, the use of power laws in physics, particularly in the atmospheric sciences, continues to gain ground in both understanding and applications. Much of the development of power-law parameterizations stems from the intimate relationship between fractal geometry and chaos theory. The current understanding of the relationship between these two seemingly disparate concepts in atmospheric science primarily is due to the work of Benoit Mandelbrot, who pioneered the field of fractal geometry. Through multiple individual and collaboration efforts, Mandelbrot used fractal geometry to describe turbulence (Mandelbrot 1974, 1975), the spatial distribution of cloud and rain fields (Lovejoy and Mandelbrot 1985), and the geometry of
diffusion-limited aggregates (Mandelbrot 1992; Mandelbrot et al. 2002).

A particular subfield of meteorology, cloud microphysics, is particularly filled with the observation of power-law behavior resulting from fractal geometry. The use of in situ (e.g., Locatelli and Hobbs 1974; Mitchell 1996; Heymsfield et al. 2002) or laboratory (e.g., Lamb and Scott 1972) derived power-law relations allows for an easy and physically meaningful way to couple various quantities together. For instance, it is very common for numerical weather prediction (NWP) microphysics schemes to specify different particle classes such as “rain,” “snow,” “graupel,” and “hail,” where each particle class employs a different set of power-law parameterizations. These power-law functions generally connect the maximum dimension of each particle to their geometry (e.g., aspect ratio) and their physical properties (e.g., mass and fallspeed). The total changes in the physical properties of all particles within a given model timestep is then used to appropriately adjust the thermodynamic, dynamic, and radiative responses for the rest of the model. The fractal geometry of snow aggregates have led to multiple parameterizations of their mass-dimensional power-law functions (e.g., Schmitt and Heymsfield 2010). The use of maximum dimension in these parameterizations is particularly attractive because both laboratory and in situ cloud probe observations can utilize particle images as estimates of size. These in situ cloud probe data can then be used to construct size distributions in the form of inverse exponential distributions (Marshall and Langleben 1953) or gamma distributions (Ulbrich 1983). Therefore, a single power-law function integrated over a gamma-type distribution can be expressed analytically, thus allowing for the simple and efficient calculations of bulk particle properties like water content or mass-weighted fallspeed. As a result, the current “bulk” microphysics framework assumes a functional form for the size distribution, uses integro-differential equations to predict some microphysical quantities like particle number and mass, and then uses the integration properties of the gamma or exponential size distribution to diagnose more involved properties such as mass-weighted fall speed.

However, there are a number of issues with this current power-law and size distribution framework. For instance, it is often the case that particles of the same habit type are not well characterized by a single set of power-law functions. That is, different datasets will yield different power-law parameters. Even power-law parameters with an assumed “universal” value, such as the $2.0$ fractal dimension often cited by modeling and observational studies (Westbrook et al. 2004b,a), will yield different values in different environments or
campaigns (Schmitt and Heymsfield 2010). Ice particles in particular have physical properties that are especially sensitive to their assumed power-law parameters. This is because ice particles come in many different shapes and sizes all resulting from the contribution of many different microphysical processes such as vapor deposition, riming, and aggregation. Power-law fits to observational data are also often reported without specifying correlation coefficients or goodness of fit values (e.g., Mitchell 1996). When these values are reported, they are often quite variable depending on particle class. For instance, Locatelli and Hobbs (1974) reported numerous power-law fits to fall speed data for different particle classes (see their Table 1). Locatelli and Hobbs (1974) reports correlation coefficients between fall speed and size power-law fits anywhere from 0.20 (aggregates of unrimed radiating assemblages of dendrites or dendrites) to 0.91 (Aggregates of unrimed radiating assemblages of plates, side planes, bullets, and columns). The sparse number of data points available from observations also contributes to a lack of physical understanding of these (assumed) power-law relationships.

Newer models, called particle property models, predict the power-law prefactors (e.g., Morrison and Milbrandt 2015) or power-law exponents (e.g., Jensen et al. 2017) that are used in bulk calculations. These new frameworks have focused on improving the representation of ice particles because of their observed variability in both form and behavior. By contrast, cloud and rain particles exhibit a homogeneous, quasi-spherical form that allows for a clear geometric representation. Ice particles, on the other hand, can yield dense, quasi-spherical forms such as graupel and hail or light and eccentric forms like dendrites. Variegated geometries naturally produce nonlinear behaviors in their physical properties. Ice particle fall speed in particular is nonlinearly affected by changes in geometry. The increase in particle mass directly acts to increase fall speed through an increased gravitational force. However, the increase of projected area acts to decrease fall speed through an increase in drag. Both mass and area are functions of particle size, thus producing a competition effect. As a result, it is common for particle properties to convolve with one another in highly nonlinear and often unpredictable ways. To make matters more confusing, ice particle density often decreases as particle size increases (Heymsfield et al. 2002; Brandes et al. 2007). This means that particle density, volume, and surface area all contribute to mass and fall speed, yet power-laws derived from observations will often ignore the underlying geometric factors and their weights that produce these resulting properties (e.g., Brown and
Francis 1995). Implementation of these parameterizations in microphysics schemes therefore will assume geometric factors based on spheres or spheroids, which introduce more uncertainty in calculations.

It is only very recently that researchers have attempted to use observations to evaluate particle property model performance. Sulia and Kumjian (2017a,b) used dual-polarization radar observations to evaluate the ice particle shape prediction performance of the bulk adaptive habit model (AHM). The adaptive habit model approximates ice particles as spheroids, thus providing a single degree of freedom for specifying particle shape. For spheroids, shape can be quantified in terms of an aspect ratio of major and minor axes. Model process rates like vapor deposition, riming and melting are used to predict an average power-law exponent that appropriately scales one axis length according to the other. This allows for a single size distribution to integrate particle properties related to area and volume. However, radar observations do not provide particle-by-particle information of each particles’ shape; instead, the radar signal depends on integrated scattering properties of the sampling volume. Microphysics models that implement adaptive habit prediction such as AHM or the Ice-Spheroids Habit Model with Aspect-Ratio EvoLution (ISHMAEL) can, at best, compare integrated properties. Therefore it is very difficult to use radar observations as a way to evaluate predicted spheroid shapes or to compare appropriate power-law quantities.

In situ cloud probes can provide a much more attractive alternative, because particle images can permit estimations of an entire distribution of ice particle shapes. In theory, these probes not only can allow for a direct aspect ratio distribution comparison, but can be used to estimate power-law exponents for appropriate shape evolution. The main limitation for performing such a comparison lies in a fundamental problem associated with in situ imaging. Particles tend to rotate and cant as they fall. The degree to which they orient themselves is primarily determined by each particles’ Reynolds number (Klett 1995; Siewert et al. 2014), which tends to span many orders of magnitude. In theory, this means that in situ estimates of particle shapes using proxies such as fitted ellipses should represent a convolution of the 3D ice particle shape and their orientations. However, the degree to which orientations distort the estimated shape is unknown and thus requires a general methodology for incorporating orientations in estimated ellipse fit distributions. Furthermore, particles like snow aggregates exhibit a number of different geometric forms that are
not necessarily well represented by spheroids. Models often assume spheres (Thompson et al. 2008) or oblate spheroids (Jensen et al. 2017) as proxies for aggregate shape, however, recent ground-based observations of aggregates (Jiang et al. 2019) calls into question their usefulness of such proxies. Instead, Jiang et al. (2019) found that very few aggregates were well represented by oblate spheroids, and rather were often better represented as prolate spheroids. Yet the lack of a single, well-defined shape further confuses estimations of aggregate geometry and how that geometry might relate to a single set of power-law relations. Therefore, model representation of snow aggregate geometry also requires a general approach that does not necessarily fall within the power-law framework.

1.2 The purpose and scope of this dissertation

The purpose of this dissertation is to develop general techniques for estimating 2D and 3D representations of ice particle shape for both observations and models. However, in pursuit of this goal, one of the most useful and fundamental properties of power-law functions, the aggregation property, becomes its greatest weakness. The power-law aggregation property is used when power-law functions are multiplied together with the same independent variable. This allows for their parameters to absorb one another as follows

\[ f_1(x) f_2(x) = a x^b \cdot c x^d = a c x^{b+d} = f x^g. \]  

(1.1)

When this occurs, the information that governs each individual component is lost. For imaging ice particles, this means that it is not possible to separate out a shape component with an orientation component from 2D ellipse fits. A similar problem occurs when convolving snow aggregate shapes and densities together to formulate mass or fall speed.

The methodologies presented in the following chapters promote a different strategy to account for these unnatural and natural convolutions. Instead, variables that convolve are assumed to follow a continuous probability distribution much like the particle size distribution. To account for the generality of possible distribution functions, we assume these variables belong to a class of functions known as Fox’s H-function (Fox 1961) or simply H-functions (Mathai et al. 2010). The beauty of the H-function lies in its convolution and
scaling properties and its ability to efficiently compute distribution moments. Because of
the esoteric nature of the $H$-function, the next chapter presents its properties and notations.
These properties are then used in chapters 3 and 4 as motivation for the presented methodologies and results. Chapter 3 presents a general methodology for projecting bulk distributions of ice particle shape, whereas chapter 4 develops an ellipsoidal aggregate model that describes a bivariate $H$-function distribution of ellipsoid aspect ratios. Chapter 5 ties chapters 2, 3, and 4 together by exploiting $H$-function properties in a way that extends the current bulk microphysics modeling power-law framework to include multiple distribution parameters.
Chapter 2

Mathematical Background

2.1 Distribution moments, Mellin transforms, and the gamma function

The Mellin integral transform is defined as

\[ f^* (s) \equiv \mathcal{M}_s \{ f (x) \} = \int_{x=0}^{\infty} x^{s-1} f (x) \, dx. \]  \hfill (2.1)

\( f (x) \) is recoverable by use of the inverse Mellin integral transform, which is defined as the following Mellin-Barnes type integral

\[ f (x) = \mathcal{M}^{-1} \left[ \mathcal{M}_s \{ f (x) \} \right] = \frac{1}{2\pi i} \int_{s=c-i\infty}^{c+i\infty} x^{-s} f^* (s) \, ds. \]  \hfill (2.2)

This theorem holds as long as \( f^* (s) \) is analytic in the strip \( a < \text{Re} (s) < b \) and if it tends to zero uniformly as \( \text{Im} (s) \to \pm \infty \) for any real value \( c \) between \( a \) and \( b \).

For example, imagine \( f (D) = N_0 \frac{1}{D_n} \exp \left( - \frac{D}{D_n} \right) \) represents a number distribution function for a particular particle class. Calculating a particular bulk quantity, like liquid water content (LWC), can be represented with the following integral

\[ \text{LWC} \equiv \frac{\pi}{6} N_0 \rho_l D_n^3 \int_{D_n=0}^{\infty} \left( \frac{D}{D_n} \right)^3 \exp \left( - \frac{D}{D_n} \right) d \left( \frac{D}{D_n} \right) = \pi N_0 \rho_l D_n^3, \]  \hfill (2.3)

where \( D_n \) is a characteristic size used to appropriate scale these types of integrations and \( m (D) = \frac{\pi}{6} \rho_l D^3 \) is the mass of each particle (assuming spherical particles). Therefore, for a general moment, \( r = s - 1 \), the integration over this size spectrum is analogous to the
following Mellin-transform from Equation (2.1)

\[ \mathcal{M}_3 \{ f(D) \} = N_0 D_n^{s-1} \int_{D_n=0}^{\infty} \left( \frac{D}{D_n} \right)^{s-1} \exp \left( -\frac{D}{D_n} \right) d\left( \frac{D}{D_n} \right) = N_0 D_n^{s-1} \Gamma(s), \quad (2.4) \]

where \( \Gamma(s) \) is the gamma function, which for positive integers can be represented by

\[ \Gamma(n) = (n - 1)!. \quad (2.5) \]

Now applying the inverse Mellin transform from Equation (2.2) gives the following Mellin-Barnes integral

\[ \mathcal{M}^{-1} \{ \mathcal{M}_3 \{ f(D) \} \} = N_0 \frac{1}{D_n} \frac{1}{2\pi i} \int_{s=c-i\infty}^{c+i\infty} \left( \frac{D}{D_n} \right)^{-s} \Gamma(s) ds. \quad (2.6) \]

The contour integral in Equation (2.6) is called the Cahen-Mellin integral. Using the Residue theorem of complex analysis allows for the evaluation of Equation (2.6) in terms of an infinite series representation. This can be done by evaluating the residues of each pole in Equation (2.6) for \( s \equiv s_k = 0, -1, -2, \ldots \). For these “simple” gamma function poles, the residues are just the first term of the Laurent series expansion near each pole: \( s = s_k \).

Summing the residues from all these poles yields

\[ \frac{1}{2\pi i} \int_{s=c-i\infty}^{c+i\infty} \left( \frac{D}{D_n} \right)^{-s} \Gamma(s) ds = \text{Res}_{s=s_k} \left( \frac{D}{D_n} \right)^{-s} \Gamma(s) ds \]

\[ = \sum_{k=0}^{\infty} (-1)^k \frac{\left( \frac{D}{D_n} \right)^k}{k!} \]

\[ \equiv \exp \left( -\frac{D}{D_n} \right), \quad (2.7) \]

where the final equality is simply the Taylor series representation of the exponential function, which was the original distribution function. This property of the exponential function exists for other analytic functions and serves as the foundation for any \( H \)-function. Essentially, any function whose Mellin transform yields a ratio of gamma functions like Equation (2.6) can be represented in terms of an \( H \)-function.

The Mellin transform also generalizes to multiple dimensions. For instance, the dou-
The double Mellin transform is given as

\[ f^* (s_1, s_2) \equiv \mathcal{M}_{s_1, s_2} \{ f(x, y) \} = \int_{x=0}^{\infty} \int_{y=0}^{\infty} x^{s_1-1} y^{s_2-1} f(x, y) \, dy \, dx. \tag{2.8} \]

The inverse double Mellin transform is analogous to the inverse Mellin transform

\[ f(x, y) = \mathcal{M}^{-1} [ \mathcal{M}_{s_1, s_2} \{ f(x, y) \} ] = \frac{1}{(2\pi i)^2} \int_{s_1=c_1-i\infty}^{c_1+i\infty} \int_{s_2=c_2-i\infty}^{c_2+i\infty} x^{-s_1} y^{-s_2} f^* (s_1, s_2) \, ds_2 \, ds_1. \tag{2.9} \]

### 2.2 The H-function

#### 2.2.1 Definition and notations

Fox’s H-function (Fox 1961) is defined by the following notations and Mellin-Barnes integral representation

\[ H(z) = H_{m,n}^{p,q}(z) \]

\[ = H_{p,q}^{m,n} \left[ z \begin{bmatrix} (a_1, A_1) & (a_2, A_2) & \cdots & (a_p, A_p) \\ (b_1, B_1) & (b_2, B_2) & \cdots & (b_q, B_q) \end{bmatrix} \right] \]

\[ = H_{p,q}^{m,n} \left[ z \begin{bmatrix} \prod_{j=1}^{m} \Gamma (b_j + B_j s) \prod_{j=1}^{n} \Gamma (1 - a_j - A_j s) \\ \prod_{j=n+1}^{p} \Gamma (a_j + A_j s) \prod_{j=m+1}^{q} \Gamma (1 - b_j - B_j s) \end{bmatrix} \right] \tag{2.10} \]

where the contour \( \mathcal{L} \) is taken in the complex plane \( s \) such that the path is to the right of the poles of \( \Gamma (b_j + B_j s) \) and to the left of the poles of \( \Gamma (1 - a_j - A_j s) \). Empty products are interpreted as unity. The notations for the \( H \)-function can be quite confusing since \( m, n, p, \) and \( q \) represent both the number of gamma functions in the numerator and denominator of the integrand as well as the type of gamma function (i.e. whether there is \( s \) or \(-s\) in the...
gamma function). To determine the Mellin-Barnes representation type from the \(m, n, p, q\) indices and the parameter sets, note that the total overall number of gamma functions is given by \(p + q\). Then, \(m\) refers to the number of left hand numerator gamma function poles whereas \(n\) refers to the number of right hand numerator gamma function poles. \(p\) and \(q\) refer to the total number of ‘A’ type and ‘B’ type gamma functions, respectively. Finally, notice that the parameter sets run from numerator to denominator; that is, \(1 \leq j \leq m + n\) are gamma functions in the numerator and \(m + n < j \leq p + q\) are gamma functions in the denominator. The symmetry of \(\Gamma((b_j + B) s)\) and \(\Gamma((a_j + A) s)\) terms with \(\Gamma((1 - b_j - B) s)\) and \(\Gamma((1 - a_j - A) s)\) terms reflects the substitution \(z = \frac{1}{z}\).

If \(A_j = B_j = C\), where \(C\) is a constant, then the H-function reduces to that of the Meijer G-Function (Meijer 1941)

\[
G(z) = G_{p,q}^{m,n}(\left\{ \begin{array}{c} a_1, a_2, \cdots a_p \\ b_1, b_2, \cdots b_q \end{array} \right\}) = \frac{1}{2\pi i} \int_{L} \prod_{j=1}^{m} \frac{\Gamma(b_j + s)}{\Gamma(b_j)} \prod_{j=1}^{n} \frac{\Gamma(1-a_j-s)}{\Gamma(1-a_j)} \prod_{j=n+1}^{p} \frac{\Gamma(a_j+s)}{\Gamma(a_j)} \prod_{j=m+1}^{q} \frac{\Gamma(1-b_j-s)}{\Gamma(1-b_j)} z^{-s} \, ds. \tag{2.11}
\]

A number distribution H-function can be considered with the following form (cf. Carter and Springer 1977):

\[
f(x) = kH(cx), \tag{2.12}
\]

where \(k\) and \(c\) are distribution constants necessary to normalize \(f\) such that \(\int_{0}^{\infty} f(x) \, dx = N_t\). Equation (2.12) can be expressed with the zeroth and first distribution moments which gives

\[
f(x) = N_t \frac{1}{x_n} H\left(\frac{x}{x_n}\right), \tag{2.13}
\]

where \(c^{-1} \equiv x_n = \frac{M_2I(2)}{M_1I(3)}\).

For example, the generalized gamma distribution can be written as the following normalized H-function distribution:

\[
n(x) = \frac{N_t}{\Gamma(b_1 + B_1)} x_n^{1.0} \left[ \left( \begin{array}{c} x \\ x_n \end{array} \right) \right] (b_1, B_1). \tag{2.14}
\]
For a number distribution function that represents linear combinations of H-functions (similar to Thompson et al. 2008), the distribution can be represented as

\[ f(x) = f_1(x) + f_2(x) = N_{t1} \frac{1}{x_{n1}} H_1 \left( \frac{x}{x_{n1}} \right) + N_{t2} \frac{1}{x_{n2}} H_2 \left( \frac{x}{x_{n2}} \right). \] (2.15)

### 2.2.2 Properties

The \( H \)-function exhibits several useful scaling properties (Mathai et al. 2010). For instance, reciprocal arguments can be represented as

\[ H_{m,n}^{p,q} \left[ \frac{1}{z} \right] \left( a_p, A_p \right) \left( b_q, B_q \right) = H_{q,p}^{n,m} \left[ \frac{1}{z} \right] \left( 1 - b_q, B_q \right) \left( 1 - a_p, A_p \right). \] (2.16)

Arguments to a power can be represented as

\[ H_{m,n}^{p,q} \left[ z^k \right] \left( a_p, A_p \right) \left( b_q, B_q \right) = k H_{p,q}^{m,n} \left[ z^k \right] \left( a_p, kA_p \right) \left( b_q, kB_q \right), \] (2.17)

where \( k > 0 \). H-functions multiplied by power functions can be represented as

\[ z^\sigma H_{m,n}^{p,q} \left[ z \right] \left( a_p, A_p \right) \left( b_q, B_q \right) = H_{p,q}^{m,n} \left[ z \right] \left( a_p + \sigma A_p, a_p \right) \left( b_q + \sigma B_q, B_q \right), \] (2.18)

where \( \sigma \in \mathbb{C} \).

Derivatives of the \( H \)-function are given in Cook (1981) as

\[ \frac{d^r}{dz^r} H(z^k) = H_{p+1,q+1}^{m,n+1} \left[ z^k \right] \left( \frac{r}{k} A_p, A_p \right) \left( b_q - \frac{r}{k} B_q, B_q \right) \left( 0, k \right), \] (2.19)

where \( k > 0 \). A similar equation can be derived for \( k < 0 \) using the reciprocal property of \( H \)-functions. Integration of the \( H \)-function and distribution moments of \( H \)-function
distributions are in terms of the gamma function ratios in Equation (2.10)

\[ I(r+1) \equiv \int_{x=0}^{\infty} x^r kH(cx) \, dx \]

\[ = kc^{-1-r} \prod_{j=n+1}^{m} \Gamma(a_j + A_j (r+1)) \prod_{j=m+1}^{q} \Gamma(1 - b_j - B_j (r+1)) \]

\[ \prod_{j=1}^{p} \Gamma(b_j + B_j (r+1)) \prod_{j=1}^{n} \Gamma(1 - a_j - A_j (r+1)) \]

(2.20)

Notice that this definition also doubles as the Mellin transform of the \( H \)-function when \( r = s - 1 \). Fourier and Laplace transforms of the \( H \)-function are \( H \)-functions of higher order (see Cook 1981).

The convolution property of univariate \( H \)-functions is given in Carter and Springer (1977). If \( X_1, X_2, \ldots, X_N \) are independent \( H \)-function variates with probability density functions \( f_1(x_1), f_2(x_2), \ldots, f_N(x_N) \), respectively, where

\[ f_Z(z) = k_j H_{P_{jk},A_j}^{m_{jk},n_{jk}} \left[ c_j x_j \left( \begin{array}{c} a_{jp_j}, A_{jp_j} \\ b_{jp_j}, B_{jp_j} \end{array} \right) \right], \]

(2.21)

for \( j = 1, 2, \ldots, N \), then the probability density function of the variate

\[ Y = \prod_{j=1}^{N} X_j \]

(2.22)

is given by

\[ h(y) = \left( \prod_{j=1}^{N} k_j \right) H_{\sum_{j=1}^{N} m_j, \sum_{j=1}^{N} n_j} \left[ c_j y_j \left( \begin{array}{c} a_{N_{jk}}, A_{N_{jk}} \\ b_{N_{jk}}, B_{N_{jk}} \end{array} \right) \right] \]

(2.23)

with the parameter sets given in Carter and Springer (1977). These equations and parameter sets can be easily proven by directly applying the Mellin transform and by rearranging terms.
2.3 The bivariate H-function

2.3.1 Definition and notations

The bivariate $H$-function is given by Kellogg and Barnes (1987, 1989) as

$$H(x, y) = H_{m_1, n_1, m_2, n_2, m_3, n_3}^{p_1, q_1, p_2, q_2, p_3, q_3} \left[ \begin{array}{c} (e_j, E_j) \\ (a_j, A_j) ; (c_j, C_j) \\ (f_j, F_j) \\ (b_j, B_j) ; (d_j, D_j) \end{array} \right]$$

$$= \frac{1}{(2\pi i)^2} \int_{\mathcal{L}_1} \int_{\mathcal{L}_2} \chi_1(s_1) \chi_2(s_2) \chi_3(s_1 + s_2) x^{-s_1} y^{-s_2} ds_1 ds_2,$$

(2.24)

where

$$\chi_1(s_1) = \frac{m_1 \prod_{j=1}^{p_1} \Gamma(b_j + B_j s_1) \prod_{j=1}^{n_1} \Gamma(1 - a_j - A_j s_1)}{\prod_{j=n_1+1}^{p_1} \Gamma(a_j + A_j s_1) \prod_{j=m_1+1}^{q_1} \Gamma(1 - b_j - B_j s_1)}$$

(2.25a)

$$\chi_2(s_2) = \frac{m_2 \prod_{j=1}^{p_2} \Gamma(d_j + D_j s_2) \prod_{j=1}^{n_2} \Gamma(1 - c_j - C_j s_2)}{\prod_{j=n_2+1}^{p_2} \Gamma(c_j + C_j s_2) \prod_{j=m_2+1}^{q_2} \Gamma(1 - d_j - D_j s_2)}$$

(2.25b)

$$\chi_3(s_1 + s_2) = \frac{m_3 \prod_{j=1}^{p_3} \Gamma(e_j + E_j (s_1 + s_2)) \prod_{j=1}^{n_3} \Gamma(1 - f_j - F_j (s_1 + s_2))}{\prod_{j=n_3+1}^{p_3} \Gamma(f_j + F_j (s_1 + s_2)) \prod_{j=m_3+1}^{q_3} \Gamma(1 - e_j - E_j (s_1 + s_2))}.$$

(2.25c)
2.3.2 Properties

If \( Z = X^a Y^b \) and \( X \) and \( Y \) are bivariate \( H \)-function random variates with rational \( a \) and \( b \) then the distribution of \( Z \) is given by Kellogg and Barnes (1987) as

\[
f_Z(z) = K g_1^{a-1} g_2^{b-1} H_{P,Q}^{M,N} \left[ \begin{array}{c} g_1^a g_2^b \eta_1 \\ \eta_2 \end{array} \right],
\]

(2.26)

where \( \eta_1 \) and \( \eta_2 \) are parameter sets given by Kellogg and Barnes (1987).
Chapter 3

A Method for Estimating Bulk 2D Projections of Ice Particle Shape

3.1 Introduction

Characterization of individual ice particle geometry represents an integral part of many modern numerical weather prediction (NWP) models. A single length scale such as particle diameter allows for an efficient, albeit crude, way to connect various macroscopic quantities together. To do this, traditional “bulk” models assign size spectra \textit{a priori} such that various moments of each size spectrum correspond to relevant bulk ice quantities like ice water content or radar reflectivity. Bulk models will predict some of these various distribution moments, whereas other relevant moments can be diagnosed through analytical integration. However, the simplicity of this traditional bulk approach can often lead to unphysical ice particle properties across the size spectrum, such as representing all ice particles with a constant density (e.g., Morrison et al. 2005) or with reduced-density spheres (e.g., Thompson et al. 2008). As a result, most schemes need multiple ice categories such as “graupel” or “snow” to account for different densities and shapes. This means that artificial or ad hoc transfer functions are necessary to convert ice from one category to another (Harrington et al. 2013a). Ice particles represented by spheres do not properly account for the various shape effects that result from different habits. Shape provides nonlinear growth and depletion by adjusting vapor gradients around particle edges during vapor deposition and sublimation (Marshall and Langleben 1953), thermal gradients during melting (Kintea et al. 2015) and by modifying collection areas during riming (Fukuta and Takahashi 1999) and aggregation (Connolly et al. 2012). As a result, the key nonlinearities resulting from these process rates are often either ignored or are inconsistent with laboratory data (Bailey and Hallett 2009) and numerical studies (Westbrook et al. 2008). Therefore, even if the size distribution of a traditional scheme happens to be consistent with observations, the various
moments of the distribution that represent bulk quantities can still have large errors (Petty and Huang 2011; Wu and McFarquhar 2016).

Despite these inconsistencies between models and observations, bulk models will often rely on empirical or semi-empirical dimensional relations that characterize entire particle properties (e.g., mass, fallspeed or density) across a single size spectrum (e.g., Brown and Francis 1995; Baker and Lawson 2006; Lawson and Baker 2006; Lawson et al. 2006a; Brandes et al. 2007). However, any dimensional relation derived from in situ data can be severely biased or otherwise subject to ambiguity. Part of this uncertainty stems from limitations of the in situ cloud probe imaging process (Brenguier et al. 2013), but much of the uncertainty is also the result of how one describes entire properties of any particle in terms of only a single dimension. For instance, Wu and McFarquhar (2016) found that different measures of size derived from the same in situ observations can vary the estimated ice water content by 3 times and the estimated number distribution function and mass-weighted terminal velocity by 6 times.

Newer bulk modeling frameworks, called Particle Property Methods (PPM), partially mitigate these consistency issues by predicting bulk ice particle properties (e.g., shape, density, or rime fraction) themselves. One such framework is called the Adaptive HABit model (AHAB) (Chen and Lamb 1994; Harrington et al. 2013a) which predicts two axis lengths, \(a\) and \(c\), such that ice particles are modeled as reduced-density spheroids. To first order, oblate spheroids approximate plate-like crystals such as dendrites, and prolate spheroids approximate column-like crystals such as needles. Here, we use the convention given in Chen and Lamb (1994) where the \(c\)-axis of each spheroid is along the spheroid’s symmetry axis and the \(a\)-axis is orthogonal to \(c\). These two axis lengths both have generalized gamma distribution size spectra and \(c\) is related to \(a\) by a power-law relation. Evolution of spheroidal aspect ratios (defined as \(\varphi = \frac{c}{a}\)) and effective densities are dictated by mass distribution hypotheses for each growth or depletion process. Adaptive habit evolution has since been extended to various hybrid-bin (Hashino and Tripoli 2007, 2008, 2011a) and bulk (Harrington et al. 2013a,b; Chen and Tsai 2016; Jensen et al. 2017) implementations.

Evaluation of modeled ice particle shapes using observations requires a common basis for comparison. Dual-polarization radar is one possible observational tool for such a comparison because products like differential reflectivity can be useful for inferring hy-
drometeor shapes. However, these products reflect the shapes of all particles within a given radar volume. Therefore, although dual-polarization radar can help constrain the bulk distribution of ice particle shapes, the individual information of each particle shape is washed out. On the other hand, in situ cloud probe images maintain individual particle shape information through each image. This allows for a direct aspect ratio comparison between model and observations. Cloud probes operate by shining a laser onto a linear photodiode array (see chapter 5 in Brenguier et al. 2013). Particles within the swept-out cloud probe volume block the laser signal from reaching the photodiode array, thereby producing “shadowed” or “projected” particle images. The individual particle projections can then be fit with various shapes such as circles or ellipses such that size or shape information of the projection can be quantified.

Retrievals of aspect ratios using either in situ or radar observations have to be performed with an assumption about particle orientation. Several theoretical studies have investigated the orientation of single spheroidal ice particles (King 1985, 1986; Klett 1995; Siewert et al. 2014) but few have dealt with projections of an entire aspect ratio distribution. One exception is Jiang et al. (2017), who projected various aspect ratio spectra but did not connect these assumed spectra to microphysics schemes or observations. This need for a consistent characterization of ice particle projection spectra is also important for calculating particle fallspeeds (Böhm 1989) and collection areas during riming (Erfani and Mitchell 2017) and aggregation (Connolly et al. 2012). Currently, microphysical processes ignore these effects by assuming that particles fall with their major dimension in the horizontal (Böhm 1989; Harrington et al. 2013a). However, laboratory studies suggest that particle orientations depend upon each particles’ Reynolds number (List and Schemenauer 1970), which itself depends upon particle mass and therefore particle size. This nonlinear dependence has also been shown using lidar (e.g., Noel and Sassen 2005) for both planar and columnar crystals. As a result, projection quantities themselves represent a key set of nonlinearities that remain absent in current microphysics schemes.

This study develops a methodology for estimating projected aspect ratios of modeled ice particle distributions. The method is general enough such that equations derived in this chapter can be used for estimating single particle average aspect ratios, developing projection error estimates and bounds, and comparing modeled aspect ratio distributions with those derived from cloud probe ellipse fit data. In Section 3.2, we show the geometry of
projecting single spheroids onto a 2D plane, which allows us to develop mapping equations for spheroid eccentricity and aspect ratio. By differentiating the mapping equations that relate spheroid shapes with their projections, we show how propagation of uncertainties in angle and spheroid shape affect projections. In Section 3.3, we derive the aspect ratio and eccentricity distributions that are consistent with those in bulk microphysics schemes. In Section 3.4, we derive the projected eccentricity distributions from the spheroid eccentricity distributions in Section 3.3 with assumed orientation distributions. In Section 3.5, we test our theoretical projection method with example distribution parameters by comparing with a Monte Carlo procedure.

### 3.2 Theory

Jiang et al. (2017) project ellipsoidal aspect ratios by performing Euler angle rotations on each ellipsoid and by finding tangent points with respect to a projection plane. Here, we take a different approach by simplifying as much of the rotation and projection geometry problem as we can analytically. There are many reasons why this is worthwhile:

1. Spheroidal axial symmetry can allow us to combine and reduce some of the terms that constitute the complicated projection expressions given in the Appendix of Jiang et al. (2017).

2. The Euler angle rotation matrix method from Jiang et al. (2017) is computationally expensive, especially when projecting multiple distributions of particles that have potentially complex orientations.

3. It is not obvious, for a given distribution or sets of distributions, how many samples are required for robust statistical analyses of projected quantities.

4. Bulk size distributions given in microphysics schemes are continuous and have closed-form integral representations. Similarly, it is possible to derive projection quantities in closed-form, as we show below.

5. Analytical expressions for projection quantities allow us to efficiently explore the projection parameter spaces based on both model parameters and orientation assump-
tions. This also allows us to evaluate current observational techniques that are used to report these aspect ratio quantities (e.g., Korolev and Isaac 2003; Brandes et al. 2007; Hogan et al. 2012).

6. Microphysical quantities such as fallspeed and radiative quantities like extinction are indirectly dependent on the projected area. For spheroids, projected area is proportional to the projected aspect ratio. Therefore, this analysis could help provide appropriate and convenient scaling factors or expressions that incorporate orientation effects in bulk microphysics schemes.

Jiang et al. (2017) state that they were unaware of realistic aspect ratio distributions. However, we show a way to derive aspect ratio spectra that is consistent with both traditional bulk modeling approaches and the adaptive habit approach. We first start with the general projection of single spheroids and we then extend this analytic approach to these derived bulk model aspect ratio distributions.

3.2.1 Single spheroid projection

The single spheroid projection problem can be set up like in Figure 3.1 where a spheroid (shown here as oblate) is initially oriented with its c axis perpendicular to the 2D projection plane. In this sense, the c axis length is along the z axis and the a axis length is along the x axis (the third length b = a, is along the y-axis). To orient the reader, four colored circles are shown along the outside of the spheroid/ellipse for each rotation step. If one considers a parallel light source that illuminates the spheroid from above, then the resulting projection underneath is a circle with radius of length a (first row in Figure 3.1). The first rotation, \( \alpha \), is about the z axis, which acts to rotate the spheroid’s x axis counterclockwise. The second rotation, \( \beta \), is about this new x axis, \( x' \). The third rotation, \( \gamma \), is about the new z axis, \( z' \).

The important aspect about this spheroid rotation convention is that two out of the three rotations, \( \alpha \) and \( \gamma \), do not change the aspect ratio of the 2D projection. This is because these two rotations are about the spheroid’s c axis, which is an axis of symmetry. This means that using this Z – X – Z Euler angle rotation convention allows us to parameterize...
the changing projection about only one angle, $\beta$. We can make one additional simplification to transform the real aspect ratios to projection analogs if we consider transforming the aspect ratio quantities themselves. This is shown in Figure 3.2 which represents the second
rotation, $\beta$, for both an oblate (left) and prolate (right) spheroid. Notice that canting of the oblate spheroid decreases the projected ellipse minor axis length $L$ whereas canting of the prolate spheroid increases the projected ellipse major axis length $L$ while $a$ is held constant.

For $\beta = 90^\circ$, the projected length $L$ is equal to the particle length, $c$.

**Figure 3.2.** Single spheroid projection geometry. The spheroid and corresponding 2D ellipse origins are marked with an orange filled circle whereas foci are marked with green filled circles. Right triangles: 1 (purple), 2 (green), and 3 (blue), are shown on each spheroid/ellipse and are enlarged outside the diagram for convenience. The dashed lines represent the projection of both the spheroid origin and focus onto the 2D ellipse. Notice that the spheroid $a$ axis is represented in both the spheroid and ellipse and that the hypotenuse of triangles 1 and 3 are also the maximum axis lengths.

Drawn on each spheroid are two right triangles labeled 1 and 2. The hypotenuse of triangle 1 is the spheroid’s major dimension whereas the two sides are the minor dimension
and the spheroid’s linear eccentricity $l_{\text{ob}}$ (oblate) or $l_{\text{pro}}$ (prolate). Triangle 2 represents the projection of each spheroid focus length, $l$, onto the 2D plane (given by $l_{\text{ob}} \sin \beta$ and $l_{\text{pro}} \sin \beta$). Finally, in order to retrieve a shape quantity, we can take the projected linear ellipse eccentricity $l_{\text{proj}}$ and divide by $a$. This division cancels the length quantity from the linear eccentricities such that we are left with a simple mapping:

\begin{align}
\text{Oblate} : & \quad \varepsilon_{\text{proj}} = \varepsilon_{\text{ob}} \sin \beta \\
\text{Prolate} : & \quad \varepsilon'_{\text{proj}} = \varepsilon'_{\text{pro}} \sin \beta,
\end{align}

where $\varepsilon_{\text{proj}} = \frac{l_{\text{proj}}}{a}$ is the eccentricity variable for the oblate projection and $\varepsilon'_{\text{proj}} = \frac{L}{l_{\text{proj}}}$ is the second eccentricity variable for the prolate projection. Aspect ratio, eccentricity, and second eccentricity all could represent the shape of spheroids, while (second) eccentricity shows a very simple transformation between the oblate (prolate) spheroid and its projection. Because we will be using Equation (3.1) in later sections it is important to know the relationships among aspect ratio, eccentricity, and second eccentricity. These transformations for both oblate and prolate spheroids are given in Figure 3.3 for each variable and their differentials.

Similarly, we can also use the Pythagorean theorem for triangle 3 in Figure 3.2 to map the spheroid aspect ratios to the projected aspect ratio. This gives us an aspect ratio mapping equation for oblate and prolate spheroids:

$$\varphi_{\text{proj}} = \frac{L}{a} = \sqrt{\cos^2 \beta + \varphi^2 \sin^2 \beta} = \sqrt{1 - (1 - \varphi^2) \sin^2 \beta}.$$  (3.2)

We can verify Equation (3.2) by analytically integrating the equation with a given orientation distribution and comparing the average, or expected, projected aspect ratio with results from Jiang et al. (2017). Because both spheroidal aspect ratios in Jiang et al. (2017) are defined as the ratio of the minor dimension over the major dimension, we use a similar definition for aspect ratio: $\Phi = \frac{D_{\text{minor}}}{D_{\text{major}}} = \min(\varphi, \varphi^{-1})$. The random orientation assumption given in Jiang et al. (2017) is consistent with a canting distribution of $\sin \beta$ since this term specifies a solid angle. The analytical solution for randomly oriented oblate and prolate
Oblate \( \varphi < 1.0 \)  

Prolate \( \varphi > 1.0 \)

**Figure 3.3.** Transformations among aspect ratio (\( \varphi \)), eccentricity (\( \varepsilon \)), and second eccentricity (\( \varepsilon' \)) for oblate and prolate spheroids using the convention that \( \varphi = \frac{c}{a} \). The top row corresponds to transformations between any two variables whereas the bottom row represents transformations between the differentials of each variable.

spheroids is therefore:

\[
\text{Oblate} : \quad \langle \Phi_{\text{proj}} \rangle_{\text{rand}} = \int_{\beta=0}^{\pi/2} \sin \beta \sqrt{1 - (1 - \Phi^2) \sin^2 \beta} \, d\beta
\]

\[
= 2F_1 \left( -\frac{1}{2}, 1; \frac{3}{2}; 1 - \Phi^2 \right)
\]

\[
= \frac{1}{2} + \frac{1}{2} \frac{\Phi^2}{\sqrt{\Phi^2 - 1}} \sec^{-1}(\Phi)
\]

(3.3a)
Prolate: \( \langle \Phi_{\text{proj}} \rangle_{\text{rand}} = \int_{\beta=0}^{\pi} \frac{\sin \beta}{\sqrt{1 - (1 - \Phi^{-2}) \sin^2 \beta}} d\beta \)

\[
= 2F_1 \left( \frac{1}{2}, 1; \frac{3}{2}; 1 - \Phi^{-2} \right) \\
= \frac{\Phi}{\sqrt{1 - \Phi^2}} \cos^{-1}(\Phi),
\]

(3.3b)

where \( 2F_1 (a, b; c; x) \) is Gauss’ hypergeometric function. These analytical solutions for \( 0.001 \leq \Phi \leq 1.0 \) are shown in Figure 3.4 alongside average projected aspect ratio values for \( \Phi = 0.1, 0.2, 0.4, 0.6, 0.8, 1.0 \) from Jiang et al. (2017). The corresponding values between Jiang et al. (2017) and Equation (3.3) are all within 0.1 of each other, which is the precision given in Jiang et al. (2017).

Also shown in Figure 3.4 are analytical solutions for the average projected aspect ratios if \( \beta \) follows a uniform distribution. These solutions are given in terms of the following elliptic integrals:

Oblate: \( \langle \Phi_{\text{proj}} \rangle_{\text{uniform}} = \frac{2}{\pi} \int_{\beta=0}^{\pi} \sqrt{1 - (1 - \Phi^2) \sin^2 \beta} d\beta \)

(3.4a)

\[
= \frac{2}{\pi} E \left( 1 - \Phi^2 \right)
\]

Prolate: \( \langle \Phi_{\text{proj}} \rangle_{\text{uniform}} = \frac{2}{\pi} \int_{\beta=0}^{\pi} \frac{1}{\sqrt{1 - (1 - \Phi^{-2}) \sin^2 \beta}} d\beta \)

(3.4b)

\[
= \frac{2}{\pi} \Phi K \left( 1 - \Phi^2 \right)
\]

where \( E \) and \( K \) are the complete elliptic integrals of the second and first kind, respectively.

These tests not only validate our method, but they also give insight into what we can conclude from averaging aspect ratio values, as is common in the literature (e.g., Korolev and Isaac 2003; Brandes et al. 2007; Hogan et al. 2012; Garrett et al. 2015). Some of
these insights are not necessarily obvious using previous results such as Jiang et al. (2017) because these previous tests only show behavior for specific spheroid aspect ratios within a given range. Our analytical expressions however give behavior for the entire range of possible spheroid shapes. For instance, Figure 3.4 clearly shows the asymmetric behavior of rotating and projecting aspect ratios of randomly oriented oblate spheroids vs. prolate spheroids. Randomly oriented oblate spheroids using the orientation convention of Jiang et al. (2017) have average projected aspect ratio values that tend toward 0.5 as the real, spheroidal values tend toward 0. Similarly, uniformly oriented oblate spheroids have average projected aspect ratio values that tend toward \( \frac{2}{\pi} \approx 0.6366 \) as the real, spheroidal values tend toward 0. Because both these orientation assumptions yield average projected aspect ratios that tend toward finite numbers, the absolute errors (dashed lines) associated with the difference between the oblate and average projected aspect ratio values increase monotonically for more eccentric particles.

However, prolate particles deviate from this behavior. Average projected aspect ratios of randomly and uniformly oriented prolate spheroids have the same limits as the real prolate aspect ratio; as prolate aspect ratios tend toward 0, so do the average projected aspect ratios. However, the absolute error for both orientations reach maximum values at finite values. Differentiating Equations (3.3b) and (3.4b) with respect to \( \Phi \) yield a random orientation absolute error maximum at \( \Phi \approx 0.433447 \) and a uniform orientation absolute error maximum at \( \Phi \approx 0.341622 \). These maxima occur as a result of taking the reciprocal of \( \varphi \) and averaging projected aspect ratios of \( \frac{D_{\text{minor}}}{D_{\text{major}}} \) instead of \( \frac{D_{\text{major}}}{D_{\text{minor}}} \) which changes the limiting behavior. Since spheroid volume and area are linear with respect to \( \varphi \) and not \( \Phi \), these results suggest that proper care should be employed when choosing aspect ratio quantities for different habit types and when averaging aspect ratio values. Although defining prolate aspect ratios using \( \Phi \) allows for the decreasing of absolute errors across the aspect ratio spectrum, this benefit becomes irrelevant if one takes the reciprocal to relate to geometric quantities (i.e., volume or projected area).

Uniform or random orientations are generally specified for particles with very low or very high Reynolds numbers whereas particles with intermediate Reynolds numbers will wobble with a Gaussian canting about their preferred orientation (i.e., maximum dimension in the horizontal) (Pruppacher and Klett 1997). For these intermediate Reynolds number particles, there are two relevant projection viewing directions: side incidence and fallspeed.
Figure 3.4. Comparison of average projected aspect ratios for each spheroid aspect ratio, $\Phi$, Equation (3.2) (solid, Equations (3.3) and (3.4)), analytical errors (dashed, $\langle \Phi_{\text{proj}} \rangle - \Phi$), and results from Jiang et al. (2017) (dots). Random orientations are specified as in Jiang et al. (2017).

direction. For planar (oblate) crystals, these viewing directions correspond to Gaussian orientations about $\beta = 90^\circ$ for side incidence and Gaussian orientations about $\beta = 0^\circ$ for fallspeed direction. For columnar (prolate) crystals, both view directions correspond to Gaussian orientations about $\beta = 90^\circ$ (refer to Figure 3.2). Therefore, aspect ratio retrieval estimates are best performed if particles are viewed from side incidence whereas projected area estimates are best performed when viewing particles along their fallspeed direction.
For small angles, these Gaussian assumptions can be simplified by replacing $\beta$ with $\sin \beta$ (cf. Klett 1995, and Table 3.1). Doing this for calculating the average aspect ratio of oblate (planar) particles viewed along their fall direction yields the approximate form:

$$
\langle \Phi_{\text{proj}} \rangle_{\text{Gaussian}} \approx \frac{2}{\pi} \frac{\exp \left( \frac{1}{4\sigma^2} \right)}{I_0 \left( \frac{1}{4\sigma^2} \right)} \int_{\beta=0}^{\pi} \sqrt{1 - (1 - \Phi^2) \sin^2 \beta} \exp \left( -\frac{1}{2\sigma^2} \sin^2 \beta \right) d\beta. \quad \text{(3.5)}
$$

If we use the substitution $u = \sin^2 \beta$ in Equation (3.5), then this integral takes the following form:

$$
\langle \Phi_{\text{proj}} \rangle_{\text{Gaussian}} \approx \frac{1}{\pi} \frac{\exp \left( \frac{\kappa}{2} \right)}{I_0 \left( \frac{\kappa}{2} \right)} \int_{u=0}^{1} u^{-\frac{1}{2}} \left[ 1 - (1 - \Phi^2) u \right]^\frac{1}{2} (1 - u)^{-\frac{1}{2}} \exp \left( -\kappa u \right) du, \quad \text{(3.6)}
$$

where $\kappa = \frac{1}{2\sigma^2}$. Surprisingly, even though symbolic programming languages (e.g., Mathematica or Maple) will not produce a closed-form solution to integrals of the type shown in Equation (3.6), Equation (3.6) can still be represented in closed-form using Humbert’s function (see Srivastava and Karlsson 1985) which has the following integral and bivariate $H$-function representations

$$
\Phi_1(a,b;c;x,y) = \frac{1}{B(a,c-a)} \int_{t=0}^{1} t^{a-1} (1-xt)^{-b} (1-t)^{c-a-1} \exp(zt) dt,
$$

$$
= \frac{\Gamma(1-b)\Gamma(c)}{\Gamma(a)} H_{1,1,0,1,0,1}^{1,1,0,1,1,1} \left[ \begin{array}{c} x \\ -y \end{array} \right| \begin{array}{c} (1-c,1) \\ (1-b,1) \\ (1-a,1) \\ (0,1);(0,1) \end{array} \right] \quad \text{(3.7)}
$$

Where $\Re(c) > \Re(a) > 0$.

This puts Equation (3.6) into the following concise and elegant form

$$
\langle \Phi_{\text{proj}} \rangle_{\text{Gaussian}} \approx \frac{\exp \left( \frac{\kappa}{2} \right)}{I_0 \left( \frac{\kappa}{2} \right)} \Phi_1 \left( \frac{1}{2}, -\frac{1}{2}; 1; (1 - \Phi^2), -\kappa \right). \quad \text{(3.8)}
$$
Replacing \( \sin \beta \) with \( \cos \beta \) in the Gaussian term (i.e. side view) yields a similar equation:

\[
\langle \Phi_{\text{proj}} \rangle_{\text{Gaussian}} \approx \exp \left( -\frac{\kappa^2}{2} \right) I_0 \left( \frac{\kappa}{2} \right) \Phi_1 \left( \frac{1}{2}, -\frac{1}{2}; 1; \left( 1 - \Phi^2 \right), \kappa \right).
\] 

(3.9)

Evaluation of Equations (3.8) and (3.9) can be performed using the ‘hyper2d’ function from the mpmath Python library.

We can use Equation (3.9) to investigate how the common Gaussian canting assumption changes the average projected aspect ratios for single spheroid particles. This is shown in Figure 3.5 for \( \sigma = 5^\circ, 10^\circ, 20^\circ, \) and \( 40^\circ \) where we plot the absolute errors of \( \langle \Phi \rangle_{\text{Gaussian}} \) for both the analytical approximation (dashed, Equation (3.9)) and for the standard Gaussian distribution (see Table 3.1). For values of \( \sigma \) about \( 10^\circ \), the analytical equation can be seen to provide a very good approximation to using the standard Gaussian. Often times, even though snowflakes and plates are assumed to have \( \sigma = 40^\circ \) and \( \sigma = 10^\circ \), respectively, authors will report average aspect ratio quantities as actual particle aspect ratios (e.g., Korolev and Isaac 2003; Brandes et al. 2007; Hogan et al. 2012; Garrett et al. 2015). However, Figure 3.5 suggests that this is only strictly appropriate for particles that have both small values of \( \sigma \), which dictates the canting angle standard deviations, and values of \( \phi \) that do not significantly deviate from unity. For planar crystals with an aspect ratio of 0.1 and \( \sigma = 10^\circ \), the absolute error is 0.08 whereas for \( \sigma = 40^\circ \) the absolute error is 0.380. Equation (3.9) shows that these errors get even worse for flatter crystals and tend to asymptote towards values dictated by the Gaussian orientation alone.

### 3.2.2 Uncertainty analysis for individual projected spheroids

We can use Equations (3.1) and (3.2) to investigate how orientation uncertainty can affect the corresponding projected eccentricities and aspect ratios. This analysis can be useful from an observational perspective since any measurement of a crystal has orientation uncertainty. Typically, those who report or average aspect ratios for different habit types will assume that each crystal is observed exactly from its side. In our convention shown in Figure 3.2, this assumption for spheroidal particles corresponds to \( \beta = 90^\circ \) where \( L = c \). From Equation (3.1a), we can write the projected eccentricity uncertainty as (Equation 3.47
Figure 3.5. Gaussian orientation assumption average absolute errors for planar crystals viewed at side incidence. Solid lines represent the standard (actual) Gaussian orientation probability distribution whereas the dashed line represent the analytical expression given in Equation (3.9). Each color represents a different canting angle standard deviation, $\sigma$.

from Taylor 1997):

$$
\delta\varepsilon_{\text{proj}} = \sqrt{\left( \frac{\partial\varepsilon_{\text{proj}}}{\partial\beta} \cdot \delta\beta \right)^2 + \left( \frac{\partial\varepsilon_{\text{proj}}}{\partial\varepsilon} \cdot \delta\varepsilon \right)^2} = \sqrt{\varepsilon^2 (\delta\beta)^2 \cos^2\beta + (\delta\varepsilon)^2 \sin^2\beta}.
$$

(3.10)

Similarly, we can write down the projected aspect ratio uncertainty using Equa-
tion (3.2) as:

\[
\delta \phi_{\text{proj}} = \sqrt{\left( \frac{\partial \phi_{\text{proj}}}{\partial \beta} \cdot \delta \beta \right)^2 + \left( \frac{\partial \phi_{\text{proj}}}{\partial \phi} \cdot \delta \phi \right)^2}
\]

\[
= \frac{\sin \beta}{\phi_{\text{proj}}} \sqrt{(1 - \phi^2)^2 (\delta \beta)^2 \cos^2 \beta + \phi^2 (\delta \phi)^2 \sin^2 \beta}.
\]

(3.11)

Similar equations exist for prolate spheroids since the mapping equations are analogous as shown in Equation (3.1).

Figures 3.6 and 3.7 show how the uncertainties of the projected eccentricity and aspect ratio for an oblate spheroid depend on uncertainties in the angle and actual eccentricity (aspect ratio) using Equations (3.10) and (3.11). The top row of each figure shows how the uncertainty of each projected variable is affected by uncertainties in the spheroid eccentricity (aspect ratio) whereas the left column shows how uncertainties in the assumed angle \( \beta \) affect the projected uncertainties. Other subplots in each figure show different combinations of each variable uncertainty. The maximum \( \delta \beta = 10^\circ \) was chosen based on the variance that oblate crystals are often assumed to have during sedimentation in calm air (Sassen 1986; Klett 1995; Ryzhkov et al. 2011).

The top row in Figure 3.6 (i.e. the assumed angle is the true angle) shows that uncertainties in \( \epsilon_{\text{proj}} \) are dependent only on the angle of the oblate spheroid and the uncertainty associated with the true eccentricity. As \( \beta \) increases from 0° to 90°, the absolute error in the projected eccentricity also increases. However, the first column of Figure 3.6 (i.e. the chosen spheroid eccentricity is the actual spheroid eccentricity) shows nonlinear behavior for different values of \( \beta \) and \( \epsilon \). For larger values of \( \delta \beta \), there becomes a noticeable asymmetry where the projected eccentricity error is dependent on both the chosen angle and spheroid eccentricity. For values of \( \beta \) close to 90° uncertainties stay small even for large values of \( \epsilon \). However, for \( \beta \) close to 0° the error in \( \epsilon_{\text{proj}} \) scales linearly with increases in \( \epsilon \) for a given \( \delta \beta \). Values of \( \beta \) between 0° and 90° give a nonlinear increase in the projected eccentricity uncertainty for larger values of \( \epsilon \). These subplots suggest that, conversely, if angles are close to 90° then errors in the projected eccentricity remain small regardless of the particle’s actual eccentricity. If uncertainties of angle (\( \delta \beta \)) and spheroid eccentricity (\( \delta \epsilon \)) are about the same order (such as the middle, right panel where \( \delta \beta = 5^\circ \) and \( \delta \epsilon = 0.1 \)) then the absolute projected eccentricity error increases monotonically for both increases in
Figure 3.6. Contour plots of Equation (3.10) for different values of $\delta\beta$ and $\delta\varepsilon$.

Figure 3.7 is the same as Figure 3.6 except that these subplots show the results for aspect ratio using Equation (3.11). However, unlike Figure 3.6, it is apparent that behavior of Equation (3.11) for $\varphi < 1.0$ is nonlinear regardless of model uncertainties. The largest errors for $\delta\beta = 0^\circ$ occur at aspect ratios closer to unity and angles closer to 90$^\circ$. However, errors for $\beta$ close to 0$^\circ$ remain small regardless of the particle’s actual aspect ratio. While eccentricity errors consistently remain low when particles are observed from the side, pro-
jected aspect ratio errors are more sensitive. If $\beta$ is very close to $90^\circ$, then absolute errors for aspect ratios are lower than that of eccentricity. However, even if $\beta$ deviates only a few degrees, then aspect ratio absolute errors quickly increase past that of eccentricity. More importantly, these errors become significantly worse as particles become more and more eccentric.

While Figures 3.6 and 3.7 show *absolute* uncertainties for different combinations of chosen angles and spheroid shapes, it is not initially obvious how these uncertainties relate
Figure 3.8. (Left) Equation (3.14) plotted for $45^\circ \leq \beta \leq 90^\circ$. (Right) Relative projected error for $\varphi_{\text{proj}}$ (orange line) and $\varepsilon_{\text{proj}}$ (blue line) for different values of $\beta$ and $\delta\beta = 10^\circ$.

to one another in a relative sense. This is because changes in the projected aspect ratio and project eccentricity quantities are related nonlinearly (given by the relationships shown in Figure 3.3). If we assume that the orientation angle $\beta$ dominates the total uncertainty given by Equations (3.10) and (3.11) then we can reduce the absolute uncertainty equations into
simplified forms

\[ \delta \epsilon_{\text{proj}} = \lim_{\delta \epsilon \to 0} \sqrt{\epsilon^2 (\delta \beta)^2 \cos^2 \beta + (\delta \epsilon)^2 \sin^2 \beta} \]  

(3.12a)

\[ \delta \epsilon_{\text{proj}} \approx \epsilon \cos \beta \delta \beta \]

\[ \delta \varphi_{\text{proj}} = \lim_{\delta \varphi \to 0} \frac{\sin \beta}{\varphi_{\text{proj}}} \sqrt{(1 - \varphi^2)^2 (\delta \beta)^2 \cos^2 \beta + \varphi^2 (\delta \varphi)^2 \sin^2 \beta} \]  

(3.12b)

\[ \delta \varphi_{\text{proj}} \approx \frac{1}{\varphi_{\text{proj}}} \sin \beta \cos (1 - \varphi^2) \delta \beta. \]

If we divide through by each projected quantity, then we can express the relative uncertainties as:

\[ \frac{\delta \epsilon_{\text{proj}}}{\epsilon_{\text{proj}}} = \cot \beta \cdot \delta \beta \]  

(3.13a)

\[ \frac{\delta \varphi_{\text{proj}}}{\varphi_{\text{proj}}} = \frac{1}{\varphi_{\text{proj}}} (1 - \varphi^2) \sin \beta \cos \beta \cdot \delta \beta. \]  

(3.13b)

Notice that both Equations (3.13a) and (3.13b) depend linearly on \( \delta \beta \) but the relative projected aspect ratio error depends nonlinearly on the spheroid aspect ratio. This means that for certain ranges of \( \varphi \), the relative uncertainty of \( \varphi_{\text{proj}} \) will be greater than \( \epsilon_{\text{proj}} \). We can set Equations (3.13a) and (3.13b) equal to one another to see, for a chosen \( \beta \), where the relative projected aspect ratio error equals the relative projected eccentricity error. By performing some algebra, it is easy to show that this occurs when \( \varphi_{\text{proj}} = \epsilon_{\text{proj}} \). Therefore, solving for \( \varphi \) gives the remarkably simple expression:

\[ \varphi_{\text{int}} = \sqrt{\frac{2}{1 - \cot^2 \beta}}, \quad \beta > 45^\circ, \]  

(3.14)

where \( \varphi_{\text{int}} \) is the value of \( \varphi \) where the relative projected errors of aspect ratio and eccentricity equal one another. The restriction on \( \beta \) is to ensure that both relative error quantities intersect at a real value of \( \varphi_{\text{int}} \). Equations (3.13a), (3.13b) and (3.14) are shown in Figure 3.8. For \( \beta = 90^\circ \) (not shown) both relative projected error quantities are 0% for every value of \( \varphi \). However, for \( \delta \beta = 10^\circ \) and \( \beta = 80^\circ \) the projected aspect ratio relative error becomes greater than the projected eccentricity relative error for \( \varphi < 0.696 \) and tends toward about 98.9% as \( \varphi \) tends toward 0. The values of \( \varphi_{\text{int}} \) are relatively high with respect to many observed planar crystals. These results suggest that comparisons of modeled ice
particle shapes with observations should be performed using eccentricity information and not aspect ratios. While averaging of aspect ratio quantities could provide more accurate information about the 3D geometric quantities, the use of eccentricity instead provides a direct shape comparison that contributes smaller relative errors.

### 3.3 Bulk spheroid distributions

In Section 3.2, we showed that single spheroids linearly map eccentricity quantities onto their projected ellipses for any given canting angle, $\beta$. However, bulk models either implicitly or explicitly predict that ice particle aspect ratios vary across the size spectrum. While Harrington et al. (2013a) presents a $c$-axis AHAB distribution, they did not provide an equation for the aspect ratio distribution or eccentricity distribution. Similarly, aspect ratio information of ice particles in traditional bulk schemes are included implicitly in the formulation of mass-dimensional relationships. In this section we show how to derive the various diagnostic parameters that determine aspect ratio and therefore (second) eccentricity distributions. We employ the framework and notation of Harrington et al. (2013a) to develop an aspect ratio spectrum. We then extend this spectrum to one consistent with a traditional bulk approach. The relationships we derive are general as long as one prescribes mass-dimensional or width-dimensional relationships.

#### 3.3.1 Adaptive Habit framework

The size distribution (as a number density function) for AHAB spheroid $a$-axis lengths is given in Harrington et al. (2013a) with the equation:

$$ n(a) = \frac{N_i}{\Gamma(\nu)} \frac{1}{a_n} \left( \frac{a}{a_n} \right)^{\nu-1} \exp \left( -\frac{a}{a_n} \right), $$

(3.15)

where $N_i$ is the total grid box ice particle number concentration, $a_n$ is the characteristic $a$-axis length, $\nu$ is the gamma distribution shape factor and $\Gamma$ is the gamma function. This form of this size distribution is what many bulk microphysics schemes assume (e.g., Ferrier 1994; Thompson et al. 2004; Morrison et al. 2005). The $c$-axis is specified by a power-law
relation given by:

\[ c = \alpha_s a^{\delta_s}, \quad (3.16) \]

where \( \delta_s \) is the time-averaged growth history of both size distributions, \( \alpha_s = a_0^{1-\delta_s} \) and \( a_0 = 0.1 \mu m \) is the initial \( a \)-axis length. This means that the AHAB spheroid aspect ratio is given by a similar power-law relationship:

\[ \varphi \equiv \frac{c}{a} = \alpha_s a^{\delta_s-1}. \quad (3.17) \]

The adaptive habit distribution function for particle aspect ratios can be derived by transforming Equation (3.15) using Equation (3.17) and by normalizing this new distribution. This yields the following number density function:

\[ n(\varphi) = \frac{N_i}{\Gamma(\nu, \phi_n^{-\frac{1}{\delta_s-1}})} \frac{1}{\varphi_n |\delta_s - 1|} \left( \frac{\varphi}{\phi_n} \right)^{\frac{\nu}{\delta_s-1}-1} \exp \left[ - \left( \frac{\varphi}{\phi_n} \right)^{\frac{1}{\delta_s-1}} \right]. \quad (3.18) \]

Notice that the distribution given in Equation (3.18) is the more general Amoroso distribution (Amoroso 1925) as opposed to the generalized gamma distribution. This is because \( \delta_s < 1.0 \) yields negative exponents for \( \varphi \). Additionally, notice that if \( n(a) \) follows an inverse exponential distribution \( (\nu = 1.0) \) then Equation (3.18) becomes a Weibull distribution.

Values of \( |\delta_s - 1| \) that approach zero lead to a Dirac delta distribution at \( \varphi = 1.0 \). Additionally, values of \( \delta_s < 1.0 \) correspond to a distribution of oblate particles whereas values of \( \delta_s > 1.0 \) correspond to distribution of prolate particles. However, notice an important asymmetry associated with these distributions. The scaling of the distribution associated with deviations of \( |\delta_s - 1| \) from unity is different for oblate versus prolate distributions. We can separate out the oblate distribution from the prolate distribution as follows:

\[ \text{Oblate: } n(\varphi) = \frac{N_i}{\Gamma(\nu, \phi_n^{-\frac{1}{\delta_s-1}})} \frac{1}{\varphi_n |\delta_s - 1|} \left( \frac{\varphi}{\phi_n} \right)^{\frac{\nu}{\delta_s-1}+1} \exp \left[ - \left( \frac{\varphi}{\phi_n} \right)^{\frac{1}{\delta_s-1}} \right], \quad 1 \geq \varphi > 0 \quad (3.19a) \]
and

Prolate: \[ n(\varphi) = \frac{N_i}{\Gamma(\nu, \varphi_n^{\frac{1}{\delta_s-1}})} \frac{1}{\varphi_n^{\frac{1}{\delta_s-1}}} \left( \frac{\varphi}{\varphi_n} \right)^{\nu-1} \exp \left[ -\left( \frac{\varphi}{\varphi_n} \right)^{\frac{1}{\delta_s-1}} \right], \quad 1 \leq \varphi < \infty. \]

(3.19b)

Because the aspect ratio and eccentricity quantities behave monotonically across the size spectrum, we can generalize these distributions for a given size range \( D_{\text{min}} \leq D \leq D_{\text{max}} \) by using incomplete gamma functions.

Our mapping functions are linear with respect to (second) eccentricity. Therefore, we can perform another change of variables from aspect ratio to eccentricity (oblate) and second eccentricity (prolate) using transformations given in Figure 3.3 and using Equation (3.19). These corresponding eccentricity distributions are:

Oblate: \[ n(\varepsilon_{\text{ob}}) = \cdots \]

\[
\frac{N_i}{\Gamma(\nu, \varphi_n^{\frac{1}{\delta_s-1}})} \frac{1}{\varphi_n^{\frac{1}{\delta_s-1}}} \varepsilon_{\text{ob}} \left( \frac{\varphi_n}{\sqrt{1 - \varepsilon_{\text{ob}}^2}} \right)^{\nu+1} \exp \left[ -\left( \frac{\varphi_n}{\sqrt{1 - \varepsilon_{\text{ob}}^2}} \right)^{\frac{1}{\delta_s-1}} \right]
\]

Prolate: \[ n(\varepsilon'_{\text{pro}}) = \cdots \]

\[
\frac{N_i}{\Gamma(\nu, \varphi_n^{\frac{1}{\delta_s-1}})} \frac{1}{\varphi_n^{\frac{1}{\delta_s-1}}} \frac{\varepsilon'_{\text{pro}}}{\sqrt{\varepsilon'_{\text{pro}}^2 + 1}} \left( \frac{\sqrt{\varepsilon'_{\text{pro}}^2 + 1}}{\varphi_n} \right)^{\nu+1} \exp \left[ -\left( \frac{\sqrt{\varepsilon'_{\text{pro}}^2 + 1}}{\varphi_n} \right)^{\frac{1}{\delta_s-1}} \right].
\]

(3.20a)

(3.20b)

Equation (3.20) are non-standard distributions that have some interesting properties. For instance, moments of these distributions take a different form than the Amoroso distributions of Equation (3.18).
Oblate:

\[
E[e_{ob}^n] = \frac{N_i}{\Gamma\left(\nu, \varphi_n^{-1/\delta_s-1}\right)} \frac{1}{\varphi_n |\delta_s - 1|} \int_{\varphi=0}^{1} (1 - \varphi^2)^{\frac{n}{2}} \left(\frac{\varphi}{\varphi_n}\right)^{\frac{\nu}{\delta_s-1}-1} \exp \left[-\left(\frac{\varphi}{\varphi_n}\right)^{\frac{1}{\delta_s-1}}\right] d\varphi
\]

\[
= \frac{N_i}{2} \frac{\Gamma\left(\frac{n+1}{2}+1\right)}{\Gamma\left(\nu, \varphi_n^{-1/\delta_s-1}\right)} H_{1.2}^{2.0} \left[ \varphi_n \left(\frac{\nu}{2} + 1, \frac{1}{2}\right) \right] (0, \frac{1}{2}, (\nu, |\delta_s - 1|))
\]

(3.21a)

Prolate:

\[
E[e_{pro}^n] = \frac{N_i}{\Gamma\left(\nu, \varphi_n^{-1/\delta_s-1}\right)} \frac{1}{\varphi_n |\delta_s - 1|} \int_{\varphi=1}^{\infty} (\varphi^2 - 1)^{\frac{n}{2}} \left(\frac{\varphi}{\varphi_n}\right)^{\frac{\nu}{\delta_s-1}-1} \exp \left[-\left(\frac{\varphi}{\varphi_n}\right)^{\frac{1}{\delta_s-1}}\right] d\varphi
\]

\[
= \frac{N_i}{2} \frac{\Gamma\left(\frac{n+1}{2}+1\right)}{\Gamma\left(\nu, \varphi_n^{-1/\delta_s-1}\right)} H_{2.1}^{0.2} \left[ \varphi_n \left(1 + \frac{n}{2}, \frac{1}{2}\right) \right] (1 - \nu, \delta_s - 1, 0, \frac{1}{2})
\]

(3.21b)

A derivation for these \(H\)-function representations is given in Appendix A.2. It is very interesting to note that if \(n = 0\) then each equation in Equation (3.21) should reduce down to \(N_i\). However, if \(n = 0\) then the multiplicative terms of \(s\) (i.e., the second elements in each parameter sets of Equation (3.21)) are not identical. This is particularly curious since the incomplete gamma function that normalizes each distribution is represented in terms of the \(G\)-function (see Equation (2.11)). The \(G\)-function is defined such that these second elements are unity. Generally, Equation (2.17) can be used to rewrite these equations to meet this requirement but this is not the case for our \(H\)-functions because of the gamma function term with \(\nu\) and \(\delta_s\). Numerical integrations of each equation (not shown) actually prove these forms to be correct. It turns out that we can reconcile this conundrum using a little known property of this type of \(H\)-function that permits “generalizing constants” as shown in Bodenschatz (1992). Appendix A.3 presents a proof for these \(H\)-function
normalizations.

The number distribution functions of Equation (3.20) can be expressed as bivariate $H$-functions if $n \equiv s_1 - 1$ and another Mellin transform is applied to $\phi_n$. This gives the following distributions

\begin{equation}
 n(\varepsilon_{\text{ob}}) = \frac{N_i}{2} \frac{1}{\Gamma(v, \varphi_n^{(1-\delta)_{\frac{1}{2}}})} H_{0,1,0,2,0,1,0}^{1,0,2,0,0,0} \left[ \begin{array}{c}
 \varepsilon_{\text{ob}} \\
 \phi_n \\
 \end{array} \right] ; \left( \frac{1}{2}, \frac{1}{2} \right) ; (v, 1 - \delta_{\frac{1}{2}}, 0, \frac{1}{2}) \right]
\end{equation}

\begin{equation}
 n(\varepsilon'_{\text{pro}}) = \frac{N_i}{2} \frac{1}{\Gamma(v, \varphi_n^{(1-\delta)_{\frac{1}{2}}})} H_{0,1,1,1,1,0}^{1,0,0,1,0,1} \left[ \begin{array}{c}
 \varepsilon'_{\text{pro}} \\
 \phi_n \\
 \end{array} \right] ; \left( 1 - v, \delta_{\frac{1}{2}} - 1 \right) ; \left( \frac{1}{2}, \frac{1}{2} \right) ; (0, \frac{1}{2}) \right].
\end{equation}

### 3.3.2 Traditional bulk model frameworks

It is possible to diagnose an aspect ratio distribution of the form of Equation (3.18) if one assumes a traditional mass-dimensional relationship. The general form for a traditional mass-dimensional relationship is given as:

\begin{equation}
 m_i(D) = \alpha_0 D^{\beta_0}.
\end{equation}

Therefore, one can relate traditional particle masses to those specified by AHAB if we assume an average effective particle density $\bar{\rho}_i$ and the volume of a spheroid (i.e. $V_i = \frac{4}{3} \pi a^3 \phi = \frac{4}{3} \pi \alpha_0 a^{2+\delta}$). This gives us the general AHAB mass-dimensional form:

\begin{equation}
 m_i(a) = \frac{4}{3} \pi \alpha_0 \bar{\rho}_i a^{2+\delta}.
\end{equation}

However, because the traditional relationship Equation (3.23) is almost always in
terms of the maximum particle dimension and not axis lengths, we have to determine \textit{a priori} whether the traditional bulk particles are oblate (i.e. $D = 2a$) or prolate (i.e. $D = 2c$). Substituting these expressions for $D$ into Equation (3.24) gives us expressions for both oblate and prolate spheroids:

Oblate: \[ m_i(D) = \frac{\pi}{6} \rho_i D_0^{1-\delta_s} D^{2+\delta_s} \]  

Prolate: \[ m_i(D) = \frac{\pi}{6} \rho_i D_0^{2-\frac{2}{\delta_{*}}} D^{1+\frac{2}{\delta_{*}}} , \]  

where $D_0 = 2 \max (a_0, c_0)$ is the initial maximum dimension. If we compare Equation (3.24) with Equation (3.25), then we can diagnose $\delta_s$:

Oblate: \[ \delta_s = \beta_m - 2 \]  

Prolate: \[ \delta_s = \frac{2}{\beta_m - 1} . \]  

$\varphi_n$ can then be diagnosed by combining Equations (3.16), (3.17) and (3.26). This yields:

Oblate: \[ \varphi_n = D_0^{3-\beta_m} D_n^{\beta_m - 3} \]  

Prolate: \[ \varphi_n = D_0^{\beta_m - 3} D_n^{3-\beta_m} . \]

To solve for $D_0$, we assume that $D_0$ is determined when the mass-dimensional relationship for a given habit is equal to the mass-dimensional relationship of a sphere:

\[ \frac{\pi}{6} \rho_i D_0^3 = \alpha_m D_0^{\beta_m} \]

\[ \Rightarrow D_0 = \left( \frac{6 \alpha_m}{\pi \rho_i} \right)^{\frac{1}{3-\beta_m}} . \]

Equations (3.25) and (3.28) explicitly assumes that the average density is a constant although one could assume a power-law relationship like in Thompson et al. (2008) to derive similar equations.

The aspect ratio and eccentricity distributions for oblate particles are the same as Equations (3.19) and (3.20) since the $a$-axis spectrum follows a gamma distribution and the $c$-
axis follows a generalized gamma distribution. For prolate distributions where \( D = 2c \), then the reverse occurs: The \( c \)-axis follows a gamma distribution and the \( a \)-axis follows a generalized gamma distribution. As a result, \( \delta \), becomes \( \frac{1}{\delta_c} \) for these prolate distributions.

3.4 Transformation to projected eccentricity distribution

In this section, we show how to extend the results of the single particle projections to a bulk distribution. Doing so requires combining the spheroidal eccentricity distributions with an assumed orientation distribution. Here we just show the derivation for oblate spheroids, but the derivation for prolate spheroids is completely analogous.

If we assume that eccentricity distributions of spheroids are independent with respect to arbitrary canting angle probability distributions then we are able to write down a joint density function as:

\[
n (\varepsilon_{ob}, \beta) = n(\varepsilon_{ob}) \tilde{n}(\beta),
\]

where \( \tilde{n}(\beta) \) is an assumed probability density function in \( \beta \). Although theoretical and laboratory studies tend to suggest that \( \varepsilon \) and \( \beta \) are not completely independent from one another since both implicitly depend on size (List and Schemenauer 1970; Klett 1995; Pruppacher and Klett 1997), we make this assumption so as to provide a first order approximation for the projection analysis.

The convolution properties of the \( H \)-function translate over to the bivariate \( H \)-function distributions given in Equation (3.22). This can be verified by applying a Mellin Transform for the eccentricity variable. For example assume that \( u = \sin \beta \) can be represented as an \( H \)-function distribution. Then taking the Mellin transform of \( \varepsilon_{proj} \) and exploiting the assumed independence of \( \varepsilon_{ob} \) and \( u \) gives

\[
\mathcal{M}_{s_1} \{ \varepsilon_{proj} \} = \mathcal{M}_{s_1} \{ \varepsilon_{ob} u \} = \mathcal{M}_{s_1} \{ \varepsilon_{ob} \} \cdot \mathcal{M}_{s_1} \{ u \}.
\]

This means that the inverse Mellin transform allows for \( n(\varepsilon_{proj}) \) to be represented in terms of a bivariate \( H \)-function. It is important to note that while the function itself is bivariate, the distribution function is still univariate, i.e. the function is still normalized according to
$\varepsilon_{\text{proj}}$. $\varphi_n$ is still a constant for a particular distribution and not a random variable. The effect of this procedure has the effect of producing additional $s_1$ gamma function factors from the distribution of $u$. Although we could these bivariate functions in the results section, we instead elect to perform a change of variables for numerical simplicity. This change of variable methodology follows below.

Using our mapping functions given by Equation (3.1) on Equation (3.29) yields

$$ n\left(\varepsilon_{\text{ob}}, \beta\right) \mapsto n\left(\varepsilon_{\text{ob}}, \varepsilon_{\text{proj}}\right) = n(\varepsilon_{\text{ob}}) \tilde{n}\left(\beta \left(\varepsilon_{\text{ob}}, \varepsilon_{\text{proj}}\right)\right) \cdot |J|, \quad (3.31) $$

where the Jacobian is given by:

$$ |J| = \left| \begin{array}{cc} \frac{\partial \varepsilon_{\text{ob}}}{\partial \varepsilon_{\text{ob}}} & \frac{\partial \varepsilon_{\text{ob}}}{\partial \varepsilon_{\text{proj}}} \\ \frac{\partial \varepsilon_{\text{proj}}}{\partial \varepsilon_{\text{ob}}} & \frac{\partial \varepsilon_{\text{proj}}}{\partial \beta} \end{array} \right| = \begin{vmatrix} 1 & 0 \\ \varepsilon_{\text{proj}} \sqrt{\varepsilon_{\text{ob}}^2 - \varepsilon_{\text{proj}}^2} & \varepsilon_{\text{ob}} \sqrt{\varepsilon_{\text{ob}}^2 - \varepsilon_{\text{proj}}^2} \end{vmatrix} = \frac{1}{\sqrt{\varepsilon_{\text{ob}}^2 - \varepsilon_{\text{proj}}^2}}. \quad (3.32) $$

The choice to transform the joint distribution in terms of both 3D and 2D eccentricity distributions is such that the more complicated 3D eccentricity distribution will be unchanged.

The new joint distribution, corresponding to the projection kernel, is therefore given by:

$$ n\left(\varepsilon_{\text{ob}}, \varepsilon_{\text{proj}}\right) = n(\varepsilon_{\text{ob}}) \tilde{n}\left(\beta \left(\varepsilon_{\text{ob}}, \varepsilon_{\text{proj}}\right)\right) \frac{1}{\sqrt{\varepsilon_{\text{ob}}^2 - \varepsilon_{\text{proj}}^2}}. \quad (3.33) $$

Finally, we can integrate Equation (3.33) with respect to the spheroid eccentricity in order to find the corresponding projection distribution. Doing this procedure for both oblate and prolate spheroids gives the following equations:

Oblate: $n\left(\varepsilon_{\text{proj}}\right) = \int_{\varepsilon_{\text{ob}} = \varepsilon_{\text{proj}}}^{1} n(\varepsilon_{\text{ob}}) \tilde{n}\left(\beta \left(\varepsilon_{\text{ob}}, \varepsilon_{\text{proj}}\right)\right) \frac{1}{\sqrt{\varepsilon_{\text{ob}}^2 - \varepsilon_{\text{proj}}^2}} d\varepsilon_{\text{ob}} \quad (3.34a)$

Prolate: $n\left(\varepsilon'_{\text{proj}}\right) = \int_{\varepsilon'_{\text{pro}} = \varepsilon'_{\text{proj}}}^{\infty} n(\varepsilon'_{\text{pro}}) \tilde{n}\left(\beta \left(\varepsilon'_{\text{pro}}, \varepsilon'_{\text{proj}}\right)\right) \frac{1}{\sqrt{\varepsilon'^2_{\text{pro}} - \varepsilon'^2_{\text{proj}}}} d\varepsilon'_{\text{pro}}. \quad (3.34b)$

Notice that the integral of the spheroid (second) eccentricity starts from the projected...
(second) eccentricity due to the constraint that the former is no less that the latter (as dictated by Equation (3.1)). If we want to find the distribution for the projected aspect ratio then we can perform an additional transformation using Figure 3.3 after we integrate Equation (3.34).

For truncated distributions (such as to represent sampling size ranges of various cloud probes), we can modify Equation (3.34) in the following way:

\[
\text{Oblate : } n(\varepsilon_{\text{proj}}) = \int_{\varepsilon_{\text{ob}}=\max[\varepsilon_{\text{ob}}(D_{\text{min}}), \varepsilon_{\text{proj}}]}^{\varepsilon_{\text{ob}}(D_{\text{max}})} n(\varepsilon_{\text{ob}}) \tilde{n}(\beta(\varepsilon_{\text{ob}}, \varepsilon_{\text{proj}})) \frac{1}{\sqrt{\varepsilon_{\text{ob}}^2 - \varepsilon_{\text{proj}}^2}} d\varepsilon_{\text{ob}}
\]

(3.35a)

\[
\text{Prolate : } n'(\varepsilon'_{\text{proj}}) = \int_{\varepsilon'_{\text{pro}}=\max[\varepsilon'_{\text{pro}}(D_{\text{min}}), \varepsilon'_{\text{proj}}]}^{\varepsilon'_{\text{pro}}(D_{\text{max}})} n(\varepsilon'_{\text{pro}}) \tilde{n}(\beta'(\varepsilon'_{\text{pro}}, \varepsilon'_{\text{proj}})) \frac{1}{\sqrt{\varepsilon'_{\text{pro}}^2 - \varepsilon'_{\text{proj}}^2}} d\varepsilon'_{\text{pro}}
\]

(3.35b)

where the limits of integration reflect the requirement that projections can only appear more circular.

Orientation distributions \( \tilde{n}(\beta) \) for this paper are defined over the interval \( 0 \leq \beta \leq \frac{\pi}{2} \). We tested several different distributions to describe \( \tilde{n}(\beta) \) where Table 3.1 shows the analytic forms for each orientation distribution we use. For Gaussian distributions, we use the standard form where \( \tilde{n}(\beta) \propto \exp\left(-\frac{(\beta - \mu)^2}{2\sigma^2}\right) \).

### 3.4.1 Monte Carlo projection method

To test our theoretical method, we also calculate eccentricity and aspect ratio projections with a Monte Carlo approach. We first specify either the \( a \)-axis distribution (for AHAB or traditional planar size spectra) or the \( c \)-axis distribution (for traditional columnar size spectra) using Equations (3.15) and (3.16) and the distribution parameters \( N_i, \nu, \delta_* \), and \( \varphi_n \). For simplicity, \( N_i \) is normalized to unity for all tests. Each time we draw from Equation (3.15), we use the distribution parameters to calculate the corresponding \( c \)-axis length using Equation (3.16). For traditional columnar spectrum tests, the \( c \)-axis spectrum and \( a \)-axis spectrum are switched. Then, we draw from one of the \( \beta \) distributions given in Ta-
Table 3.1. Orientation probability density functions used throughout paper.

<table>
<thead>
<tr>
<th>Orientation</th>
<th>( \tilde{n}(\beta) ) (0 ≤ ( \beta ) ≤ ( \frac{\pi}{2} ))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Uniform Random (Jiang et al. 2017)</td>
<td>( \frac{2}{\pi} \sin \beta )</td>
</tr>
<tr>
<td>Beta</td>
<td>( \frac{1}{B(\frac{1}{2}(a+1),\frac{1}{2}(b+1))} (\sin \beta)^a (\cos \beta)^b )</td>
</tr>
<tr>
<td>Gaussian (Klett 1995) (top-down view)</td>
<td>( \frac{2}{\pi} \exp\left(\frac{1}{4\sigma^2}\right) \ln \left(\frac{1}{\frac{1}{4\sigma^2}}\right) \exp\left[-\frac{\sin^2 \beta}{2\sigma^2}\right] )</td>
</tr>
<tr>
<td>Gaussian (Klett 1995) (side view)</td>
<td>( \frac{2}{\pi} \exp\left(-\frac{1}{4\sigma^2}\right) \ln \left(-\frac{1}{4\sigma^2}\right) \exp\left[\frac{\sin^2 \beta}{2\sigma^2}\right] )</td>
</tr>
<tr>
<td>Gaussian</td>
<td>( \sqrt{\frac{2}{\pi}} \frac{1}{\sigma} \operatorname{erf}\left(\frac{\mu}{\sqrt{2}\sigma}\right) - \operatorname{erf}\left(\frac{\mu - \frac{\pi}{2}}{\sqrt{2}\sigma}\right) \exp\left(-\frac{(\beta - \mu)^2}{2\sigma^2}\right) )</td>
</tr>
</tbody>
</table>

Table 3.1 to calculate the projected quantities using Equations (3.1) and (3.2). This procedure is repeated \( 10^6 \) times to develop projection distributions which we normalize by dividing by the bin width and total counts so that the distribution is a probability density.

3.5 Results

3.5.1 Idealized test results

To get a sense for how the projection process changes aspect ratio and eccentricity distributions, we perform several idealized tests. To do this, we choose two different spheroid distributions (oblate and prolate) each characterized by \(|\delta_n - 1| = 0.1\), \( \min \left(\phi_n, \phi^{-1}_n\right) = 0.5 \) and \( \nu = 1.0 \). The original and projection distributions for these tests are shown in Figure 3.9. Circles represent results using the Monte Carlo method whereas lines represent the results when numerically integrating Equation (3.34). The top row of panels show the real eccentricity (blue) and aspect ratio (orange) distributions whereas the bottom two rows show the corresponding projected (second) eccentricity and projected aspect ratio distributions when \( \beta \) follows a uniform, cosine, or sine distribution. The cosine and sine distributions were chosen so as to represent a simple deviation from horizontally oriented particles viewed along their fallspeed direction. For instance, this might be the case if one
observes ice particles using Optical Array Probes (OAPs) (McFarquhar et al. 2017). It is also worth noting the relationship between the aspect ratio and the (second) eccentricity as shown before in Figure 3.3. While the oblate eccentricity starts at 0 (sphere), the distribution itself tends toward 1.0 which represents a parabola. Analogously, the prolate second
eccentricity value of 0 represents a sphere and an infinite eccentricity represents a parabola.

**Figure 3.10.** Same as Figure 3.9 but with \( \nu = 4.0 \). Oblate projection examples have a different ordinate range to highlight distribution features.

For uniform \( \beta \) distributions, the projected eccentricity and aspect ratio distributions have local peaks close to their spheroidal values. However, some of these counts get shifted toward more circular values where the distribution tends toward uniformity. The cosine and
sine $\beta$ distributions have the same general behavior, but the tails toward the circular end of the distribution are different. Cosine orientations act to produce a projected eccentricity distribution that is roughly uniform for values less than the spheroidal mode, but exponentially falls off for values greater than the mode. The prolate sine distribution on the other hand is roughly linear for projected eccentricity values less than the spheroidal mode. These behaviors can be explained by Equation (3.34). The introduction of $\cos \beta$ in the projection kernel acts to cancel the Jacobian component. As a result, the projection kernel is not dependent on the projected eccentricity. Therefore, the integration of this projection kernel yields a nearly uniform distribution. Similarly, the introduction of $\sin \beta$ in projection kernel yields a projected eccentricity term with the form of an arctangent which produces quasi-linear behavior as $\varepsilon_{\text{proj}}$ approaches zero.

For $\nu = 4.0$ (Figure 3.10) the behavior of these orientation assumptions is nearly identical. The main difference between Figure 3.9 and Figure 3.10 is that the projection features are more pronounced: The tails from the circular projections extend farther toward the spheroid mode. This seems to be partly explained by the narrowing of each spectrum and also by the shifting of the mode toward more eccentric values. Therefore, higher values of $\nu$ seem to suggest a tendency for orientation effects to become more maximized for a given set of other model parameters.

### 3.5.2 Traditional M-D tests

For these tests, we use mass-dimensional relationships of hexagonal plates (HexPl) and hexagonal columns (HexCol) given in Table 1 of Mitchell (1996) to investigate how their shapes might be affected when projected. For consistency with observations, we assume that these particles wobble with Gaussian orientations of $\sigma = 10^\circ$ and $\sigma = 40^\circ$ about their side incidence (i.e. $\mu = 90^\circ$). OAPs can be mounted in such a way that the viewing direction is either side incidence or fallspeed direction but side incidence should provide the best shape estimates. Therefore, these tests can be thought of as best case scenarios for ice particle shape estimates. Since the in situ observations used to derive these mass-dimensional relationships assume truncated size spectra (dependent on cloud probe instrument limitations), we similarly truncate the maximum size in the range 0.15mm to 2.5mm which is a typical range for OAPs. To diagnose $\phi_n$, we specify the number and
mass concentrations such that we can integrate the mass distribution to solve for $D_n$. For simplicity, we choose $N_i = 1000 \text{ m}^{-3}$ and $q_i = 1.0 \text{ g m}^{-3}$. We then solve for $\phi_n$ using Equations (3.27) and (3.28) assuming the density of plates is $\rho_i = 0.9 \text{ g cm}^{-3}$ and the density of hexagonal columns is $\rho_i = 0.8 \text{ g cm}^{-3}$.

$$\nu = 1.0$$

$\nu = 4.0$

![Figure 3.11](image)

**Figure 3.11.** Traditional M-D test using hexagonal plates from Mitchell (1996). A different ordinate range between spheroid distributions and projection distributions is used so that projection features are highlighted. For these spheroid distributions: $\delta_s = 0.45$ and $D_0 = 5.235 \mu\text{m}$. $\phi_n = 0.0318$ for $\nu = 1.0$ and $\phi_n = 0.0574$ for $\nu = 4.0$. The maximum dimension is truncated from $D_{\text{min}} = 0.150\text{mm}$ to $D_{\text{max}} = 2.50\text{mm}$.
For hexagonal plates (Figure 3.11) with $\sigma = 10^\circ$, the projections for $\nu = 1.0$ and $\nu = 4.0$ have tails that are very similar. However, for $\sigma = 10^\circ$, the aspect ratio distribution peaks at a slightly lower value for $\nu = 4.0$ and this peak is more pronounced. The increase of $\sigma = 10^\circ$ to $40^\circ$ significantly changes the projections for both values of $\nu$. Although the spheroid distributions have narrow peaks, $\sigma = 40^\circ$ acts to nearly destroy these peaks altogether and smooth out each distribution such that they are nearly identical to one another.

$\nu = 1.0$

$\nu = 4.0$

![Graphs showing aspect ratio distributions for hexagonal plates with $\sigma = 10^\circ$ and $\sigma = 40^\circ$.]

Figure 3.12. Same as Figure 3.11 but for hexagonal columns. For these spheroid distributions: $\delta_0 = 2.70$ and $D_0 = 76.8 \mu m$. $\phi_n = 8.17$ for $\nu = 1.0$ and $\phi_n = 8.82$ for $\nu = 4.0$. 49
For hexagonal columns (Figure 3.12), $\sigma = 10^\circ$ does not change the truncated aspect ratio and second eccentricity spheroid distribution shapes much at all. However, we notice an interesting feature associated with truncation. For $\nu = 1.0$ and $\sigma = 10^\circ$, the projection mode exists at about the same aspect ratio (second eccentricity) of the spheroid distributions. For $\nu = 1.0$ and $\sigma = 40^\circ$, the distribution reverses itself and its mode shifts to more circular values. Additionally, the impact of truncation on the projections produces cusps in these plots at an aspect ratio of about 1.5 and a second eccentricity of 1.0. However, because $\nu = 4.0$ acts to change the location of the truncation with respect to the Amoroso spheroid distributions, these truncation effects do not appear when increasing $\sigma$. Instead, the effect of increasing $\sigma$ acts to reduce the amplitude of the mode as well as produce a more concave down behavior. Therefore, these results seem to suggest that the combination of truncation and increases in $\sigma$ can significantly obfuscate interpretations of observed aspect ratio and eccentricity projections.

### 3.5.3 Relative entropy

The previous tests showed that a combination of orientation assumptions, model parameters and size truncation can shift the modality of the projected eccentricity and aspect ratio spectra. However, it is not obvious which combinations of these parameters act to switch the projections from appearing like their spheroidal counterparts to appear like their orientations. We can visualize this transition in Figure 3.13 where the surface plot represents the oblate spheroid distribution from Figure 3.9 projected assuming Gaussian canting about side incidence (left) and fallspeed direction (right). As $\sigma$ increases, both distributions become more uniform (see left, middle plot from Figure 3.9). Also plotted in Figure 3.13 is the relative entropy or Kullback-Leibler Divergence (cf. Wu and McFarquhar 2018) between the spheroid and projection eccentricity distributions for different values of $\sigma$. Here, we define relative entropy as:

$$D_{KL}(n_{sph}||n_{proj}) = \int_{\varepsilon=0}^{1} n_{sph}(\varepsilon) \ln \left[ \frac{n_{sph}(\varepsilon)}{n_{proj}(\varepsilon)} \right] d\varepsilon. \quad (3.36)$$
Relative entropy in this context can be viewed as the log difference expectation of $n_{sph} = n(\varepsilon)$ if we observe $n_{proj} = n(\varepsilon_{proj})$. Therefore, with our definition of relative entropy, we can view the projection process as introducing entropy from the orientations into the eccentricity distributions. Ideally, we would like for $D_{KL} = 0$, which indicates that the projection distributions are the same (i.e. $\sigma \to 0^\circ$ for side incidence, left surface plot). For side incidence viewing directions, increases in $\sigma$ lead to increases in relative entropy (green line). On the other hand, if we assume that these oblate spheroids are viewed from their fallspeed direction then we see relative entropy decrease as $\sigma$ increases. For large values of $\sigma$, we begin to see the peak associated with the spheroid eccentricity distribution’s mode. Since relative entropy is invariant under coordinate transformations, the values we present here are exactly the same as if we instead use aspect ratios instead of eccentricities. The
advantage to using eccentricity is that the distribution density values remain lower and do not diverge for circular projections.

![Figure 3.14](image)

Figure 3.14. Relative entropy values between model and projection distributions across the model parameter space for oblate particles with Gaussian canting about side incidence.

We can use the concept of relative entropy to determine regions of model and orientation parameters where we can be confident that shape information from the observed ice shape distributions or projections are representative of the actual particle geometry and not the orientations. To do this, we calculate relative entropy values for the two commonly used \( \nu \) values of 1.0 and 4.0 and the two commonly assumed values of \( \sigma \), 10° and 40°, across the model parameter space \( \delta_* \) and \( \varphi_n \). Although \( \delta_* \) and \( \varphi_n \) are not necessarily independent

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of one another (see Equation (3.17)) and \( \nu \) is not always fixed as a constant (e.g., Milbrandt and Yau 2005a), the use of these variables allows us to plot relative entropy values on linear scales that represent realistic model distributions. These parameter spaces are shown in Figure 3.14 as surfaces for each \( \nu \) and \( \sigma \) combination. For \( \nu = 1.0 \) and \( \sigma = 10^\circ \), which is commonly assumed for oblate particles (Ryzhkov et al. 2011), relative entropy values stay well below 1.0. As \( \delta_\ast \) decreases so does relative entropy. Conversely, as \( \phi_n \) decreases, relative entropy increases. However, if \( \nu = 4.0 \) (top, right) the relative entropy becomes more sensitive to decreases in \( \phi_n \) while becoming less sensitive to \( \delta_\ast \). The relative entropy values are overall higher across this parameter space, especially at lower values of \( \phi_n \). The same plots but with \( \sigma = 40^\circ \) (indicative of, for instance, dry snowflakes) show similar behavior to \( \sigma = 10^\circ \) but relative entropy values are larger at every point. For \( \nu = 4.0 \) the relative entropy values remain large regardless of \( \delta_\ast \) for low values of \( \phi_n \).

### 3.6 Discussion and conclusions

Many studies have used a measure of aspect ratio for estimating particle shape in observational and theoretical studies (Korolev et al. 2000; Korolev and Isaac 2003; Hogan et al. 2012; Garrett et al. 2015; Jiang et al. 2017). However, this work seems to suggest that projected eccentricities might be a more appropriate variable in some cases. For analyzing the shape of single particles viewed from the side, orientations act to produce projected eccentricity quantities with lower relative errors for aspect ratios less than about 0.7. Since most ice particles (with the possible exception of graupel) have aspect ratios lower than 0.7, it is more appropriate to report or average projected eccentricities for a direct shape comparison. For a distribution of particle shapes, we showed that the upper bound of the aspect ratio distributions shown in Figure 3.9 can yield singularities for uniform, cosine, and Gaussian distributions whereas the projected eccentricity distributions are well-behaved. Some of the assumptions we make above can also be relaxed. For instance, since in situ particle imagers can only operate in a limited size range, we can similarly truncate our model distributions. Furthermore, if we assume that particle orientations are not independent of eccentricity (and hence particle size), then we can truncate the size (eccentricity) distribution so that orientations are approximately independent of eccentricity within each size range.
Implementation of our method can also be applied in reverse: One could back out model distribution parameters using a particular observational data set distribution and by assuming a particular orientation. Because our method is general and theoretical, the inverse problem itself is appropriate for method-of-moments (Heymsfield et al. 2002) or variance minimization (McFarquhar et al. 2015; Wu and McFarquhar 2018) parameter estimation techniques. Doing so only requires a relationship between spheroid and projection eccentricity moments. The ratio of projected to spheroid eccentricity moments is represented by the following integral:

\[
\chi_n = \frac{\mathbb{E}\left[\varepsilon_{\text{proj}}^n\right]}{\mathbb{E}\left[\varepsilon_{\text{ob}}^n\right]} = \frac{\int_{\beta=0}^{\pi/2} \int_{\varepsilon_{\text{ob}}=0}^{1} n(\varepsilon_{\text{ob}}) \tilde{n}(\beta)(\varepsilon_{\text{ob}} \sin \beta)^n d\varepsilon_{\text{ob}} d\beta}{\int_{\varepsilon_{\text{ob}}=0}^{1} n(\varepsilon_{\text{ob}}) \varepsilon_{\text{ob}}^n d\varepsilon_{\text{ob}}} \quad (3.37)
\]

\[
= \int_{\beta=0}^{\pi/2} \tilde{n}(\beta) \sin^n \beta d\beta,
\]

where \(n\) is the moment of each distribution. By analogy, second eccentricity moments between prolate and projected distributions can be related to one another with the same \(\chi_n\) shown in Equation (3.37). Figure 3.15 comparing numerical integration of each moment equation to Equation (3.37) illustrates that Equation (3.37) is valid regardless of model parameters or truncation. This moment ratio is therefore only dependent on each moment, \(n\), and the parameters that dictate \(\tilde{n}(\beta)\). It is important to keep in mind that the assumed form of \(\tilde{n}(\beta)\) depends on the type of cloud probe used to derive ellipse fit data. For instance, it is sometimes assumed that the deceleration of air within a Cloud Probe Imager (CPI) presents low Reynolds number ice particles in random orientation (Schmitt and Heymsfield 2005; Um and McFarquhar 2007) while open path OAPs present particles with their maximum dimension in the horizontal (McFarquhar et al. 2017). Therefore, estimating the power-law exponent, \(\delta_*\), which relates the \(a\)-axis and \(c\)-axis just requires that each (second) eccentricity distribution moment scales appropriately with the values of \(\chi_n\) given in Table 3.2. The simplicity of this integral allows for most relevant orientations to produce closed-form scaling factors, \(\chi_n\). These analytical forms are shown in Table 3.2. Therefore, one can easily
solve for $\delta_*$ using the method-of-moments parameter estimation technique for any given in situ ellipse fit data set. For example, integration of spheroidal eccentricity moments can be performed analytically for even integers of $n$. Therefore, the equation that matches $n = 2$ moments for oblate crystals to projections is given by:

$$n = 2 : \left( \frac{D_n}{D_0} \right)^{2\delta_* - 2} \frac{\Gamma \left( \nu + 2\delta_* - 2, \frac{D_{\text{min}}}{D_n}, \frac{D_{\text{max}}}{D_n} \right)}{\Gamma \left( \nu, \frac{D_{\text{min}}}{D_n}, \frac{D_{\text{max}}}{D_n} \right)} + \frac{E \left[ \varepsilon_{\text{proj}}^2 \right]}{\chi^2} - 1 = 0,$$

(3.38)

where $\Gamma(z,x_1,x_2)$ is the generalized gamma function given by the integral:

$$\Gamma(z,x_1,x_2) = \int_{t = x_1}^{x_2} t^{z-1} e^{-t} dt = \Gamma(z,x_1) - \Gamma(z,x_2).$$

(3.39)

$v$ and $D_n$ can be determined through standard size distribution parameter estimation techniques for the invariant $a$-axis length distribution whereas $D_{\text{min}}$ and $D_{\text{max}}$ are dictated by the cloud probe viewing volume. An analogous equation exists for prolate spheroids.

<table>
<thead>
<tr>
<th>Orientation</th>
<th>$\chi_n = \frac{E \left[ \varepsilon_{\text{proj}}^n \right]}{E \left[ \varepsilon_{\text{ob}}^n \right]}$ or $\frac{E \left[ \varepsilon_{\text{proj}}^n \right]}{E \left[ \varepsilon_{\text{proj}}^n \right]}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Uniform</td>
<td>$B \left( \frac{n+1}{2}, \frac{1}{2} \right)$</td>
</tr>
<tr>
<td>Beta</td>
<td>$\frac{B \left( \frac{n+1}{2}, \frac{n+3}{2} \right)}{B \left( \frac{n+1}{2}, \frac{n+1}{2} \right)}$</td>
</tr>
<tr>
<td>Sine</td>
<td>$\frac{1}{2} B \left( \frac{1}{2}, \frac{1}{2} + \frac{n}{2} \right)$</td>
</tr>
<tr>
<td>Cosine</td>
<td>$\frac{1}{4} f_1 \left( \frac{n+1}{2}; 1 + \frac{a}{2}, \frac{1}{2\sigma^2} \right) B \left( \frac{n+1}{2}, \frac{1}{2} \right) \exp \left( \frac{1}{4\sigma^2} \right)$</td>
</tr>
<tr>
<td>Gaussian (Klett 1995, side view)</td>
<td>$\frac{1}{4} \frac{f_1 \left( \frac{n+1}{2}; 1 + \frac{a}{2}, \frac{1}{2\sigma^2} \right) B \left( \frac{n+1}{2}, \frac{1}{2} \right)}{\exp \left( \frac{1}{4\sigma^2} \right)} \exp \left( -\frac{\sigma^2}{2} \right) \text{erf} \left( \frac{\pi - 2i\sigma^2}{2\sqrt{2}\sigma^2} \right)$</td>
</tr>
<tr>
<td>Gaussian side view ($\mu = \frac{\pi}{2}$): $n = 1$</td>
<td>$\frac{1}{2} \exp \left( -\frac{\sigma^2}{2} \right) \text{erf} \left( \frac{\pi - 2i\sigma^2}{2\sqrt{2}\sigma^2} \right)$</td>
</tr>
<tr>
<td>Gaussian side view ($\mu = \frac{\pi}{2}$): $n = 2$</td>
<td>$\frac{1}{2} + \frac{1}{4} \exp \left( -\frac{\sigma^2}{2} \right) \text{erf} \left( \frac{\pi - 4i\sigma^2}{2\sqrt{2}\sigma^2} \right)$</td>
</tr>
</tbody>
</table>

We can also use the methods presented in this paper when calculating bulk projected area quantities for radiation and microphysical processes. For example, notice that the
Figure 3.15. Values of projected and oblate eccentricity moments for different values of $n$ (top) and their ratio (bottom) using both numerical integration (lines) and analytical expressions from Table 3.2 (circles). $\nu = 4.0$, $\delta = 0.9$, $\varphi = 0.5$. Distributions are truncated from $D_{\text{min}} = 0.150\text{mm}$ to $D_{\text{max}} = 2.50\text{mm}$.
projected area, $A_{\text{proj}}$, for AHAB can be written solely in terms of $\varphi$ and $\beta$:

$$A_{\text{proj}} = \pi a^2 \varphi_{\text{proj}} = \pi a_0^2 \varphi^{\frac{2}{\delta - 1}} \varphi_{\text{proj}}(\varphi, \beta),$$

(3.40)

where $\varphi_{\text{proj}}$ is given by Equation (3.2). Therefore orientation averaged quantities of projected area take the form:

$$\langle A \rangle_{\text{proj}} = \int_{\varphi=0}^{\infty} \int_{\beta=0}^{\frac{\pi}{2}} n(\varphi) \tilde{n}(\beta) A_{\text{proj}}(\varphi, \beta) d\beta d\varphi$$

$$= \pi a_0^2 \int_{\varphi=0}^{\infty} \varphi^{\frac{2}{\delta - 1}} n(\varphi) \left\{ \int_{\beta=0}^{\frac{\pi}{2}} \tilde{n}(\beta) \varphi_{\text{proj}}(\varphi, \beta) d\beta \right\} d\varphi$$

(3.41)

$$= \pi a_0^2 \int_{\varphi=0}^{\infty} \varphi^{\frac{2}{\delta - 1}} n(\varphi) \left\{ \langle \varphi_{\text{proj}} \rangle_{\tilde{n}(\beta)}(\varphi) \right\} d\varphi,$$

where the limits of integration for $\varphi$ now reflect the entire size distribution range of $a = 0$ to $a = \infty$ such that the gamma function in Equation (3.18) is complete instead of incomplete. $\langle \varphi_{\text{proj}} \rangle_{\tilde{n}(\beta)}(\varphi)$ is the orientation averaged projected aspect ratio that correspond to hypergeometric-type expressions given by Equations (3.3), (3.4), (3.8) and (3.9) and others. Although integration of Equation (3.41) is analytically complicated because of these hypergeometric functions, we can accurately approximate these functions with power-law or polynomial type functions within a predetermined aspect ratio range. This allows for these bulk quantities to be calculated with a linear combination of gamma functions. Some power-law approximations of $\langle \varphi_{\text{proj}} \rangle_{\tilde{n}(\beta)}(\varphi)$ are given in Table 3.3 where each fit was determined from a nonlinear least squares fitting. From this equation for uniformly oriented spheroids, we see that the maximum reduction in bulk projected area is by a factor of $\frac{2}{\pi}$. As a reference, Mason (1994) provided estimates of cloud albedo due to different habit types and showed that replacing plates with columns of the same mass reduced cloud albedo by about $\frac{1}{3}$. Therefore, reductions in projected area due to particle orientation, at most, represent about half that due to ice crystal habit type.
Table 3.3. Power-law approximations of $\langle \phi_{\text{proj}} \rangle_{\beta}(\phi)$ in the range $0.001 \leq \min(\phi, \phi^{-1}) \leq 1.0$. Gaussian orientations are specified by particle fallspeed direction where $\sigma$ is given in radians in the range $0 \leq \sigma \leq 40^\circ$.

<table>
<thead>
<tr>
<th>Orientation</th>
<th>Oblate/Prolate</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Uniform</td>
<td>Oblate</td>
<td>$\frac{2}{\pi} + \left(1 - \frac{2}{\pi}\right) \phi^{1.44}$</td>
</tr>
<tr>
<td></td>
<td>Prolate</td>
<td>$\frac{2}{\pi} \phi$</td>
</tr>
<tr>
<td>Random</td>
<td>Oblate</td>
<td>$\frac{1}{2} + \frac{1}{2} \phi^{1.4}$</td>
</tr>
<tr>
<td></td>
<td>Prolate</td>
<td>$0.2149 + 0.7851 \phi$</td>
</tr>
<tr>
<td>Gaussian</td>
<td>Oblate</td>
<td>$\sqrt{\frac{2}{\pi}} \sigma^{-0.126} + 0.24 \sigma^{0.6} \phi^{2} \cdot \text{erf}\left(\frac{\pi}{2\sqrt{2} \sigma}\right)$</td>
</tr>
<tr>
<td></td>
<td>Prolate</td>
<td>$\sqrt{\frac{2}{\pi}} \left(\sigma^{-0.1393} - 1.4 \sigma^{9.308}\right) \phi \cdot \text{erf}\left(\frac{\pi}{2\sqrt{2} \sigma}\right)$</td>
</tr>
</tbody>
</table>

Proper care must be taken when applying the ideas and methodology presented in this paper to models and for any joint effort to combine model and observations. Although we assume spheroidal geometry for our projection method, many if not most observed atmospheric ice particles do not necessarily exhibit this type of symmetry. In fact, Korolev et al. (2000) used CPI images to estimate that these “irregular” particles constitute about 97% of all ice particles in Arctic clouds. Some irregular particles could be appropriately represented by spheroids but others might not. Despite this, the spheroidal approximation is still used by a large number of microphysics models as a way to represent ice particle geometry. As such, it is important that models begin to incorporate orientation effects in bulk calculations so that bulk microphysical and radiative quantities scale appropriately. With that said, it is important to realize that the additional axis length of a spheroid simply allows for an additional degree of freedom in representing a measure of geometry. Because of the natural variability of these observed irregular particles and aggregates, a special study is required for estimating the potential errors associated with using the spheroid approximation. But for pristine particles like plates, dendrites, columns, and needles, that do exhibit spheroidal symmetry, we can expect that our methodology will provide results that are more consistent with observations. Moreover, our methodology could also be used to investigate orientation distributions themselves. For instance, instruments like the 2D-S OAP (Lawson et al. 2006b) capture two orthogonal projections at the same time. Therefore, the projection problem is well constrained for spheroidal particles since the 2D-S captures two independent projection measures and two unknown quantities, $\beta$ and $\epsilon_{ob} (\epsilon'_{pro})$, for any
If we do make common spheroidal assumptions about ice particles and their orientations then we are able to analytically derive certain projected quantities. For instance, values of $\frac{1}{\chi_n}$ for traditional Gaussian orientations about side incidence across the $(n, \sigma)$ parameter space are shown in Figure 3.16. For $\sigma = 10^\circ$, the relative change in the mean $(n = 1)$ eccentricity is about 0.78%. However, for $\sigma = 40^\circ$ the relative change increases to about 150%. For distributions of snow with $\nu = 1$, $\delta_* = 0.5$, and $\phi_n = 0.1$ (cf. Mitchell 1996), relative entropy increases from 0.394 when $\sigma = 10^\circ$ to 1.42 when $\sigma = 40^\circ$. Furthermore, higher values of $\nu$ necessarily lead to larger relative entropy values regardless of other model parameters (Figure 3.14). This means that for particles like aggregates, which can be both highly eccentric and fall with large canting angle deviations, one can infer very little of the underlying 3D shape without first specifying appropriate orientations. Because of this uncertainty and the tendency for randomly or uniformly oriented projected aspect ratios to tend toward unity (see Figures 3.9 and 3.10 and Jiang et al. 2017), reported aspect ratios of “oblate” aggregates should be seriously questioned.
Chapter 4
The Shape and Density Evolution of Snow Aggregates

4.1 Introduction

Snow aggregates represent a dominant proportion of observed ice precipitation on Earth, yet the processes that dictate formation and structure are still poorly understood (Connolly et al. 2012). The resulting snow aggregate geometry is important for accurately describing and predicting snow precipitation rates (Heymsfield and Westbrook 2010; Westbrook and Sephton 2017), collection rates (Mitchell 1988), and radiation properties (Petty and Huang 2010). A common and simple approach for characterizing measures of aggregate geometry is to use a Euclidean object as a volumetric shell for the calculation of various physical properties. The link between this assumed proxy and its physical properties is completed by specifying a density, which acts to appropriately scale volume with mass. Current microphysics models often assume spheres or oblate spheroids as proxies (e.g., Thompson et al. 2008; Jensen et al. 2017) although there are other models that incorporate more complex geometries (e.g., Hashino and Tripoli 2011a,b). In general, each individual aggregate is assumed to have a mass that scales with length (however length is defined) according to a power-law relation. Euclidean geometry is useful because it permits the analytical separation of density and volume in the formulation of mass:

\[ m_i = \rho_i \cdot V_i = \left( \alpha_\rho D^{\beta_\rho} \right) \cdot \left( \alpha_V D^{\beta_V} \right) = \alpha_m D^{\beta_m}, \]  

(4.1)

where \( \alpha_m = \alpha_\rho \alpha_V \) and \( \beta_m = \beta_\rho + \beta_V \). \( \alpha_m \) and \( \beta_m \) are coefficients that can be derived from fits to in situ data (e.g., Locatelli and Hobbs 1974; Mitchell 1996). The prefactor, \( \alpha_m \) of Equation (4.1) is often thought to primarily contain information on particle density whereas \( \beta_m \) is often thought to primarily contain information on particle shape (Erfani and Mitchell 2017). This formulation is well suited for microphysics models because integration of these
power-law type functional relations over gamma distributed particle lengths yield closed-form expressions in terms of Gamma functions. However, bulk microphysics models will often use mass-dimensional relationships where both constants represent a combination of shape and density (e.g., Brown and Francis 1995). This convolution obfuscates the relative contribution of both shape and density to the characterization of particle properties. Current theories that mathematically link an aggregate’s morphology to its physical properties, such as that developed by Böhm (1989), are predicated on the ability to appropriately segregate shape and density.

However, the Euclidean concepts of “shape” and “density” themselves suggest some sort of structural consistency; such consistency is rarely noticed through casual observations of falling snowflakes. Various monomer configurations can produce wildly different physical properties. Configurations where the aggregate is more porous can reduce drag through the reduction of surface area relative to fall direction. However, configurations where the aggregate is more spatially “open” (such as linear chains) can act to increase this same surface area, thus producing an opposite effect on fallspeed. These various configurations also change how each aggregate absorbs and scatters electromagnetic radiation at different radar wavelengths (Petty and Huang 2010; Botta et al. 2011; Lu et al. 2013). Near-field electric interactions among individual aggregate elements act to both enhance and diminish the returned radar signal. This interference effect is further complicated by each aggregates’ orientation with respect to the direction of radiation propagation.

Paradoxically, although aggregates exhibit a variety of geometric forms, both observations (e.g., Korolev and Isaac 2003) and numerical studies (e.g., Westbrook et al. 2004a,b) support claims of universality. For instance, Westbrook et al. (2004a) performed Monte Carlo simulations of aggregates and compared their projected mean aspect ratios to those derived by Korolev and Isaac (2003) from CPI in situ data of stratiform ice. Westbrook et al. (2004a) found that aggregates evolve to produce mean projected aspect ratios that asymptote toward a value of about 0.6 regardless of the initial monomer aspect ratio or habit type. This value seems to be consistent with the 0.6 to 0.8 aspect ratio range estimated by Korolev and Isaac (2003). Remarkably, these two aspect ratios are also consistent with radar scattering calculations using horizontally oriented, soft oblate spheroids (Hogan et al. 2012) and 2DVD observations (Brandes et al. 2007), respectively. While models have used these aspect ratios to characterize aggregates, the relationship between the assumed aspect
ratio and the underlying shape it implies has remained ambiguous. Estimating 3D structure from 2D images is particularly troublesome because of how any particular aggregate can be oriented while it falls. The correct distribution of aggregate orientations is still largely uncertain but thought to depend upon both environment (whether natural or unnatural) and aggregate morphology (see Pruppacher and Klett 1997).

This orientation uncertainty led Jiang et al. (2017) to test the implications of projecting spheroids of a fixed aspect ratio in a way that is analogous to observations. The results of their tests showed a tendency for oblate and prolate spheroids to appear much more spherical than their true 3D aspect ratios. This implies that if aggregates are well represented by oblate spheroids then the mean aspect ratio is actually much lower than what the often assumed 0.6 or 0.8 aspect ratio would suggest. In fact, Dunnavan and Jiang (2019) show that the projection problem for spheroids can be done analytically, and they derived closed-form equations for the errors produced by projecting oriented spheroids of various aspect ratios. For distributions of flat or thin spheroids, Dunnavan and Jiang (2019) show that the resulting distributions of projected aspect ratios are not only sensitive to orientation, but also to the size distribution shape factor, $\nu$. If aspect ratio is assumed to depend on size, a simple increase of $\nu$ from 1 to 4 can increase the 2D to 3D relative entropy of aspect ratios by more than three times. This increase in entropy can destroy any indication of the actual 3D shapes even if aggregates are truly oblate. These results all suggest that in most cases of single aggregate imaging, the projection process itself ruins any attempt at estimating or inferring 3D geometry. This is highlighted by the fact that any observed projected aspect ratio could potentially correspond to any spheroid more eccentric than its 2D projection or image.

Fortunately, recent developments in imaging technology permit a much better treatment of 3D aggregate reconstructions. One such instrument used for reconstructions is the Multi-Angle Snowflake Camera (MASC) (Garrett et al. 2015) which can simultaneously image aggregates from multiple viewing angles. The use of three or more images of the same aggregate has already been shown to greatly reduce uncertainties associated with 3D retrievals (Kleinkort et al. 2017). A recent study by Jiang et al. (2019) uses a database of MASC captured aggregates along with a machine learning algorithm to estimate best fit ellipsoids for each aggregate. They found that very few of the aggregates were well represented by oblate spheroids. Even more surprising was the result that, in many cases,
aggregates were better represented by prolate spheroids rather than oblate spheroids. Furthermore, Jiang et al. (2019) found that the orientation angle of aggregate maximum dimensions were rarely horizontal but rather preferentially canted based on turbulence intensity. Overall, the inconsistency of assumed aggregate shapes combats the apparent consistency exhibited by previously universal measures. This conundrum therefore presents a fundamental challenge associated with estimating 3D aggregate properties from 2D analogs: A single set of geometric relationships derived from observations cannot necessarily describe multiple aggregate properties. This observation suggests that improving aggregate representation in models requires either incorporating multiple sets of geometric measures (e.g., maximum dimension and area ratio) in calculations or an entirely new paradigm altogether.

One such paradigm has been the use of fractal geometry instead of Euclidean measures as a way to describe aggregates (e.g., Westbrook et al. 2004a; Maruyama and Fujiyoshi 2005; Ishimoto 2008; Schmitt and Heymsfield 2010). The fractal approach takes Equation (4.1) in its convolved form and assumes that each aggregate mass scales according to the constituents of each monomer. Each individual monomer constituent is assumed to be identical in mass and size. The fractal dimension, $D_f$, characterizes how the spatial distribution of these elements varies with grid scale. As a result, boxcounting methods such as those described in Karperian (1999–2013) can be used to estimate $D_f$, which is then assumed to represent $\beta_m$ in Equation (4.1). The fractal description therefore circumvents the issues of defining and estimating shape and density individually. Using this boxcounting approach, Schmitt and Heymsfield (2010) was able to relate 3D fractal dimensions of simulated aggregates to the 2D fractal dimensions calculated from their various projections. They found that, in general, the 2D and 3D fractal quantities were related by a scaling factor, $S$, which was seemingly invariant with respect to viewing direction. $S$ was well described for aggregates with 25 or more monomers and was around 1.30 in value. The mathematical approach developed by Schmitt and Heymsfield (2010) therefore allows one to use 2D in situ projections or images to estimate or infer the 3D aggregate fractal dimensions. However, this approach still has drawbacks. Even small deviations in $S$ can lead to substantial changes in bulk quantities: Mere differences of 0.02 in $S$ can lead to a change in calculated ice water content of more than 10% (Schmitt and Heymsfield 2010). Furthermore, the method still relies on the methodology of one-to-one mass dimensional relationships, which do not by themselves capture the correct dispersion of, for instance,
particle fallspeeds (Passarelli 1978a,b; Sasyo and Matsuo 1985). Schmitt and Heymsfield (2010) also found that the observed 3D mean fractal dimension itself varied from about 2.0 to 2.3 with an apparent dependence on temperature. Other authors (e.g., Westbrook et al. 2004a; Maruyama and Fujiyoshi 2005; Ishimoto 2008) have reported similar values for $D_f$ that fall well within the range of Schmitt and Heymsfield (2010), leading them to claim another universal feature of aggregates: a constant, or near constant, fractal dimension.

The fractal dimension for aggregates, while useful for describing how aggregate mass scales with size, is not the only type of fractal measure. For instance, the fractal dimension can be generalized to a probability distribution for each grid box. To do this, the boxcounting spatial information in each grid box is described by a partition function rather than a binary unit. Moments of this partition function over various grid sizes can then be used to infer whether the object is non-fractal, mono-fractal, or multi-fractal. More importantly, the statistical moments of the partition function serve a similar function as moments of particle size distributions: Moments of the size distribution correspond to the bulk composition of (assumed) identical aggregates; moments of the multi-fractal partition function for any particular aggregate correspond to the bulk composition of each (assumed) identical cluster of water molecules. Positive moments of the partition function amplify denser regions of the aggregate whereas negative moments amplify rarer ones (Chhabra and Jensen 1989). The amplification effect of various moments therefore can act to provide more information about the spatial distribution of aggregate mass.

Another important, but much less frequently mentioned, fractal quantity is lacunarity. Lacunarity can be loosely thought of as the “gappiness” of a particular fractal; that is, lacunarity represents the size distribution of holes throughout a particular fractal. In this sense, lacunarity is a measure of porosity or density. Low values of lacunarity represent less gaps overall whereas higher values represent more gaps. Furthermore, fractals with low values of lacunarity exhibit more rotational or translational invariance, whereas fractals with high values of lacunarity are more sensitive to orientation. Lacunarity can serve many purposes for describing snow aggregates. For instance, one can imagine lacunarity as a density-like measure that acts to appropriately scale the aggregate mass with size; as aggregates grow, so should the number of gaps in between monomers. Lacunarity can also be used to evaluate the invariant or variant nature of how 2D image or projection properties correspond to the 3D aggregate geometry. Therefore, this could be useful for supplement-
ing the method of Schmitt and Heymsfield (2010) for in situ images. In general, aggregate features (e.g., maximum dimension, area ratio, and fractal dimension) are assumed to be more or less spatially invariant. As far as we are aware, however, this assumption has not been tested for various types of aggregates and it is not clear whether certain types of aggregates yield higher values of lacunarity than others. It is somewhat surprising how previous Monte Carlo aggregation studies have not so much as mentioned lacunarity even though it has many potential uses for ice microphysics. Lacunarity is potentially important since it can act to provide more depth for any fractal analysis. For instance, Mandelbrot (1994) showed that Cantor dust sets of the exact same fractal dimension can still have features that differ “violently” from one another. This suggests that fractal dimensions alone might not be enough to properly capture the many physical properties of aggregates. Additionally, Mandelbrot (1992); Blumenfeld and Mandelbrot (1997) shows that lacunarity can be used to estimate the prefactor component of the fractal power-law scaling relationship. This suggests that lacunarity could also perhaps be used to better select prefactor values if these power-law relations like Equation (4.1) are to be used in models. Current methods for calculating the prefactor component, $\alpha_m$, often rely on extrapolation approaches using, for instance, in situ area ratio data (see Schmitt and Heymsfield 2010). However, this type of extrapolation relies on the questionable assumption that initial aggregates are uniformly dense spheres. Such extrapolations might need to be rescaled in a more physical manner.

Despite large uncertainties associated with estimating aggregate geometry from projections and assigning these measures to a single length scale, both Euclidean and fractal descriptions of aggregates seem to yield consistent or universal values. The question we ask is whether this is by design or by fluke. Does each individual snow aggregate evolve into a truly universal shape and density or do certain “chimeras” of the same fractal dimension still differ “violently” from one another? In other words, exactly how quantitatively different are any two “identical” snowflake aggregates? With these questions in mind, consider that the Euclidean viewpoint can be thought of as a special case of the fractal viewpoint. This relationship is demonstrated in Figure 4.1 (top) which shows a visualization for how spheroidal proxies of different shape and density could relate to various ranges of fractal dimensions. Uniformly filled spheres are assumed to fill space uniformly, meaning that $D_f = 3.0$. However, if one imagines deforming the sphere into a disc-like plate ($\phi = \frac{c}{a} \to 0$), then the plate tends toward $D_f = 2.0$. If instead, one stretches the sphere...
Figure 4.1. (Top) Examples of the possible relationship between spheroidal geometry and fractal dimension for different combinations of shape and density. (Bottom) Modeled aggregate image from Figure 12 of Westbrook et al. (2008) conceptualized as a reduced density ellipsoid of volume $V_i$. $V_{i0}$ represents a reduced density sphere of the same maximum dimension, $2a$.

into a thin needle ($\varphi = \frac{c}{a} \rightarrow \infty$), then the geometry of the needle tends toward that of a line where $D_f = 1.0$. The changes in the density structure (or rather porosity) yield the
sort of chimeric behaviors in $D_f$ that Mandelbrot (1994) warned about. From a Euclidean perspective, this leads to the possibility that particles with a particular fractal dimension could correspond to many different combinations of shape and density or even for the same fractal dimension to correspond to different lacunarities, and therefore different porosities.

Previous Monte Carlo modeling efforts such as Westbrook et al. (2004a,b); Maruyama and Fujiyoshi (2005) not only simulated the evolution of aggregate sizes and shapes, but also the evolution of aggregate fallspeeds and size distributions. Unlike previous Monte Carlo papers that explicitly resolve aggregate properties, we instead intentionally sever this link. Instead, we focus on look at how Euclidean descriptions of shape and density and estimates of fractal quantities evolve for different types of monomer geometries and their combinations. We can then use the resulting distributions of aggregate geometry to infer their statistical properties. For simplicity, we assume each monomer is well described by spheroidal geometry (i.e., $\phi = \frac{c}{a}$ and $\rho_i = const$). Therefore, by performing these tests, we attempt to link a priori shape and density information of primary habits (i.e., planar and columnar particles) to the resulting Euclidean and fractal evolution of aggregate geometry.

### 4.2 Observations

To provide a basis for our Monte Carlo simulations, we first present recent observations of estimated ellipsoid shapes derived from the MASC imager. The gradient descent method used to estimate these observed ellipsoid aspect ratios is describe in detail by Jiang et al. (2019). Figure 4.1 (bottom) shows a schematic for what best fit ellipsoids look like when superimposed onto an aggregate. For consistency, we assume each ellipsoid dimension is arranged as: $a \geq b \geq c$. Notice that two aspect ratio measures are required to specify the ellipsoid shape although it is not clear which ratios are the most convenient. For this reason, we define the following aspect ratios:

$$\phi_{ba} \equiv \frac{b}{a} \quad (4.2a)$$

$$\phi_{ca} \equiv \frac{c}{a} \quad (4.2b)$$
\[ \varphi_{cb} \equiv \frac{c}{b}. \]  

(4.2c)

The ellipsoid volume can therefore be neatly expressed as:

\[ V_i = \frac{4}{3} \pi abc = \frac{4}{3} \pi a^3 \varphi_{ba} \varphi_{ca} = V_{i0} \varphi_{ba} \varphi_{ca}, \]  

(4.3)

or

\[ V_i = \frac{4}{3} \pi abc = \frac{4}{3} \pi a^3 \varphi_{cb}^2 \varphi_{cb} = V_{i0} \varphi_{cb}^2 \varphi_{cb}. \]  

(4.4)

Notice that the ellipsoid volume, \( V_i \) (green shell), is related to a spherical volume of radius \( a \), \( V_{i0} \) (blue shell), by simple aspect ratio scaling factors.

Figure 4.2 shows a comparison of ellipsoid aspect ratio distributions of snow aggregates derived from two separate locations: The North Slope of Alaska (NSA) and Alta, Utah (Alta). Each row represents the probability distribution \( n(\varphi) \) for the three different aspect ratio definitions in Equation (4.2). The distributions of these aspect ratios seem to be rather well behaved; each distribution is uni-modal with fewer counts observed at the extremes \( \varphi \to 0 \) and \( \varphi = 1.0 \). The form of the distributions also seem to be similar to that of the Beta distribution which is described by the probability density function:

\[ n(\varphi) = \frac{1}{B(\alpha, \beta)} \varphi^{\alpha-1} (1 - \varphi)^{\beta-1} \sim \text{Beta}(\alpha, \beta), \]  

(4.5)

where \( B(\alpha, \beta) \) is the Beta function. As such, we have overlaid Beta distribution fits (green lines) over these distributions which seem to do a great job capturing the distribution shapes for both MASC observation cases. Moreover, although these two datasets were taken independently from one another and from two very different geographic locations, the ellipsoid distributions are almost identical. To illustrate this further, Table 4.1 shows a comparison of the mean, standard deviation, and skewness for each aspect ratio quantity. The mean aspect ratio quantities in particular are remarkably close to one another between each case.

The consistency of the Beta-like marginal distributions of \( \varphi_{ba}, \varphi_{ca}, \) and \( \varphi_{cb} \) with that of the observations (Figure 4.2) suggests the possibility of modeling a joint aspect ratio distribution (describing all possible ellipsoids) using a bivariate Beta distribution. The use of Beta distributions in general is particularly attractive for bulk modeling since moments of
Figure 4.2. Ellipsoidal aggregate aspect ratio probability distributions derived from the MASC imager following Jiang et al. (2019) for: $\phi_{ba} = \frac{b}{a}$, $\phi_{ca} = \frac{c}{a}$, $\phi_{cb} = \frac{c}{b}$, where $a \geq b \geq c$. Histograms are shown for all 950 ellipsoids derived from the NSA MASC aggregate database (left column) and all 414 ellipsoids derived from the Alta MASC aggregate database (right column). Beta distribution fits are shown as green lines, where the best fit Beta distribution parameters $\alpha$ and $\beta$ are shown for each aspect ratio, rounded to 2 decimal places.

Univariate Beta distributions can be expressed using the Gamma functions commonly used in bulk models; similarly, some bivariate Beta distribution product moments can also be calculated using Gamma functions. However, bivariate Beta distributions often have strong
Table 4.1. Statistical properties of ellipsoid retrieval distributions.

<table>
<thead>
<tr>
<th>Location</th>
<th>Aspect Ratio</th>
<th>Mean</th>
<th>Standard Deviation</th>
<th>Skewness</th>
</tr>
</thead>
<tbody>
<tr>
<td>North Slope of Alaska (NSA)</td>
<td>( \varphi_{ba} )</td>
<td>0.6160</td>
<td>0.1589</td>
<td>+0.0366</td>
</tr>
<tr>
<td></td>
<td>( \varphi_{ca} )</td>
<td>0.4186</td>
<td>0.1333</td>
<td>-0.0585</td>
</tr>
<tr>
<td></td>
<td>( \varphi_{cb} )</td>
<td>0.6904</td>
<td>0.1702</td>
<td>-0.8035</td>
</tr>
<tr>
<td>Alta, Utah (Alta)</td>
<td>( \varphi_{ba} )</td>
<td>0.6269</td>
<td>0.1491</td>
<td>+0.0294</td>
</tr>
<tr>
<td></td>
<td>( \varphi_{ca} )</td>
<td>0.4397</td>
<td>0.1304</td>
<td>+0.1497</td>
</tr>
<tr>
<td></td>
<td>( \varphi_{cb} )</td>
<td>0.7068</td>
<td>0.1462</td>
<td>-0.6946</td>
</tr>
</tbody>
</table>

restrictions on the domain of each variable (Nadarajah and Kotz 2005). For instance, the bivariate Beta distributions developed by Olkin and Trikalinos (2015) have the restriction that the sum of each variable can be less than unity, equal to unity, or greater than unity, but not simultaneously greater than and less than unity. Our Monte Carlo generated best fit ellipsoid probability distributions (Section 4.4) show that each combination of aspect ratios can be both greater than and less than unity. Fortunately, the bivariate distributions described in Nadarajah and Kotz (2005) avoid these restrictions entirely. We use the first bivariate distribution given in Nadarajah and Kotz (2005) (their equation 4). This bivariate distribution is specified by the relationships:

\[ \varphi_{ca} = \varphi_{ba} \cdot \varphi_{cb}, \]  

\[ \varphi_{ba} = \varphi_{ba} \]  

where Lemma 1 from Nadarajah and Kotz (2005) is used to specify the following Beta distributions: \( n(\varphi_{ba}) \sim \text{Beta}(\alpha_{ba}, \beta_{ba}) \), \( n(\varphi_{ca}) \sim \text{Beta}(\alpha_{ba}, \beta_{ba} + \beta_{cb}) \), and \( n(\varphi_{cb}) \sim \text{Beta}(\alpha_{ba} + \beta_{ba}, \beta_{cb}) \). Then one can derive the following bivariate distribution for two of the aspect ratios:

\[
\frac{1}{B(\varphi_{ba}, \beta_{ba})B(\varphi_{ba} + \beta_{ba}; \beta_{cb})} \varphi_{ca}^{\alpha_{ba} + \beta_{ba} - 1} (\varphi_{ba} - \varphi_{ca})^{\beta_{cb} - 1} \varphi_{cb}^{\beta_{ba} - \beta_{cb}} (1 - \varphi_{ba})^{eta_{ba} - 1} = \frac{\Gamma(\alpha_{ba} + \beta_{ba} + \beta_{cb})}{\Gamma(\alpha_{ba})} H^{0.0,1.0,1.0}_{0.0,1.1,1.1,1,1} \begin{bmatrix} \varphi_{ba} \\ \varphi_{ca} \end{bmatrix} \left( \begin{array}{c} \alpha_{ba} - 2, 1 \\ \varphi_{ba} - \varphi_{ca} \end{array} \right) \begin{array}{c} \varphi_{ca} \\ \varphi_{cb} \end{array} \begin{array}{c} \alpha_{ba} + \beta_{ba} + \beta_{cb} - 1, 1 \\ \alpha_{ba} + \beta_{ba} - 2, 1 \end{array}, \right)
\]  

\[ (4.7) \]
where the bivariate $H$-function representation (not given in Nadarajah and Kotz (2005)) can be obtained by applying the double Mellin transform and inverse Mellin transform for each aspect ratio (Equations (2.8) and (2.9)). This particular bivariate distribution has triangular support $0 < \varphi_{ca} \leq \varphi_{ba} < 1.0$. The nice aspect of this joint distribution is that product moments are represented in terms of complete Beta functions:

$$\langle \varphi_{ba}^m \varphi_{ca}^n \rangle \equiv E_{mn} = \frac{B(m + n + \alpha_{ba}, \beta_{ba}) B(n + \alpha_{ba} + \beta_{ba}, \beta_{cb})}{B(\alpha_{ba}, \beta_{ba}) B(\alpha_{ba} + \beta_{ba}, \beta_{cb})},$$  \hspace{1cm} (4.8)

where $m$ and $n$ represent distribution moments. These Beta functions can be represented in terms of a ratio of Gamma functions,

$$B(\alpha, \beta) = \frac{\Gamma(\alpha) \Gamma(\beta)}{\Gamma(\alpha + \beta)}.$$  \hspace{1cm} (4.9)

Furthermore, integer product moments of Equation (4.8) can be expressed algebraically using properties of the gamma function. This means that the method-of-moments technique can easily be used to estimate the three parameters: $\alpha_{ba}$, $\beta_{ba}$, and $\beta_{cb}$. Doing this for $E_{10} \equiv \overline{\varphi}_{ba}$, $E_{01} \equiv \overline{\varphi}_{ca}$ and $E_{11} \equiv \langle \varphi_{ba} \varphi_{ca} \rangle$ yields simple, algebraic expressions for each parameter:

$$\alpha_{ba} = \frac{E_{10}E_{01} - E_{10}E_{11}}{E_{11} - E_{01}E_{10}} - \frac{\overline{\varphi}_{ba} \left[ \frac{1}{\overline{\varphi}_{ca} (1 + \overline{\varphi}_{ba})} - 1 \right]}{\text{cov}(\varphi_{ba}, \varphi_{ca})}$$  \hspace{1cm} (4.10a)

$$\beta_{ba} = \alpha_{ba} \left( \frac{1}{E_{10}} - 1 \right) = \alpha_{ba} \left( \frac{1}{\overline{\varphi}_{ba}} - 1 \right)$$  \hspace{1cm} (4.10b)

$$\beta_{cb} = \alpha_{ba} \left( \frac{1}{E_{01}} - 1 \right) - \beta_{ba} = \alpha_{ba} \left( \frac{1}{\overline{\varphi}_{ca}} - 1 \right) - \beta_{ba}.$$  \hspace{1cm} (4.10c)

Figure 4.3 shows a comparison of the bivariate distribution from the NSA MASC (joint histogram) and our bivariate Beta distribution model (contours) using Equations (4.7) and (4.10a) to (4.10c). Four examples of the MASC aggregates are shown along with their estimated best fit ellipsoid as well as their locations on the bivariate histogram. Despite the simplicity of this method of moments approach, the bivariate model seems to do a remarkable job capturing the entire ellipsoid parameter space. To further illustrate the effectiveness of our mathematical model, Figure 4.4 shows how product moments of our model compare to those estimated from the MASC derived ellipsoid database for NSA and the
resulting relative error. Product moments are shown from 0 to 2 since reflectivity is often considered to be proportional to $m = n = 2$ and bulk fallspeed quantities represent fractional moments anywhere from $m = n = 0$ to $m = n = 1.5$ depending on each aggregates’ Reynolds number. Different aggregate orientations act to make $m \neq n$ through changing projected areas. Subplots a.) (MASC) and b.) (model) show the entire parameter space over all combinations of $m$ and $n$ moments and are nearly identical. Subplot c.) shows the improvement of our model to models that assume oblate spheroids of $\phi = 0.6$ (purple line)

Figure 4.3. Joint probability density function of the NSA MASC derived ellipsoid aspect ratios ($\phi_{ba}$ and $\phi_{ca}$) and associated marginal distributions. Solid lines represent the (joint) probability distribution dictated by Equations (4.7) and (4.10).
Figure 4.4. Comparison of distribution moments for MASC derived ellipsoids from NSA (a.) and the bivariate Beta distribution model (b.). Plot c.) shows product moments (or spheroid $\varphi_{ca}$ moments) when $m=n$ for: Spheres, oblate spheroids ($\varphi = \frac{c}{a} = 0.6$), MASC derived ellipsoids, and the bivariate aspect ratio ellipsoid model. Plot d.) shows the relative error of the ellipsoid aspect ratio product moment between MASC derived aggregates and the bivariate model.

and spheres (brown line). Subplot d.) shows the relative error between the MASC derived ellipsoids and our model. Notice that even the largest errors at $m=n=2$ only lead to about a 4% difference in estimated product moment. For the rest of this paper, Equations (4.7) and (4.10) serves as the mathematical basis for studying the ellipsoid distributions from the results of our Monte Carlo simulations.
4.3 Methods

4.3.1 Monte Carlo aggregation method

Aggregates are generated much differently from Westbrook et al. (2004a); Ishimoto (2008) and others in the sense that we implicitly rather than explicitly simulate the aggregation process. An initial monomer is specified as a spheroid (either oblate, prolate, or sphere) with aspect ratio of $\varphi = \frac{c}{a}$. Each monomer is itself made up of individual sphere elements with location $(x, y, z)$. For simplicity, we call these sphere elements “dipoles” which have a diameter of unity (arbitrary units). These dipoles also act as lattice sites upon each monomer where additional monomer dipole elements can attach. Each aggregation event therefore constitutes selecting an orientation for each collecting species, projecting each of the dipole elements onto the $x – y$ plane, and randomly selecting lattice sites on each species based on each projection. Only dipoles that are outermost from the center of the monomer or aggregate are chosen as attachment sites. The maximum dimension of the aggregate ensemble is calculated after each aggregation event and this length is then rotated to fall along the $x$-axis using an Euler angle rotation matrix (see Jiang et al. 2017). This maximum dimension is defined to be twice the $a$-axis length of the best fit ellipsoid. The $b$ and $c$ axes are calculated by fitting ellipses around the 2D projections in the $x – y$ and $y – z$ planes. The ellipse fits are determined by matching the second central moment of the fitted ellipse to the projected areas from each dipole. This means that aggregate dipoles can have locations outside the ellipsoid shell. Unless otherwise noted, particles are assumed to be randomly oriented during collection.

4.3.2 Calculation of fractal properties

Generalized fractal dimensions for simulated aggregates are computing using a box-counting method similar to Karperian (1999–2013) but generalized even further for multiple model runs. For a particular aggregate with a given number of monomers, monomer dipole locations are stored in terms of their Cartesian coordinates and binned for each box-counting grid size, $l$. For each aggregate, multiple successive grids are set up by using the
ellipsoid maximum dimension, $2a$, to determine the initial grid length. Figure 4.5 shows an example for what the boxcounting procedure looks like using different numbers of grid boxes for a given aggregate. Each grid is specified by a grid length, $l$, which divides the aggregate into $N_{\text{grid}} = 2^n$ components which creates a total of $2^n$ total boxes for each $x, y, z$ direction. This gives a total of $2^{3n}$ boxes for each aggregate where the length scale, $l$, is given by: $l = 2^{-n}$. The common definition for the generalized multi-fractal dimension is
given by:

\[
D_q = \frac{1}{q-1} \lim_{l \to 0} \frac{\log[Z(q,l)]}{\log l}.
\] (4.11)

\[Z(q,l) = \sum_{i=1}^{N_{\text{dip}}} P_{i,l}^q \] is a partition function where dipole probabilities, \(P_{i,l}\), are given by \(P_{i,l} = \frac{N_i}{N_{\text{agg}}}\). \(N_i\) is the total number of dipoles with locations, \((x_i, y_i, z_i)\), located in a bin with grid resolution, \(l\), that makes up the total number of dipoles for a particular aggregate, \(N_{\text{agg}}\). Equation (4.11) however is difficult to use in practice since the limiting behavior cannot be calculated numerically. Instead, the more common approach is to utilize L’Hospital’s rule to approximate this limit at a physically relevant and computationally reasonable grid scale \(l_0\)

\[
D_q \approx \frac{1}{q-1} \left. \frac{\partial \log[Z(q,l)]}{\partial \log l} \right|_{l=l_0}.
\] (4.12)

To evaluate Equation (4.12), \(D_q\) is plotted for each \(q\) value as a function of each grid size, \(l\), around \(l = l_0\). From this plot, \(D_q\) can be estimated in terms of the slope of the linear regression in log-log space. For \(q = 0\), the generalized fractal dimension is equal to the (mono-) fractal dimension or boxcounting dimension defined by

\[
D_f \equiv D_0 = \left. \frac{\partial \log N}{\partial \log l} \right|_{l=l_0} \implies N \propto l^{-D_f},
\] (4.13)

where \(N\) represents the total number of boxes that has at least one dipole. Throughout this paper, we refer to \(D_0\) as \(D_f\) for consistency with previous works (e.g., Westbrook et al. 2004b; Schmitt and Heymsfield 2010). For \(q = 1\), Equation (4.11) corresponds to the information (entropy) dimension\(^1\). For \(q = 2\), Equation (4.11) corresponds to the “correlation dimension” (Karperian 1999–2013).

While boxcounting methods for estimating generalized fractal dimensions are calculated in a standard way, calculations of lacunarity have historically been performed using a variety of methods (Smith et al. 1996). In fact, as Benoit Mandelbrot himself has stated in Mandelbrot (1994): “...I have little hope of finding a unique measure of lacunarity.” For

\[^1\]q = 1 yields a singularity using Equation (4.11). However, this singularity can be avoided by using L’Hospital’s rule. The following equation gives the appropriate information dimension:

\[
D_1 = \lim_{l \to 0} \frac{\log \sum_{i,j} P_{i,j}^q}{\log l} \quad \text{(see van Opheusden et al. 1996)}.
\]
this work, we characterize lacunarity as the efficiency, or the square of the coefficient of variation, CV, of the multi-fractal partition function

$$\lambda_l \equiv \text{Eff}_l = (\text{CV}_l)^2 = \left( \frac{\sigma_l}{\mu_l} \right)^2 = \frac{Z(2,l)}{|Z(1,l)|^2} - 1,$$

(4.14)

where $\sigma_l$ represents the standard deviation of dipole probabilities for each model run, and $\mu_l$ represents the mean of dipole probabilities for each model run. Notice that the form of Equation (4.14) provides a nice conceptual relationship with the multifractal moments $q = 1$ and $q = 2$. In general, lacunarity is orientation dependent, meaning that different aggregate orientations will yield different values. As a result, it is common to sample and average over multiple grid orientations. Therefore, an average lacunarity can be calculated as

$$\Lambda = \frac{1}{GE} \sum_{g=1}^{G} \sum_{l=1}^{E} \lambda_l.$$  

(4.15)

We found in our initial tests that averaging over multiple particle orientations did little to change fractal quantities when we had many model runs. Rather, the spread in fractal quantities was dominated by the multiple model runs. Therefore, for runs where we calculated only mono-fractal quantities we set $G = 1$ whereas for runs where we calculate multi-fractal quantities we set $G = 20$.

### 4.3.3 Model configurations

Since fractal calculations require better dipole resolution and Euclidean calculations require many separate runs, we perform separate simulations for each case. For calculating the evolution of ellipsoid quantities, we use a total of about 520 dipoles to represent each monomer whereas for fractal simulations we use a total of about 4200 dipoles. The number of dipoles for each monomer is slightly variable when reorienting each monomer during aggregation. This is because dipole indices are given in terms of integer values which means some dipoles are rounded to the same location. For Euclidean only runs, we build up 2000 aggregates whereas for fractal runs we build up only 20. We can calculate mean fractal quantities (generalized fractal dimension and lacunarity) for each model run and then average over each simulation. In this sense, each model run represents a different
realization of aggregates with $N_{\text{mon}}$ number of monomers for given initial conditions. For our tests, we have a fixed dipole size of 0.01 (arbitrary units). We found in our initial tests that only three $l$ grid scales of $N_{\text{grid}} = 4, 8, 16$ (see Figure 4.5) were necessarily to maintain consistent fractal results throughout evolution. Grid scales that are too close to that of the size of the entire aggregate (i.e., $N_{\text{grid}} = 2$) or too close to the size of the dipole (i.e., $N_{\text{grid}} = 32, 64$) will not capture the appropriate fractal scaling.

For tests where we aggregate monomers of different aspect ratio, we perform two sets of simulations. We first hold monomer volume constant and we then hold the maximum dimension constant. For aggregating particles of different orientation we use two extreme cases: random and horizontal. Random orientation of Euler angles follows that of Jiang et al. (2017) whereas horizontal orientations are identical except that the second rotation is held constant at zero which keeps the maximum dimension always in the horizontal. For multi-fractal runs, we average $D_q$ over 20 orientations for each aggregate realization. $q$ values for multi-fractal analysis were computed in linear intervals from $-10$ to $+10$ to determine multi-fractal behavior.

### 4.4 Results

#### 4.4.1 Monomers of the same habit and aspect ratio

We first start with the aggregation of identical monomers. Although this situation is physically implausible (due to a lack of fallspeed dispersion) we start with this scenario so as to form a basis of comparison for future simulation where we test different combinations of size and shape.

Figure 4.6 shows the evolution of aggregate ellipsoid aspect ratios for different initial monomer aspect ratios and $N_{\text{mon}} = 2, 3, 10, 50, 100$. The symmetry of spherical monomers restrict aggregates with $N_{\text{mon}} = 2$ to always produces prolate spheroids with $\phi = 0.5$. However, as more and more monomers are added, the ellipsoid bivariate aspect ratio distribution shifts toward aspect ratios of unity. When $N_{\text{mon}} = 100$, the dominant shape is close to prolate spheroids with two separate modes ($\phi_{ba} = \phi_{ca} \approx 0.4$ and $\phi_{ba} = \phi_{ca} \approx 0.8$). For oblate
Figure 4.6. Evolution of ellipsoid distributions for different monomer aspect ratios for Monte Carlo simulations (joint histograms) and mathematical model (contours). Contours range from 2 to 12 in increments of 2.

Spheroids (plates) and prolate spheroids (columns) with aspect ratios of $\varphi_{\text{mon}} = 2$, the ellipsoid evolution from $N_{\text{mon}} = 3$ to $N_{\text{mon}} = 100$ is nearly identical to that of spheres. The only monomer type that deviates from this evolution is that of prolate spheroids with aspect ratio of $\varphi_{\text{mon}} = 10$. For this case at $N_{\text{mon}} = 2$, the distribution mode is close to $\varphi_{ba} \approx \varphi_{ca} \approx 0.2$ but much of the ellipsoid parameter space is open. By $N_{\text{mon}} = 10$, all cases have distributions that look identical. However, for $N_{\text{mon}} = 50, 100$, the $\varphi_{\text{mon}} = 10$ case has its mode concentrated more toward unity and has much less overall spread in values.
Figure 4.7. Fractal and Euclidean evolution of single monomer aggregates under random orientations. Red lines correspond to prolate spheroid monomers, blue lines correspond to oblate spheroid monomers, and black lines correspond to sphere monomers. Fractal quantities (left column) were calculated over 20 model runs whereas Euclidean quantities (right two columns) were calculated over 2000 model runs. Lines represent the mean values over all runs whereas shaded regions represent ±1 standard deviation. Dotted lines for fractal quantities represent cases where \( \min(\varphi, \varphi^{-1}) = 0.05 \).

A comparison of the fractal evolution alongside the Euclidean evolution of shape and density is shown in Figure 4.7. Each mean quantity essentially behaves as a power-law with respect to the number of monomers in each aggregate. For fractal dimension, aggregates composed of spherical monomers behave very much like Westbrook et al. (2004b); Schmitt and Heymsfield (2010) where the mean fractal dimension for low numbers of monomers are higher than those of more monomers. After a couple dozen monomers, the mean fractal dimension is essentially constant with \( D_f \approx 2.2 \). However, for eccentric plates and columns the mean fractal dimension monotonically increases throughout evolution. Aggregates composed of thin columns, \( \varphi_{\text{mon}} = 10 \) seem to significantly lower the fractal dimension. This behavior is even more exaggerated when \( \varphi_{\text{mon}} = 20 \) whereas the fractal dimension for plates with \( \varphi_{\text{mon}} = 0.05 \) is essentially unchanged. The mean lacunarity seems to mirror that of the fractal dimension for each monomer type. Lacunarity seems to be generally monotonically increasing (increasing porosity) throughout evolution with aggregates composed of planar monomers tending toward that composed of spheres. Ag-
gregates composed of thin columns however have lacunarity that is higher than plates and spheres but tends to decrease slightly after about 25 monomers.

The evolution of the mean ellipsoid shapes and densities (as volume fractions of total aggregate volume) are shown in the center and right columns of Figure 4.7. For plates and spheres, $\overline{\phi_{ba}}$ and $\overline{\phi_{ca}}$ (top center) increases until $N_{\text{mon}} \approx 10$ and then slowly decreases. This behavior is also shown for the first product moment (top right). Overall, it seems as though aggregates composed of plates, regardless of monomer aspect ratio, exhibit a consistent evolution behavior. Column aggregates on the other hand have mean aspect ratio quantities that increase until $N_{\text{mon}} \approx 50$. This extended evolution for thin column aggregates results in best fit ellipsoids that end up becoming more spherical than either plates or spheres. Volume fractions (densities) of aggregates are in general decreasing with number of monomers which corresponds to increasing lacunarity. However, for all model runs, the use of ellipsoids instead of spheres acts to substantially decrease the spread of potential density values. This decrease in spread is most likely due to the ability of ellipsoids to better represent the shape of aggregates. Even so, it seems that the different realizations of aggregates do not substantially increase the spread of various density values for ellipsoids. Moreover, although the mean aspect ratio quantities for thin plates are very similar to that of spheres, the density values are much lower. This discrepancy in evolution suggests that a single density relationship for aggregates is not sufficient to fully capture ellipsoidal aggregate geometry for all types of aggregates.

### 4.4.2 Monomers of the same habit but different aspect ratios

Figure 4.8 shows a comparison of mean Euclidean and fractal quantities for cases where we randomly select monomer aspect ratios of either 0.1 or 0.5 when we build each aggregate. For comparison, the $\min (\phi_{\text{mon}}, \phi_{\text{mon}}^{-1}) = 0.1$ and sphere monomers are included as well. The sphere monomer case can be thought as a proxy for $\min (\phi_{\text{mon}}, \phi_{\text{mon}}^{-1}) = 0.5$ since the fractal and Euclidean properties are nearly identical.

For monomers of the same $a$-axis length but different aspect ratios, both fractal and Euclidean properties are very similar for each habit. For these cases, the mean fractal dimension is roughly halfway between that of $\phi_{\text{mon}} = 0.1$ plates and $\phi_{\text{mon}} = 0.5$ (spheres).
Figure 4.8. Evolution of the mean ellipsoid and fractal properties for mixed aspect ratio cases of plate aggregates (blue) and column aggregates (red) and spheres (black). Solid lines correspond to results for min(\(\varphi_{\text{mon}}, \varphi_{\text{mon}}^{-1}\)) = 0.1 from Figure 4.7 and mixed cases represent randomly selected aspect ratios of either 0.1 or 0.5. Dashed lines represent mixed aspect ratios with same monomer a-axis length whereas dotted lines represent mixed aspect ratios with same monomer volume. Mean aspect ratios are from top to bottom: \(\bar{\varphi}_{\text{ba}}, \bar{\varphi}_{\text{ca}}, \text{and} \langle \varphi_{\text{ba}}\varphi_{\text{ca}} \rangle\).

for \(N_{\text{mon}} \) less than about 25. However, these mixed cases become nearly identical to that of \(\varphi_{\text{mon}} = 0.1\) plate aggregates for \(N_{\text{mon}} \geq 25\). However, the mean lacunarity for these cases is always higher than that of \(\varphi_{\text{mon}} = 0.1\) plate aggregates and seems to behavior more like column aggregates with \(\varphi_{\text{mon}} = 10\). For aggregates composed of equal volume, but mixed aspect ratio monomers, the fractal behavior is similar to that of min(\(\varphi_{\text{mon}}\)) = 0.1. For instance, the behavior of \(\bar{D}_f\) follows that of \(\varphi_{\text{mon}} = 10\) but lower in value whereas for plate aggregates the behavior is very close to that of \(\varphi_{\text{mon}} = 0.1\) throughout evolution. However, unlike \(\bar{D}_f\), the mean lacunarity of this mixed case is substantially different than the \(\varphi_{\text{mon}} = 0.1\) case. The fact that \(\bar{D}_f\) does not vary much for plate aggregates whereas \(\bar{\Lambda}\) does suggests that \(\alpha_m\) and \(\beta_m\) are not necessarily related in a unique way; the same \(\beta_m\)
$D_f$ can potentially correspond to multiple values of $\alpha_m (\Lambda)$. This lack of consistency is particularly a problem if $D_0$ and $\beta_m$ are both used to solve for $\alpha_m$ using an extrapolation approach similar to Schmitt and Heymsfield (2010): Even for the same initial monomer $a$-axis lengths, different aspect ratios yield various porosity structures for plate aggregates.

In general, the Euclidean estimates of aspect ratios and densities mirror the limiting behavior of their fractal counterparts. For instance, mean aspect ratio quantities for plate aggregates are within a few percentage of that of $\phi_{mon} = 0.1$ aggregates and sphere aggregates regardless of different monomer aspect ratio combinations. Likewise, column aggregate mean aspect ratios follow the same type of behavior to that of $\phi_{mon} = 10$. However, the ellipsoid volume fractions show some important differences. Perhaps most surprising is that while the ellipsoid volume fractions for plate monomers of equal volume, but mixed aspect ratios produce aggregates that are similar to $\phi_{mon} = 0.1$ aggregates, the lacunarity is much higher. Therefore it seems that the analogy between $\Lambda$ and $\rho_i$ is rather imperfect. Nevertheless, aggregates composed of the same maximum dimension but different aspect ratios seem to behave in a consistent way regardless of habit. One possible explanation for this is that aggregates composed of similarly sized monomers will attempt to assume the characteristics of the more voluminous monomers. However, the fact that $\bar{\Lambda}$ and $\bar{\rho}_i$ are in between their extreme aspect ratio cases suggests that aggregate characteristics still depend upon each monomer type.

4.4.3 Effect of orientations

Figure 4.9 shows the ellipsoid evolution of aggregates for plate and column monomers with $\min (\phi_{mon}, \phi_{mon}^{-1}) = 0.1$ when particles are assumed to fall with their maximum dimensions in the horizontal. For both cases, the early ellipsoidal evolution $2 \leq N_{mon} \leq 5$ is much more restricted than that of random orientations (see Figure 4.6). For plates, only a few ellipsoidal aspect ratio pairs are allowed corresponding to either a stacked configuration (i.e., an oblate spheroid with $\phi = 2\phi_{mon}$), an edge touching configuration (i.e., an ellipsoid with $\phi_{ba} = 0.5$ and $\phi_{ca} = \phi_{mon}$), or any configuration in between. Intermediate cases therefore correspond to a roughly diagonal region within the ellipsoid parameter space. For columns, horizontal orientations essentially eliminates the top half of the ellipsoid aspect ratio parameter space. This makes it so that columns are either stuck more or less from end to end.
Figure 4.9. Same as Figure 4.6 but for horizontal particle orientations and \( \min(\varphi_{\text{mon}}, \frac{1}{\varphi_{\text{mon}}}) = 0.1 \).

(i.e., \( \varphi_{\text{ba}} \approx \varphi_{\text{ca}} \approx \frac{\varphi_{\text{mon}}}{2} \)), stuck more or less in a crossed “X” configuration (i.e., \( \varphi_{\text{ba}} \approx 1.0 \) and \( \varphi_{\text{ca}} \approx 2\varphi_{\text{mon}} \)), or a configuration somewhere in between. Intermediate cases therefore correspond to a roughly horizontal region within the ellipsoid aspect ratio parameter space where one peak corresponds to the peak of \( N_{\text{mon}} = 2 \) whereas the second peak corresponds closely to that of observations (Figure 4.3) and the other simulations (Figure 4.6).

When \( N_{\text{mon}} = 3 \), plate aggregates correspond to two separate regions of the aspect ratio parameter space whereas for column aggregates with \( N_{\text{mon}} = 3 \) look much like that of random orientations but with a peak at lower aspect ratios. By \( N_{\text{mon}} = 10 \), both cases are very similar to that of Figure 4.6. However, unlike their counterparts in Figure 4.6, horizontal orientations seem to yield a nearly identical evolution for \( N_{\text{mon}} = 10 \) to \( N_{\text{mon}} = 100 \) with aspect ratios that peak closer to unity.

### 4.4.4 Multifractal evolution

One potential way to determine when aggregates become fully developed is to track when the multifractal spectrum stops changing. This signifies that regardless of how the aggregate constituents are perturbed, the overall behavior stays the same. For our purposes, this suggests that visually different aggregates have physical properties that are essentially
Figure 4.10. Multi-fractal evolution of aggregates for spheres (black line), oblate spheroids (blue lines), and prolate spheroids (red lines). Solid lines represent aspect ratios of 0.1 and 10 and dashed lines represent aspect ratios of 0.05 and 20. Each panel represents the average spectrum over 20 simulation runs and $G = 20$ orientations.
the same. Figure 4.10 shows how multifractal spectrum (which in this context is $q$ vs. $D_q$) evolves for different $N_{\text{mon}}$ and for different monomer types. For those familiar with multifractal spectra, the plots in Figure 4.10 might seem strange since each spectrum is generally monotonically increasing rather than decreasing. However, this phenomenon is consistent with the simulations in van Opheusden et al. (1996) who seems to have also calculated similar plots for their snowflake aggregates (see figure 9 in van Opheusden et al. 1996). The origin of this increasing spectrum is thoroughly discussed in van Opheusden et al. (1996); van Opheusden (1998) and seems to be the result of building up aggregates whose monomers exhibit an excluded volume effect. Diffusion-limited aggregates like dendrites, by contrast, have decreasing multifractal spectra (cf. Wolf 1996).

One interesting aspect about Figure 4.10 is that negative multifractal moments are nearly identical throughout evolution and seem to asymptote toward the same value as $q \to -\infty$. It is not clear why this is the case for each case although it could be due to averaging very large and very small numbers. Therefore, we restrict our analysis to positive moments only. In general, the multi-fractal spectrum for sphere monomers evolves slower than the other cases. The spectrum monotonically increases for each $N_{\text{mon}}$ aggregate. However, as the aggregate collects more monomers, the dimensions corresponding to positive moments flattens out. This flattening out effect is much more pronounced for the planar and columnar habits and does not appear to be a result of the choice of grid scales or dipole resolutions. As discussed in van Opheusden et al. (1996), the anomolous increasing multifractal spectrum acts to swap the interpretation of $D_0$ and $D_2$. The fact that positive moments of the multifractal dimensions are generally flat is therefore reassuring since this increasing spectrum suggests the use of $D_2$ instead of $D_0$ as a proxy for $\beta_m$. 

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4.5 Discussion

4.5.1 A possible explanation for universal ellipsoid aggregate distributions

The persistent bivariate pattern of the Monte Carlo aggregate best-fit ellipsoid distributions (Figures 4.6 and 4.9) and that of observations (Figure 4.3) suggests some sort of universality of the aggregation process that exists regardless of monomer properties. Oblate spheroids are surprisingly not preferred at any time for any of our tests. Therefore, our consistent asymmetric, tri-axial configurations counter some claims that early stage aggregates are approximately oblate (Moisseev et al. 2015). Even for the aggregation of horizontally oriented planar crystals, the best-fit ellipsoid distribution produces predominately tri-axial ellipsoids that are rarely oblate.

We propose a possible explanation for this behavior. Consider the case when $N_{\text{mon}} = 2$. Since monomers are not allowed to occupy the same space (volume exclusion), any configuration is naturally asymmetric in $(x, y, z)$. If there is no preference for any particular lattice site (which is possibly the case if the major dimension is randomly oriented in the $x - y$ plane), then the next aggregation event ($N_{\text{mon}} = 3$) will have a higher likelihood of occurring along the major dimension ($a$ axis) rather than either minor dimensions ($b$ or $c$ axes). This is simply because there are more lattice sites along the major dimension than the two minor dimensions. Each additional monomer contributes less and less to the overall aggregate size. Therefore, in order to produce an oblate or spherical aggregate, aggregation events must occur with unequal probability in the $x - y$ plane to counteract the initial asymmetric aggregate shape. As a result, the probability of extending the major ellipsoid $a$-axis length is naturally larger than the other two axes; there are simply more attachment sites that are projected along the $a$ axes versus the other axes. The ellipsoid evolution therefore could possibly be thought of as a Dirichlet-type process like the Chinese restaurant process (Blei et al. 2004). The Chinese restaurant process is a type of stochastic clustering process whereby cluster locations (imagined as tables in a Chinese restaurant) will incorporate additional integers (imagined as customers) according to probabilities that are weighted based on the current occupancy of each table. This conceptual structure generates a distri-
bution on partitions of integers. The consistent bivariate aspect ratio beta distribution form suggests that the aggregation process, like the Chinese restaurant process, is exchangeable: The order in which monomers of various orientations aggregate does not affect the final distribution. Viewing aggregation as a Dirichlet process could also explain why the marginal aspect ratio distributions are so well represented as beta distributions since the multivariate Dirichlet distribution is essentially a multidimensional beta distribution. Future aggregation work could explore this possibility by using a Dirichlet Markov Chain Monte Carlo model or a Gaussian mixture model.

4.5.2 Ellipsoid fitting uncertainties

One discrepancy in our comparison between simulated and observed aggregates has been the tendency for our simulated aspect ratio distributions to have mean values shifted more toward unity than that of the MASC derived ellipsoids. Some of this discrepancy can be explained due to uncertainties produced by the gradient descent algorithm used to estimate the best fit ellipsoids. Jiang et al. (2019) tested their gradient descent algorithm on Monte Carlo generated aggregates from the IPAS simulator (Schmitt and Heymsfield 2010). The results of this test are shown in Figure 4.11 for both the histograms themselves (left column) and their ratio (right column). The overall bias introduced by the gradient descent estimate acts to reduce the apparent ellipsoid aspect ratios in a way that is more consistent with our Monte Carlo simulations. For example, \( \phi_{cb} \) derived from the gradient descent algorithm produces very few values near unity but the actual Monte Carlo generated aggregates used had more values closer to unity.

The main assumption for use of Equation (4.7) in model calculations is that the aggregate \( a \)-axis lengths (or equivalently \( V_{in} \)) is statistically independent of \( \phi_{ba} \) and \( \phi_{ca} \). This allows for distribution moments of \( V_i \) (or mass, \( m_i \)) to simply be the product of each distributions’ moments. However, if \( a \) is correlated with \( \phi_{ba} \) and \( \phi_{ca} \), then the moments of \( V_i \) could be significantly different. From the MASC database we found that the correlation coefficients between \( a \) and each aspect ratio were very low. For instance, the correlation coefficient values for the NSA database are: \( \text{corr}(a, \phi_{ba}) = -0.0919 \) and \( \text{corr}(a, \phi_{ca}) = +0.0545 \). This suggests that we can indeed consider the \( a \)-axis and the aspect ratios to be independent of one another such that the volume (mass) distribution is
Figure 4.11. Comparison of 3D ellipsoids estimated using the Monte Carlo aggregation method and their gradient descent (GD) retrieval estimates. The left column shows the histograms of all counts \((N = 176)\) for both ellipsoid estimates. The right column shows their ratio (3D ellipsoid divided by the gradient descent retrieval estimates). Uncertainty values of 1.0 (black line) illustrate that both methods produce the same aspect ratio.

The effects of estimating \(V_i\) using Equation (4.3) is shown in Figure 4.12 where the \(V_{i0}\) and \(V_i\) from the NSA MASC are shown along with two separate Monte Carlo estimates using Equation (4.7). We first fit a Pareto distribution to the MASC dataset for \(V_{i0}\). This type of continuous distribution is similar to what a bulk microphysics model might
assumed. The second method uses a naive bootstrapping approach that randomly samples $V_i$ from the MASC NSA database. For each method, we then discretized Equation (4.7) and sampled from the $V_i$ and aspect ratio distributions to estimate $V_i$. These estimated distributions are overall very similar to that derived from the MASC database despite the biases introduced by Monte Carlo and naive bootstrapping techniques.

Despite our simplified approach to simulating snow aggregates, our comparison of best fit ellipsoids with those derived from the MASC instrument are particularly compelling. It is possible that other ellipsoid fitting methods could potentially yield different aspect ratio values and different ellipsoid evolution for each initial condition. We also assume that aggregates are formed through differential sedimentation and not through diffusion or sheer. It is thought that differential sedimentation is the dominant aggregation
mechanism in Cirrus clouds (Westbrook et al. 2004a).

4.5.3 Fractal calculation uncertainties

Since we use spheroids to approximate the geometry of monomers, we are ignoring any internal monomer structure that might influence the aggregation process and the fractal analysis. Many individual ice particles, particularly dendrites, also exhibit mono- and multi-fractal behavior (Wolf 1996). It is possible that fractal calculations of aggregates with more detailed geometry could yield different values. Therefore, since we assume homogeneous spheroids, the results presented in this paper should be considered to be an upper estimate for $D_f$ and a lower estimate for $\Lambda$.

Figure 4.13. Mean fractal dimension for prolate (column) aggregates. Dashed lines represent values reported by Schmitt and Heymsfield (2010) for monomer aspect ratios of 2.0 and 5.0.

One concern with our spheroid aggregate results is whether our implicit aggregation modeling method yields different aggregates and therefore different fractal properties than the explicit methods of Westbrook et al. (2004b); Schmitt and Heymsfield (2010) and others. Since we are not explicitly simulating the aggregation process, it is possible that our aggregates might yield different fractal properties especially since Figure 4.6 shows clearly
different fractal behavior for extreme prolate aspect ratios. To test the robustness of our prolate results, we compare the evolution of mean fractal dimensions for monomer aspect ratios that overlap that of Schmitt and Heymsfield (2010). Both sets of results are shown in Figure 4.13 where \( \phi_{\text{mon}} = 2.0 \) and \( \phi_{\text{mon}} = 5.0 \) are the aspect ratios used by Schmitt and Heymsfield (2010). For those aspect ratios, our results compare extremely well which suggests our methods are comparable. To test whether our extended runs of \( \phi_{\text{mon}} = 10, 20 \) suffer from a lack of resolution, we also re-ran the \( \phi_{\text{mon}} = 10 \) case by increasing the resolution of each monomer by three times. However, we found that increasing the number of monomer dipoles did not significantly change the mean fractal dimension. Therefore, the high sensitivity of column aggregate \( D_f \) to \( \phi_{\text{mon}} \) below that tested by Schmitt and Heymsfield (2010) seems to reflect the geometry of the aggregation problem rather than the way we compute \( D_f \) or the assumptions we use.

Through testing of the boxcounting method, we found that different regression methods can act to change the estimated fractal dimension. In this paper, we transform the boxcounting results into log-log space and then perform a linear regression to estimate \( D_f \). However, performing a non-linear regression without transforming the boxcounting data leads to a slightly higher fractal dimension. For sphere monomers, this higher fractal dimension appears to be more consistent with the results of Schmitt and Heymsfield (2010).

### 4.6 Summary and concluding remarks

Westbrook et al. (2004b) conclude their Monte Carlo aggregation paper by stating: “In summary, we have a fairly complete understanding of the geometry of the atmospheric ice crystal aggregates... The fact that the same evolution is seen for differing initial monomer populations (rods and rosettes) suggests that a single set of geometric relationships for ice aggregates can successfully be applied in a wide range of cloud conditions.” Our results however suggest a less complete picture where the apparent geometric universality as simulated by Westbrook et al. (2004a,b); Schmitt and Heymsfield (2010) is a result of the small range of their tested monomer aspect ratios and their assumption that \( D_f \) is sufficient for characterizing aggregate geometry. For instance, our results illustrate that fractal dimensions for thin column aggregates throughout evolution are much lower than the of-
ten reported \( D_f \approx 2.0 \), which even holds when \( N_{\text{mon}} \geq 100 \). For aggregates composed of very thin plates, \( D_f \) increases from about \( D_f \approx 2.0 \) to \( D_f \approx 2.1 \) when \( N_{\text{mon}} = 100 \). This suggests that the aggregate \( D_f \) evolution takes much longer for very eccentric monomers (Figure 4.10). The opposite seems to happen for lacunarity and density where the evolution is quicker for eccentric monomers but slower for more spherical monomers. For very eccentric particles (\( \min (\varphi_{\text{mon}}, \varphi_{\text{mon}}^{-1}) = 0.05 \)) the majority of density changes seems to occur from \( N_{\text{mon}} = 2 \) to \( N_{\text{mon}} = 3 \).

Our results not only support those reported in previous studies (Figure 4.13), but our tests also support the larger range of fractal dimensions \((1.6 \leq D_f \leq 2.5)\) reported in Jiang and Logan (1991) for marine snow\(^2\) aggregated through differential sedimentation. The range of fractal dimensions we estimate are also consistent with the observed \( 2.0 \leq D_f \leq 2.3 \) range estimated by Schmitt and Heymsfield (2010). The apparent temperature dependence therefore could be partially explained by different habit types: Higher altitude (lower temperature) aggregates are perhaps composed of thin plates and needles whereas lower altitude (higher temperature) are perhaps composed of more spherical planar particles. The relationship between the assumed monomer Euclidean geometry and the fractal properties of their aggregates seem to be directly related to a weighted average of monomer shape and packing factors (see Table 1 in Logan and Kilps 1995). The limiting behavior of fractal dimensions according to monomer aspect ratio mirrors the limiting behavior of spheroidal shape factors (see Figure B1 from Harrington et al. 2013a). Fractal quantities of aggregates therefore depend on the prevalence of thin, longer crystals such as needles or perhaps polycrystalline scrolls or twins. Aggregates formed in Cirrus clouds could therefore have very different fractal properties than those formed at lower levels.

The present work questions the applicability of some mass-dimensional power-law framework assumptions. Particularly troublesome is the prefactor coefficient, \( \alpha_m \), which is often solved by assuming initial aggregates are uniformly filled spheres. Our numerical results show that this assumption, while convenient for closing the system of equations in a microphysics model, is not consistent with our fractal and Euclidean geometric estimates. Instead, initial aggregates \((N_{\text{mon}} \approx 2)\) show a wide variety of different fractal dimensions and lacunarities: None of these fractal quantities corresponds to uniformly dense spheres

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\(^2\) Marine snow is not to be confused with atmospheric ice-ice snow aggregates in marine environments. Rather, marine snow refers to biological material like fish poop that drops from the surface of the ocean.
(i.e., \( \Lambda \approx 0 \) and \( D_f \approx 3.0 \)). More importantly, although plate aggregates seem to consistently produce similar values of \( D_f \), lacunarity is variable depending on different combinations of monomer sizes and shapes and generally increases from \( N_{\text{mon}} = 2 \) to \( N_{\text{mon}} \approx 25 \). The lack of consistent behavior between \( D_f \) and \( \Lambda \) implies that a single \( D_f \) value is not enough to completely characterize an aggregate’s geometry. For instance, parameterization development could utilize both measures of fractal dimension and lacunarity as described by Blumenfeld and Mandelbrot (1997); Mandelbrot (1992) to rescale the mass dimensional relationship in a more physical manner. The use of lacunarity in model development is particularly attractive since lacunarity can be easily calculated without the need for any regression technique.

Microphysics models often parameterize particle properties in terms of an assumed maximum dimension. However, this simplification means that particles with the same maximum dimension will necessarily have the same masses and fall speeds. Passarelli (1978a,b); Passarelli and Srivastava (1979); Sasyo and Matsuo (1985); Böhm (1992) and others came up with clever ways to incorporate a dispersion of fall speeds for the same particle mass or dimension. The bivariate ellipsoidal aspect ratio model presented in this paper allows for a simple, analytical way to capture the appropriate fall speed and mass dispersion. Despite the correlation of shape and density with \( N_{\text{mon}} \) (and therefore size), our estimates of the ellipsoid volume distribution are still consistent with that of observations (Figure 4.12). This consistency suggests that aggregates at any particular size represent many different stages of aggregation. For distributions of sufficiently developed aggregates, the maximum dimension and shape can be considered separate and can be specified using different functions whereas the ellipsoid distribution can be represented using Equation (4.7) as the average distribution of aggregate shapes. This would best work for plate aggregates since the mean aspect ratio quantities do not significantly change throughout most of the evolution (Figures 4.7 and 4.8). It is already common for microphysics schemes to compute bulk quantities as ratios of gamma functions. The moment approach using Equations (4.8) and (4.10) yields a closed set of equations for evolving ellipsoid shape that fits neatly into the bulk paradigm, provided that \( \bar{\phi}_{ba}, \bar{\phi}_{ca}, \) and \( \langle \phi_{ba} \phi_{ca} \rangle \) are parameterized during the aggregation process. Future aggregation work should focus on understanding the evolution and distributions of \( N_{\text{mon}} \) and monomer aspect ratios since these factors can be used, in theory, to directly predict average aggregate morphology. Characterizing these
monomer properties in models and observations will ensure appropriate estimations and parameterization of aggregate properties.

Finally, this paper reconciles historically inconsistent claims made about aggregate shapes. The early observations of Magono and Nakamura (1965) and later observations of Brandes et al. (2007) suggest snow aggregates are quasi-spherical whereas some radar results suggest aggregates are oblate (Moisseev et al. 2015) with aspect ratios of approximately 0.6 (Matrosov et al. 2005; Hogan et al. 2012; Garrett et al. 2015). In situ observations from Korolev and Isaac (2003) suggest aggregates have mean aspect ratios between 0.6 and 0.8. It is therefore not surprising that these average 2D analogs are within the aspect ratio distributions of both observed (Figures 4.2 and 4.3) and modeled (Figures 4.6 and 4.9) aggregates. The bias toward aspect ratios of unity could be explained by projection uncertainties due to orientation. Therefore, the consistency of the 0.6 aspect ratio value derived from in situ observations and that used in homogeneous oblate spheroid radar approximations should be viewed as strictly coincidental since aggregates are rarely oblate.
Chapter 5

A General N-Moment Spectral Bulk Approach for Microphysics Models

5.1 Introduction

The history of microphysical modeling is replete with numerous analytical techniques for solving various difficult integro-differential equations. Perhaps the most important and difficult equation to solve is the kinetic collection equation (KCE) given by

\[
\frac{\partial n(x, t)}{\partial t} = \frac{1}{2} \int_{x=0}^{x} K(x-y, y) n(x-y, t) dy - n(x, t) \int_{y=0}^{\infty} K(x, y) n(y, t) dy, \tag{5.1}
\]

where \( K(x, y) \) is a kernel associated with the binary collection process, \( n(z, t) \) is a distribution function associated with each species that are collecting at a time \( t \), and \( x \) and \( y \) are measures (usually size, \( D \), or mass, \( m \)) of specie \( x \) collecting specie \( y \). The first term on the right hand side represents the production rate of coagulated particles that sum to \( x \) whereas the second term represents the depletion rate of \( x \) due to their coalescence with other particles. Although this form of the KCE is only an approximate equation since covariance terms are ignored (Gillespie 1975), almost all microphysics models incorporates some version of Equation (5.1). Often, Equation (5.1) is cast into a much more convenient form for microphysics models where the distribution of coagulated particles is integrated. This moment-based equation derived by Thompson (1968) and shown in Drake (1972) is given by

\[
\frac{dM_r(t)}{dt} = \frac{1}{2} \int_{x=0}^{\infty} \int_{y=0}^{\infty} [(x+y)^r - x^r - y^r] K(x, y) n(x, t) n(y, t) dxdy, \tag{5.2}
\]
where
\[ M_r(t) \equiv \int_{x=0}^{\infty} x^r n(x,t) \, dx, \tag{5.3} \]
represents the distribution moments of \( n(x,t) \). Analytical solutions to Equations (5.1) and (5.2) have been explored using Mellin and Laplace integral transform techniques for polynomial kernels of the form: \( K \sim A + B(x+y) + Cxy \) (Golovin 1963; Scott 1968; Thompson 1968; Drake 1972; Drake and Wright 1972; Tzivion et al. 1987) and approximate analytical solutions have been explored for the hydrodynamic kernel (Passarelli 1978a; Verlinde et al. 1990; Gaudet and Schmidt 2004). For first-order polynomial kernels, Equation (5.2) is closed, meaning that higher order moments are expressed in terms of lower order moments. This allows for a predetermined set of moments \( r_i = (r_1, r_2, \ldots, r_N) \) to specify a particular distribution of collected particles with distribution moment values \( M_r \). Solutions of Equation (5.2) using this \( K \) form can be proven to be unique (Drake 1972). Therefore, a common method for evolving particles and their properties is to assume a distribution \emph{a priori} where \( N \) moments are predicted. If \( x \) and \( y \) represent masses, then \( r = 0 \) represents the total number of particles in the distribution, \( r = 1 \) represents the total mass (i.e. water content) of the distribution, and \( r = 2 \) represents a measure that is analogous to radar reflectivity.

Another important equation for microphysics is that of sedimentation (advection)
\[ \frac{\partial n(x,t)}{\partial t} = \frac{\partial}{\partial z} [\langle v_t \rangle_r n(x,t)]. \tag{5.4} \]
Again, for bulk models, Equation (5.4) can be integrated to describe how distribution moments advect
\[ \frac{dM_r(t)}{dt} = \frac{d}{dz} [\langle v_t \rangle_r], \tag{5.5} \]
where \( \langle v_t \rangle_r = \int_0^\infty x^r v_t n(x,t) \, dx \) represents the \( r \)-th \( x \)-weighted bulk fallspeed. When distributions are in terms of mass, \( r = 0 \) describes how many particles advect in a timestep whereas \( r = 1 \) describes how much mass advects in a timestep. Both these quantities are important for accurate precipitation estimates and are thus particularly sensitive to assumptions about the distribution function used in Equation (5.5) (Milbrandt and Yau 2005a; Kumjian and Ryzhkov 2012). In theory, one could use equations in the form of Equations (5.2) and (5.5) to predict \emph{all} moments of any particular particle distribution. By only
predicting a few moments, current bulk microphysics models will introduce and accrue errors across the evolving size distribution associated with the inflexibility of the assumed continuous distribution function. Although observed particle distributions are often in an “equilibrium” inverse exponential state (e.g. Westbrook et al. 2004b), the mechanisms that lead to this state and the appropriate timescale to describe this evolution are still uncertain.

Not all models however specify particle size distributions. Kogan and Belochitski (2012) for instance developed a microphysics approach that did not assume a distribution function but rather predicting full integer moments using equations of the form Equations (5.2) and (5.5). For fractional moments, related to sedimentation for instance, these authors developed power-law parameterizations as a way to estimate these quantities from the predicted full integer moments. For particles like cloud droplets or rain, the simple geometry (i.e. uniformly dense spheres) yields integer moments in their processes, making the approach of Kogan and Belochitski (2012) very useful. The methodology of Kogan and Belochitski (2012) has some important limitations however. The set of integer distribution moments is determined by finding the minimum of a cost function associated with moments compared with that from an LES bin microphysics model. Since most ice particles exhibit a wide variety of shapes and densities, the moments associated with bulk properties are inevitably fractional and not integer. This fact has led to the use of fractal methods for describing the mass-dimensional relationships for irregular particles and snow aggregates (Brown and Francis 1995; Baker and Lawson 2006; Schmitt and Heymsfield 2010). When used in sedimentation and reflectivity calculations, the mass-dimensional coefficients and other parameters algebraically absorb one another. This collapse of parameters and introduction of fractional moments into model calculations can significantly complicate both parameter estimation techniques as well as physical interpretations for how these moments relate back to individual processes and particle properties. New particle property methods for ice like ISHMAEL (Jensen et al. 2017) predict fractional moments for shape evolution which dynamically entangle model physics with distribution parameters. Therefore, it is imperative that these new schemes utilize as many fundamental, analytical techniques as possible to complement increasing model complexity.

Interestingly enough, although computing technology continues to improve rapidly, there recently has been a resurgence of older analytical methods for bulk model development. This resurgence seems to be a result of those interested in the physical mechanisms
behind the evolution and observation of particle size distributions. For example, Wu and McFarquhar (2018) uses the principle of maximum entropy and Lagrange multipliers to investigate the utility and development of the size distribution. Through their mathematical techniques and results, Wu and McFarquhar (2018) advocates for the use of the generalized gamma distribution because of its scale invariant properties. Morrison et al. (2018) recently developed a generalized re-normalization method using $N$-moments of any distribution function. The ability to combine multiple distribution parameters through normalization and re-normalization allows for the characterization of distribution variability as well as uncertainty estimates. Garrett (2019) applied the Liouville equation to derive analytical solutions to the steady-state rain size distribution. Through his solution, Garrett (2019) found that the shape of the resulting gamma distribution can be related analytically to the cloud liquid water path and the ratio of the updraft velocity to the cloud liquid water path. The use of analytical methods therefore can potentially help explain the physical mechanisms behind size/mass distribution evolution.

A promising analytical technique for exploring size distributions is the Mellin transform. The usefulness of this integral transform lies in its convolution property; that is, the distribution of two independent variables can be expressed simply in terms of the product of each distributions’ Mellin transform. Drake (1972); Drake and Wright (1972) exploited this property in their exploration of the KCE and developed solution bounds for certain initial distribution functions and collection kernels. Furthermore, Verlinde et al. (1990) also utilized the Mellin convolution methodology of Marichev (1983) in their quasi-analytical solutions to the hydrodynamic collection equation. While Verlinde et al. (1990) derived their solution with gamma distributed particles in mind, these solutions can be shown to represent a series of $H$-functions. From a modeling perspective, the gamma functions that represent $H$-function moments are computationally simple which allows for easy and efficient bulk calculations of water content, sedimentation, and other important variables. In principle, the $H$-function can be characterized by any number of parameters and can be calculated in terms of a series expansion using the Residue theorem of complex analysis. Therefore, an assumed $N$-parameter $H$-function can potentially have $N$ degrees of freedom when specifying any particular size or mass distribution.

This paper develops a general bulk modeling approach that exploits the $H$-function and its properties. The generality permitted by the $H$-function, as opposed to the general-
ized gamma distribution, can allow for bulk microphysics schemes to function in a similar way to spectral NWP models. However, unlike spectral, we instead employ Mellin transforms rather than Fourier transforms for model calculations. The advantage to using a spectral bulk approach is that there is no need for performing any inverse integral transform like what spectral NWP modeling must use to map calculations in spectral space to physical space. A major advantage to using \( H \)-function distributions is that convolutions of univariate and bivariate \( H \)-functions that represent various physical properties, such as particle shape and density, are themselves \( H \)-function distributions. The next section illustrates the effectiveness and implications of including \( H \)-function convolution properties when calculating aggregate mass and fallspeed distributions and their bulk quantities. In Section 5.3, we combine the method-of-moments procedure developed by Bodenschatz and Boedigheimer (1983) with a gradient descent algorithm to estimate \( H \)-function distribution parameters for \( N \) predicted moments. In Section 5.4 we perform idealized tests of our approach by comparing with analytical solutions of the KCE governed by the Golovin kernel.

### 5.2 Distributions of particle property convolutions

The convolution properties of univariate (Equation (2.23)) and bivariate (Equation (2.26)) \( H \)-functions allow for aggregates of various shapes, sizes, and densities to have their mass and fallspeed distributions expressed as univariate \( H \)-functions. The general form of an algebraic combination of microphysics variables is

\[
\xi = a^\xi_b \varphi_{ba} \varphi_{ca},
\]

(5.6)

where \( \xi \) is a microphysical quantity that depends on \( a, \varphi_{ba}, \) and \( \varphi_{ca} \). For example, the traditional mass-dimensional framework can be extended to include shape effects if aggregate ellipsoid \( a \) axes follow a gamma distribution with ellipsoid aspect ratios that follow the bivariate \( H \)-function distribution in Equation (4.7). The convolution properties associated
with the $H$-function allow for the following generalized number distribution function

$$
n(\xi) = N_{agg} \frac{\Gamma(\alpha + \beta_a + \beta_b)}{\Gamma(\alpha)} H^{3.0}_{2,3} \left[ \frac{\xi}{\xi_n} \right] (\alpha + \beta_a - (\zeta_{ba} + \zeta_{ca}), \zeta_{ba} + \zeta_{ca}) (\alpha + \beta_b + \beta_c - \zeta_{ca}, \zeta_{ca}) \right),
$$

where $\xi$ is an arbitrary microphysical quantity. For example, the mass distribution is given by: $\zeta_a = \beta_m$ and $\zeta_{ba} = \zeta_{ca} = 1$ which leads to

$$
n(m) = N_{agg} \frac{\Gamma(\alpha + \beta_a + \beta_b)}{\Gamma(\alpha)} H^{3.0}_{2,3} \left[ \frac{m}{m_n} \right] (\alpha + \beta_a - 2, 2) (\alpha + \beta_a - 1, 1)\right),
$$

where it is assumed that the particle density follows a power-law with size (e.g. Heymsfield et al. 2002). The fall speed distribution can be derived in a similar way using the fall speed formulation of Mitchell and Heymsfield (2005)

$$
n(v) = N_{agg} \frac{\Gamma(\alpha + \beta_a + \beta_b)}{\Gamma(\alpha)} H^{3.0}_{2,3} \left[ \frac{v}{v_n} \right] (\alpha + \beta_a - (\zeta_{ba} + \zeta_{ca}), \zeta_{ba} + \zeta_{ca}) (\alpha + \beta_a + \beta_c - \zeta_{ca}, \zeta_{ca}) \right).
$$

Figure 5.1 shows a comparison of the hybrid area ratio parameterization of Heymsfield et al. (2002) (see their Table 1) the fall speed spectrum assuming fractal aggregates (or equivalently, reduced density spheres) and the same aggregates but with ellipsoidal shapes given by MASC bivariate distribution from Figure 4.3. Each distribution was generated by constructing and sampling from the maximum dimension distribution for both spheres and ellipsoids. For ellipsoids, the aspect ratio bivariate beta distribution shown in Figure 4.3 is discretized and sampled for each drawn maximum dimension. A mean maximum dimension ($D_{max} \approx 1.0\text{mm}$) was chosen so as to approximate the range of observed aggregate sizes and masses from Locatelli and Hobbs (1974) for their “aggregates of unrimed side planes, assemblages of plates, columns, bullets.” The density parameterization for both the conventional spheres/fractal approach and ellipsoid approach are power-law functions of maximum dimension. This means that for a fixed maximum dimension, ellipsoid masses are necessarily less than that of spheres (panel b.) in Figure 5.1). This case can therefore be considered a direct in situ comparison since it is assumed that the parameterizations derived from Heymsfield et al. (2002) and others are in terms of aggregate maximum di-
Figure 5.1. Comparison of fall speed distributions computed with the methodologies of Heymsfield et al. (2002); Mitchell and Heymsfield (2005) for \( \nu = 1 \) (inverse exponential). Table 1 from Heymsfield et al. (2002) is used to specify the density with \( n = 1.5, k = 0.18, \alpha = -1 \) and Table 1 from Mitchell (1996) is used to specify the projected area with \( \sigma = 0.2285 \) and \( \zeta = 1.88 \). Shaded histograms \((N = 20,000)\) represent randomly sampling from each distribution when calculating particle fall speeds whereas solid lines correspond to Equations (5.8) and (5.9). Shaded regions are the approximate ranges of “aggregates of unrimed side planes, assemblages of plates, columns, bullets” from Locatelli and Hobbs (1974). Ellipsoidal aggregates are assumed to fall with their maximum projected area in the horizontal.

However, this comparison could be deceiving from a physical standpoint since fixing particle density necessarily changes the distribution of aggregate masses; particle mass governs much of the settling dynamics of aggregates. Therefore, we also perform calculations where both sphere and ellipsoid aggregates have the same mass distribution. To do this, we use the same mean aggregate mass for each distribution and then solve for the new characteristic size for ellipsoid aggregates. Although this doesn’t mathematically lead to an identical mass distribution, both distributions are still close to one another (panel...
b.), thus providing an additional basis of comparison.

The change in the fall speed distribution between using ellipsoids rather than spheres is quite stark. Common in situ parameterizations for bulk models in general lead to a very narrow distribution. This narrowness is due to using a fixed value to represent the fall speed-size exponent. It is common for this exponent for aggregates to be close to zero or even negative (Locatelli and Hobbs 1974; Mitchell and Heymsfield 2005). This means that the Weibullization of the inverse exponential size distribution yields very large positive exponents for the power and exponential terms in the fallspeed distribution. The introduction of ellipsoid shapes modulates the fall speed distribution so as to decrease and broaden the spectrum. Approximate observed ranges of aggregate fall speeds are surprisingly close to our ellipsoid ranges even though the mass distributions for all three cases fall well within those also reported by Locatelli and Hobbs (1974). The mass-weighted fall speeds on the other hand are closer in form to that of the mass distribution rather than the fall speed distribution. This is because the mass spectrum span multiple orders of magnitude while fall speed spans less than one. As a result, the number-weighted mean fall speed is reduced by 93.4\% for ellipsoids of the same size and 76.6\% for ellipsoids of the same mass. The mass-weighted fall speeds reduce by 60.3\% for ellipsoids of the same size and 63.0\% for the same mass. Size sorting, defined as the ratio of mass-weighted to number-weighted fall speeds, actually increase by 20.1\% for ellipsoids of the same size and 8.4\% of the same mass.

5.3 Generalized method-of-moments procedure

The previous section illustrated the utility of assuming $H$-function distributions rather than gamma distributions. This allows for convolutions of particle properties to permit multiple parameters to modulate the distribution form. Gamma distributions that employ power-law functions on the other hand will necessarily collapse all parameters into two: One for the power-law prefactor and another for the exponent. As showed in Figure 5.1, this collapsing effect can lead to unphysical or incorrect distributions. This section extends the idea of incorporating $H$-function convolutions in model calculations by modifying the bulk model framework to assume $H$-function distributions \textit{a priori} rather than gamma dis-
tributions.

The traditional method-of-moments procedure employed by bulk microphysics schemes involves a combination of normalization and re-normalization to solve for distribution parameters. For instance, Milbrandt and Yau (2005b) develops a set of predictive equations for $N_t$, $q_t$, and $Z_t$. If a liquid particle’s size is assumed to follow a gamma distribution, then $N_t \propto M_1$, $q_t \propto M_3$, and $Z_t \propto M_6$ (Milbrandt and Yau 2005a). Calculations of these moments simplify using elementary properties of the gamma function which allows for algebraic expressions for each distribution parameter. The problem of H-function parameter estimation using method-of-moments has been addressed in Bodenschatz and Boedigheimer (1983). The general procedure is to derive a set of equations for an arbitrary number of predicted moments such that the set of equations can be solved for each H-function distribution parameter. This can be done by rearranging H-function distribution moments in the form of a homogeneous equation set (cf. equation 5.3 in Bodenschatz and Boedigheimer 1983)

$$\frac{M_{r_i}M_{r_{i+2}}[I(r_{i+2}+1)]^2}{(M_{r_{i+1}})^2 I(r_{i+1}+1)I(r_{i+3}+1)} - 1 = 0,$$

where $i = 1, 2, \ldots, 2(p+q)$ is the moment order, $r_i$ are the chosen moments, and $M_{r_i}$ are the distribution moment values. Notice that for the case where the H-function is a 3-parameter gamma distribution where $x \sim \text{Gamma}(N_t, x_n, \nu)$, this set of equations simplifies to equation 6 in (Milbrandt and Yau 2005a).

These equations can be greatly simplified if the natural logarithm function is applied to both sides. For the general case, this leads to the following set of equations

$$G_i(c_j, d_j) = \ln \left[ \frac{M_{r_i}M_{r_{i+2}}}{(M_{r_{i+1}})^2} \right] + 2 \ln [I(r_{i+1}+1)] - \ln [I(r_i+1)] - \ln [I(r_{i+2}+1)] = 0$$

$$= \ln \left[ \frac{M_{r_i}M_{r_{i+2}}}{(M_{r_{i+1}})^2} \right] - \sum_{k=0}^{2} \binom{2}{k} (-1)^k \ln (I(r_{i+k}+1)) = 0$$

$$= \sum_{k=0}^{2} \binom{2}{k} (-1)^k \left[ \ln M_{r_{i+k}} - \sum_{j=1}^{p+q} (-1)^{(j-m-n)} \ln \Gamma(c_j + d_j (r_{i+k}+1)) \right] = 0,$$

(5.11)
where $G_i$ is a matrix of length $N = 2(p+q)$ and $i = 1 \ldots 2(p+q)$ are indices corresponding to each $H$-function parameter. Computationally, this yields a series of log-gamma functions. Bulk microphysics schemes generally use subroutines that compute the log-gamma function anyway, often using the Lanczos approximation, which reduces some unneeded operations. Additionally, the use of log-gamma functions avoids the possibility of multiplying and dividing by very large numbers which could lead to numerically unstable solutions. Although parameter estimation through iteration can be computationally expensive, the use of iterative solvers is still reasonably commonplace within microphysics schemes (Milbrandt and Yau 2005a,b) and numerical studies (Kumjian and Ryzhkov 2012).

To evolve the parameters of the $H$-function distribution, $N$ moments of the mass distribution at a time $t = t$ along with equations of the form Equation (5.3) can be used to predict the new $N$ moments of the distribution at $t = t + \Delta t$. For instance, at a particular time, $t$, fallspeed moments can be calculated as

$$\langle v_t \rangle_r = \frac{N_t}{c^r} \int_{x=0}^{\infty} m^r v_t n(m) dm = \frac{N_t}{c^{r+\beta_r}} \alpha_r I(r + \beta_r + 1). \quad (5.12)$$

We assume particle distributions are in terms of mass rather than size since mass represents a conservative property. We also assume mass and fall speed can be expressed in terms of power laws

$$m = \alpha_m D^{\beta_m} \implies D = \alpha_m^{-\frac{1}{\beta_m}} m^{\frac{1}{\beta_m}}. \quad (5.13a)$$

$$v_t = \alpha_r m^{\beta_r}. \quad (5.13b)$$

Additionally, the use of mass lowers the moment order required to solve Equation (5.2), thereby requiring less terms to solve. When using the hydrodynamic kernel, the kinetic collection equation can be simplified by utilizing the Wisner approximation. The approximate form suggested by Murakami (1990) and used by Milbrandt and Yau (2005a) yields a simple form

$$\Delta v_r \equiv |v_{t_x} - v_{t_y}| \approx \sqrt{\left(\langle v_{t_x} \rangle_r - \langle v_{t_y} \rangle_r \right)^2 + 0.04 \langle v_{t_x} \rangle_r \langle v_{t_y} \rangle_r}. \quad (5.14)$$

Using Equation (5.14) in Equation (5.2) and the integration properties of the $H$-function
allows for collection rates to be calculated analytically

\[
\frac{dM_r(t)}{dt} = \frac{1}{2} \int_{x=0}^{\infty} \int_{y=0}^{\infty} [(x+y)^r - x^r - y^r] K(x,y) n(x,t) n(y,t) \, dx \, dy
\]

\[
= \frac{\pi}{8} \Delta V r \int_{x=0}^{\infty} \int_{y=0}^{\infty} \sum_{j=1}^{r-1} \sum_{k=0}^{2} \binom{r}{j} \binom{2}{k} \alpha_x^{k} \alpha_y^{k} x^{\frac{2-k}{k}} y^{\frac{2-k}{k}} n(x,t) n(y,t) \, dx \, dy
\]

\[
= \frac{\pi}{8} \Delta V r N_x N_y \ldots
\]

\[
\sum_{j=1}^{r-1} \sum_{k=0}^{2} \binom{r}{j} \binom{2}{k} c_x^{\frac{2-k}{k}+1+j} c_y^{j-r-\frac{k}{k}} \alpha_x^{k} \alpha_y^{k} \Gamma(x+2-j) \Gamma(y+r+j+1).
\]

(5.15)

Alternatively, it is possible to solve Equation (5.15) assuming the full hydrodynamic kernel by using the properties of the $H$-function. The solution (derived in Appendix B.3) is a finite series of $H$-functions which can each, in theory, be evaluated in terms of an infinite series. A general technique for evaluation the $H$-function is presented in Appendix B.1.

These new moments can then be used in Equation (5.11) along with a gradient descent algorithm to predict parameters the new $H$-function parameters, $c_j$ and $d_j$. A cost function associated with the gradient descent algorithm can be defined as

\[
F(c_j, d_j) = \frac{1}{2} G_i^T(c_j, d_j) G_i(c_j, d_j).
\]

(5.16)

An initial guess of parameters, $c_j^{(0)}$ and $d_j^{(0)}$, allows for an estimate of a next guess for these parameters that minimizes Equation (5.16)

\[
c_j^{(1)} = c_j^{(0)} - c_0 \frac{\partial}{\partial c_j} F(c_j^{(0)}, d_j^{(0)})
\]

(5.17a)

\[
d_j^{(1)} = d_j^{(0)} - d_0 \frac{\partial}{\partial d_j} F(c_j^{(0)}, d_j^{(0)}),
\]

(5.17b)

where $c_0$ and $d_0$ are scaling constants. Since $G_i$ is represented in terms of a series of log-gamma functions, derivatives of $F$ are in terms of a finite series of gamma and digamma functions.

For the case of the generalized (four parameter) gamma distribution given in Equa-
tion (2.14), the first four moments: $M_{r_1}, M_{r_2}, M_{r_3}$ and $M_{r_4}$ can specify all parameters. This leads to the coupled equation set

\[
\begin{bmatrix}
\sum_{k=0}^{2} \binom{2}{k} (-1)^k \left[ \ln M_{r_{k+1}} + \ln \Gamma (b_1 + B_1 (r_{k+1} + 1)) \right] \\
\sum_{k=0}^{2} \binom{2}{k} (-1)^k \left[ \ln M_{r_{k+2}} + \ln \Gamma (b_1 + B_1 (r_{k+2} + 1)) \right]
\end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.
\] (5.18)

Equation (5.18) represents two equations with two unknowns ($b_1$ and $B_1$). Therefore, the gradient descent takes the form

\[
b_1^{(1)} = b_1^{(0)} - b_0 \sum_{k_1=0}^{2} \sum_{k_2=0}^{2} (-1)^{k_1+k_2} \left\{ M_{r_{k_1+1}} + \ln \Gamma \left[ b_1^{(0)} + B_1^{(0)} (r_{k_1+1} + 1) \right] \right\} \psi \left[ b_1^{(0)} + B_1^{(0)} (r_{k_1+1} + 1) \right]
\]

\[
B_1^{(1)} = B_1^{(0)} - B_0 \sum_{k_1=0}^{2} \sum_{k_2=0}^{2} (-1)^{k_1+k_2} \left\{ M_{r_{k_1+2}} + \ln \Gamma \left[ b_1^{(0)} + B_1^{(0)} (r_{k_1+2} + 1) \right] \right\} (r_{k_1+2} + 1) \psi \left[ b_1^{(0)} + B_1^{(0)} (r_{k_1+2} + 1) \right],
\] (5.19a)

where $\psi$ is the digamma function. Once $b_1^{(1)}$ and $B_1^{(1)}$ are solved using Equation (5.19), these values are then put back into Equation (5.19) for $b_1^{(0)}$ and $B_1^{(0)}$. This process is repeated until both parameter values converge.

### 5.4 Idealized tests using analytical solutions

We test our gradient descent approach from Section 5.3 using the first KCE solution given in Scott (1968). This analytical solution represents coagulation of gamma distributed droplet volumes using the Golovin kernel, $K(x, y) = B(x + y)$. The gamma distribution is normalized to unity and to the mean volume such that the initial distribution is given by

\[
n(x, 0) = \frac{\nu}{\Gamma(\nu)} x^{\nu-1} \exp[-\nu x].
\] (5.20)

The analytical solution from Scott (1968) is

\[
n(x, \tau) = (1 - \tau) \exp[-(\nu + \tau) x] \sum_{k=0}^{\infty} \frac{\tau^k x^{\nu+k+1} - 1 \nu^{(k+1)}}{(k+1)! \Gamma[\nu(k+1)]},
\] (5.21)
where \( x \) represents droplet volume and \( \tau \equiv 1 - \exp(-0.00153t) \) is an appropriate timescale for time \( t \) (see Equation 5.2 in Scott 1968). If \( \nu = 1 \) (an initial inverse-exponential distribution) then Equation \((5.21)\) simplifies to

\[
n(x, t) = N_0 \frac{1}{x \sqrt{t}} \exp[-x(1 + t)] I_1(2x \sqrt{t}),
\]

(5.22)

where \( I_\nu(z) \) is the modified Bessel function of the first kind. The evolution of moments is given by termwise integration of Equation \((5.21)\). This yields

\[
M_r(\tau) = \int_0^\infty x^r (1 - \tau) \exp[-(\nu + \tau)x] \sum_{k=0}^\infty \frac{\tau^k x^{\nu+k(v+1)-1} \nu^{(k+1)}}{(k+1)! \Gamma[\nu(k+1)]} dx
\]

\[
= \sum_{k=0}^\infty \frac{\tau^k (1 - \tau) \nu^{(k+1)}}{(k+1)! \Gamma[\nu(k+1)]} \int_0^\infty x^{r+\nu+k(v+1)-1} \exp[-(\nu + \tau)x] dx
\]

(5.23)

To test this methodology, we use the moments given by Equation \((5.23)\) to see how well the gamma distribution and generalized gamma distribution capture the analytical distributions given by Scott (1968). Gamma distributions require only three moments to estimate each parameter: \( N_t \equiv M_0 = 1.0, M_1, \) and \( M_2. \) This can be performed algebraically and does not require the gradient descent algorithm. Generalized gamma distributions require four moments: \( N_t \equiv M_0, M_1, M_2, \) and \( M_3 \) (Equation \((5.19)\)).

All sets of analytical solutions are shown for \( 0 \leq t \leq 300 \) seconds to illustrate the evolution of the normalized volume distribution (corresponding to Figure 6 of Scott (1968)) and water content distribution (corresponding to Figure 9 from Scott (1968)) for an initial \( \nu \) of 2. This time interval was chosen for two reasons. The first reason is that the Golovin kernel does not conserve water content after about a certain amount of time. For an initial monodisperse spectrum, mass conservation is violated at around 1300 seconds (Alfonso et al. 2008). For our tests using the initial gamma distribution specified by Scott (1968), the total water content starts to decline rapidly after \( t = 300 \) seconds. The second reason is that the analytical solution for the mass distribution becomes numerically difficult to evaluate because of the summation of large numbers from the factorial terms for large values of \( x. \)
Figure 5.2. Comparison of the analytical solutions of the KCE from Scott (1968) (solid lines) for an initial normalized gamma distribution (Equation (5.20)) and approximate solutions when assuming gamma distributions (dotted) and generalized gamma distributions (dashed). a.) Shows the evolution of the first 4 integer moments \( r = 0, 1, 2, 3 \) of the normalized volume distributions (b.)) and their volume weighted distributions (c.) for \( t = 0 \) s (black lines), \( t = 150 \) s (orange lines), and \( t = 300 \) s (red lines). The initial gamma distribution (black lines) are the same in each case (given by Equation (5.20)).

The results of these tests are shown in Figure 5.2 for \( t = 0 \) s, \( t = 150 \) s, \( t = 300 \) s (panels b. and c.) for the analytical moments from Equation (5.23) (panel a.)). When \( t = 0 \) s all three distributions are identical. The 3 parameter gamma distribution is a trivial result derived from the first three moments. However, the 4 parameter gamma distribution estimated using the gradient descent algorithm also manages to yield the correct parameter values. When \( t = 150 \) s the 3 parameter gamma distribution struggles to accurately reproduce the correct lower end of the distribution but manages to asymptote toward that of the analytical solution for larger normalized volumes. This behavior becomes exaggerated
when $t = 300 \text{ s}$ when the shape parameter $\nu$ becomes less than unity. Generalized gamma distributions on the other hand are capable of maintaining the correct distribution form throughout its evolution but tends to have its mode shifted to lower normalized volumes. The volume distributions (panel c.) for both cases tend to capture the correct bell-like shape (in log space) due to the ability for the inverse exponential from the gamma distributions to approximate that of the analytical solution. For these volume distributions the modes are shifted to larger values than that of the analytical solution. Both b.) and c.) therefore suggest that moment matching puts the burden of fitting on the exponential term rather than the power function term. This makes sense since values of $\nu$ are quite low throughout the evolution.

Since the same moments are used to specify each distribution, we elect to use relative entropy as a way to quantify the deviation of each gamma distribution from the analytical solutions. These values of relative entropy between the gamma distributions and the analytical solution of Scott (1968) are shown in Table 5.1 at each time. The definition and interpretation of relative entropy are the same as in Equation (3.36). In general, using the generalized gamma distribution rather than the gamma distribution leads to an order of magnitude reduction in relative entropy.

**Table 5.1.** Relative entropy values between gamma distributions and analytical solution of Scott (1968) in Figure 5.2

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</table>


## 5.5 Discussion and Conclusions

The bulk calculations presented in Section 5.2 illustrate some potentially important conclusions about how current microphysics schemes treat sedimentation using power-law parameterization methods. A huge restriction of these current microphysics schemes is that the fall speed power-law parameters are calculated using a fixed number-weighted Best number (e.g. Khairoutdinov and Kogan 2000). However, these fall speed parameters should in fact be calculated across a particular size/mass distribution since each parameter varies with mass. From the perspective of a bulk model, the nonlinearities presented by these relationships make it very difficult if not impossible to maintain a physical relationship between size/mass and fall speed without resorting to numerical methods. As a result, the fall speed power-law exponent for aggregates is often very small when using a representative value for a particular distribution (Mitchell and Heymsfield 2005). This has an important effect on fall speed dispersion and aggregation rates since the value of the fall speed power-law exponent directly determines the spread of fall speeds.

Our numerical results of the mass and fall speed distributions illustrates the effectiveness of using ellipsoids as opposed to spheres, or equivalently, fractals. The segregation of aggregate shapes and densities using ellipsoids permits the mass distribution, which has a more consistent basis for its validity based on both theoretical arguments from fractal geometry (Schmitt and Heymsfield 2010) and observations (Locatelli and Hobbs 1974; Brown and Francis 1995), to be governed using the conventional mass-dimensional framework. Ellipsoid shapes provide a physical mechanism that can reduce aggregate fall speeds and increase their dispersion so as to match observations (Figure 5.1). Without the implementation of ellipsoids or some equivalent in bulk calculations, models are forced to either ignore this dispersion issue or use additional parameterizations derived from different data sets (Passarelli 1978a,b; Sasyo and Matsuo 1985; Böhm 1992). These additional parameterizations therefore are not properly coupled with the underlying model physics, thus obfuscating the physical interpretation of model performance as well as potentially creating inconsistencies among these various parameterization implementations.

Our results also suggests that current bulk models overestimate number-weighted fall speeds by up to almost 100% and mass-weighted fall speeds by about 60%. If this over-
estimation is actually occurring in current bulk microphysics schemes then these schemes systematically underestimate aggregate size sorting anywhere from about 8% to 20%. This size sorting bias over time therefore could stunt precipitation rates since aggregates on average would be less massive. Both bin and bulk models have been shown to consistently underpredict the breadth and intensity of stratiform precipitation resulting from large Mesoscale Convective Systems such as squall lines (Morrison and Milbrandt 2015; Xue et al. 2017; Jensen et al. 2018; Han et al. 2019). Recent evidence derived from an observational/model comparison study suggests that models universally overpredict ice water content at altitudes above 7 km but underestimate ice water content at lower levels (Han et al. 2019). Therefore implementing an ellipsoidal parameterization in models could help explain this discrepancy in a microphysical sense.

Convolving a bivariate ellipsoid aspect ratio distribution with a gamma size distribution yields an $H$-function distribution for both mass and fall speed. It therefore makes sense to develop a framework that permits and evolves $H$-functions. The generality of $H$-functions essentially allows for as many parameters as necessary to properly represent the evolution of size/mass distributions. As shown in Section 5.3, this evolution can be performed by exploiting the intimate relationship between Mellin transforms (which serve as the definitional basis for the $H$-function) and distribution moments (which represent physical bulk quantities). Integrations of process rates (e.g. coalescence and sedimentation) allow for a closed set of equations that can predict the evolution of $H$-function distribution parameters. It is important to note that solutions to these nonlinear, coupled equation sets are not necessarily unique and are also dependent on initial (first guess) parameters as well as the algorithm used to minimize Equation (5.11). However, tests against analytical solutions to the KCE show that a single increase in parameters from 3 (gamma distribution) to 4 (generalized gamma distribution) acts to reduce the relative entropy between actual and approximate distributions by a full order of magnitude.

Often in situ observations are used to estimate size distribution parameters by assuming that they are well represented as gamma distributions. However, it is quite possible that there exist certain families more general than that of the generalized gamma (e.g. perhaps families of $n(x) \propto H_{1,1}^{1,1}(cx)$ or $n(x) \propto H_{0,2}^{2,0}(cx)$) that permit a more fundamental and functional representation. In particular, it seems that the mixed gamma and beta family proposed by Springer and Thompson (1970), $H_{P,M}^{M,0}(x)$, is particularly attractive since phys-
ical quantities like size can be represented as generalized gamma distributions whereas moderating factors like shape and density can be represented as beta distributions. As with power-law functions, it is often the case that multiple functions are capable of capturing any particular data set, especially if there is a considerable spread of values. This functional ambiguity could manifest for data sets that are sufficiently truncated because of instrumental constraints. As we have demonstrated, the convolution of certain families, such as the beta and gamma distributions, can yield a specific family for a particular variable. Efforts to estimate and report distribution parameters using mathematical techniques (McFarquhar et al. 2015) should take this property into account when exploring these various $H$-function families.
Chapter 6

Conclusions

The single particle and multiple particle (distribution) results in Chapter 3 illustrate many of the limitations of the in situ imaging process and the current methods used to report estimates of ice particle shape. For single particles, estimates of particle aspect ratios from projections are only reliable for low values of canting angle dispersion ($\sigma$) and high aspect ratios ($\Phi$). The nonlinear relationship between projected aspect ratio and canting angles leads to an unfortunate scaling behavior where the absolute error in aspect ratio monotonically increases with increasing particle eccentricity. Even planar particles that are expected to experience low values of canting angle dispersion, $\sigma \approx 10^\circ$, will have projected aspect ratios above $\Phi_{\text{proj}} > 0.1$ for $\Phi \leq 0.01$. It is commonly thought that thin plates and dendrites often exhibit these extreme aspect ratios. However, even for common assumptions of canting angle dispersion (Sassen 1986; Klett 1995), these results show that the orientation averaged aspect ratio would be 10 times greater than the actual 3D aspect ratio. It appears that in situ derived aspect ratio power-law parameterizations are still used for observations and models (Ryzhkov et al. 2019). Therefore, the power-law parameters derived from in situ observations should be re-examined to include uncertainty ranges based on estimates of orientation uncertainty. The mapping equations in chapter 3 provides a starting point for these types of estimates.

If distributions of ice particle aspect ratios (or eccentricity) are derived from in situ observations, then projected aspect ratio distributions are not only sensitive to orientations but also to the size distribution parameters. Increasing the size distribution shape parameter, $\nu$, acts to narrow both the projected aspect ratio and projected eccentricity distributions. This reduction in the particle shape dispersion maximizes orientation contributions to projected aspect ratio distributions. Distributions of $\nu = 1$ and $\nu = 4$ appear identical for large values of dispersion ($\sigma \approx 40^\circ$), thus rendering power-law estimates of aspect ratio useless. As a result, values of $\nu$ and $a_n$ should also be reported for each power-law parameterizations derived from images of planar and columnar crystals. The integral transform method provided in chapter 3 provides a direct way to project distributions of modeled spheroids or
estimate the inverse transformation from projections to spheroids. This can be achieved by exploiting the independence of eccentricity and canting angle which allows for convolutions to be specified separately as well. The ratio of distribution moments is simply given by scaling factors that depend only on the assumed orientation distribution. Current in situ methods often estimate distribution parameters using moments (McFarquhar et al. 2015). The proposed approach therefore simply extends already existing moment-based parameter estimation techniques to particle shape. Issues like shape/orientation correlations and instrument sizing limitations can be mitigated by truncated distributions; the orientation scaling factors do not change as long as there is some estimate for the length scale.

Chapter 4 shows that convolutions of ice particle shape can also be used to describe aggregates. The MASC derived ellipsoids from two separate observed cases provide evidence for a “universal” bivariate $H$-function distribution that can capture all relevant distribution product moments to within 4%. Monte Carlo simulations of the aggregation process shows that the evolution of ellipsoid aspect ratio distributions assumes the same bivariate form as that derived from MASC observations. These Monte Carlo simulations show that various aspect ratios of randomly oriented plate monomers do not significantly affect the evolution of aggregate ellipsoids. Randomly oriented column monomers, on the other hand, evolve to become more spherical than aggregates of plate monomers. The use of ellipsoids are shown to collapse much of the density variation compared to using spheres. However, different combinations of monomer aspect ratios and sizes are also shown to nonlinearly affect the ellipsoid density evolution. Future work should investigate these nonlinear relationships so as to connect monomer properties to the densities of their aggregates.

The fractal dimensions of simulated aggregates match those of previous studies like Schmitt and Heymsfield (2010). However, additional tests of thin column aggregates produce fractal dimensions that are much lower than those previous studies (Westbrook et al. 2004b,a; Schmitt and Heymsfield 2010). This discovery suggests that appropriate characterizations of monomer properties are crucial for accurate estimates of fractal dimension. This, in turn, suggests that aggregates of needles (which are perhaps formed from cirrus clouds or winter storms) exhibit different physical properties than aggregates of plates and columns (which are perhaps formed from mixed-phase clouds). Estimates of lacunarity show a wide range of values that do not exhibit a consistent evolution for different monomer properties. These lacunarity values do not appear to linearly map to specific fractal dimen-
sions. This lack of consistency suggests that the same fractal dimension can correspond to many different mass-dimensional prefactor values. Mandelbrot (1992); Blumenfeld and Mandelbrot (1997) provide methods for using lacunarity as to estimate prefactor values. These methods should be incorporated into fractal frameworks for snow aggregates as well.

A major advantage of $H$-functions lies its convolution ability. Although chapter 3 and 4 both exploit these convolution properties, the methods and results in these chapters do not directly describe particle properties other than particle shape. Therefore chapter 5 combines these convolution ideas into a single mathematical framework that can be used to improve current microphysics schemes. Using this methodology on aggregate fall speeds allows for number-weighted and mass-weighted fall speeds to be scaled in addition to mass-dimensional relationships. Scaling factors from the bivariate beta distribution allow for particles of the same size to exhibit different masses and therefore different fall speeds. When transformed, fall speed distributions can then exhibit a realistic broadening without resorting to additional parameterizations. As such, the power-law methodology is not abandoned but improved upon by appropriately moderating distributions and their moments. In addition, comparisons of analytical solutions to the KCE with more general $H$-function distributions allow for an order of magnitude decrease in relative entropy. In total, the use of $H$-functions can be used in future work to merge power-law regime behavior with behavior that is better described using other functional relations.
Appendix A

Spheroid eccentricity projection
distribution and moments

A.1 H-function representations

The following is the derivation of the $H$-function projected eccentricity distribution
for uniformly oriented oblate spheroids but the method is the same for prolate spheroids.

The probability distribution function for uniformly oriented spheroids is given by:

$$
\tilde{n}(\beta) = \frac{2}{\pi}.
$$  \hspace{1cm} (A.1)

Note that the random orientation is respect to the orientation angle $\beta$, which is different
from a general 3-D random orientation distribution in other works like Jiang et al. (2017).

We can use this $\beta$ distribution with Equation (3.33) to describe the joint distribution for
randomly oriented spheroids. Integrating this joint distribution with respect to the spheroid
eccentricity distribution gives the projected eccentricity distribution. This marginal density
can then be written as:

$$
n(\varepsilon_{proj}) = \frac{2}{\pi} \frac{2N_i}{\Gamma(v, p)^m} \int_{\varepsilon_{ob}=\varepsilon_{proj}}^{1} \frac{1}{\sqrt{1 - \frac{\varepsilon_{ob}^2}{\varepsilon_{proj}^2}}} \left(1 - \varepsilon_{ob}^2\right)^{-vm-1} p^v \exp \left[-\frac{p}{\left(1 - \varepsilon_{ob}^2\right)^m}\right] d\varepsilon_{ob}
$$

$$
= \frac{4N_i}{\pi \Gamma(v, p)} m f(n, v, m, p).
$$  \hspace{1cm} (A.2)
We now take the Mellin Transform of $f$. This gives:

\[
\mathcal{M} [f] = \int_{p=0}^{\infty} p^{s-1} \left\{ \int_{\epsilon_{ob}=\epsilon_{proj}}^{1} \frac{1}{\sqrt{1 - \frac{\epsilon_{proj}^2}{\epsilon_{ob}^2}}} (1 - \epsilon_{ob}^2)^{-vm-1} p^v \exp \left[ -\frac{p}{(1 - \epsilon_{ob}^2)^m} \right] \right\} \, \text{d}\epsilon_{ob} \, \text{d}p.
\]

(A.3)

If we assume that this integral converges, then we can swap the order of integration:

\[
\mathcal{M} [f] = \int_{\epsilon_{ob}=\epsilon_{proj}}^{1} \frac{1}{\sqrt{1 - \frac{\epsilon_{proj}^2}{\epsilon_{ob}^2}}} (1 - \epsilon_{ob}^2)^{-vm-1} \left\{ \int_{p=0}^{\infty} p^{v+s-1} \exp \left[ -\frac{p}{(1 - \epsilon_{ob}^2)^m} \right] \right\} \, \text{d}p \, \text{d}\epsilon_{ob}.
\]

(A.4)

Notice that the integral in braces is simply the gamma function integral. Therefore, this yields:

\[
\mathcal{M} [f] = \Gamma(v+s) \int_{\epsilon_{ob}=\epsilon_{proj}}^{1} \frac{1}{\sqrt{1 - \frac{\epsilon_{proj}^2}{\epsilon_{ob}^2}}} (1 - \epsilon_{ob}^2)^{ms-1} \, \text{d}\epsilon_{ob}
\]

\[
= \frac{1}{2} \left( 1 - \epsilon_{proj}^2 \right)^{ms-\frac{1}{2}} \frac{\Gamma(v+s) \Gamma\left(\frac{1}{2}\right) \Gamma(ms)}{\Gamma\left(\frac{1}{2} + ms\right)}
\]

(A.5)

\[
= \frac{1}{2} \sqrt{\pi} \left( 1 - \epsilon_{proj}^2 \right)^{ms-\frac{1}{2}} \frac{\Gamma(v+s) \Gamma(ms)}{\Gamma\left(\frac{1}{2} + ms\right)},
\]

where $\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$ and

\[
B(a,b) = \int_{x=0}^{1} x^{a-1} (1-x)^{b-1} \, dx = \frac{\Gamma(a) \Gamma(b)}{\Gamma(a+b)}
\]

(A.6)

is the Beta function.
Taking the inverse Mellin Transform gives:

\[
f = \mathcal{M}^{-1}[\mathcal{M}[f]] = \frac{1}{2} \sqrt{\pi} \left( 1 - \varepsilon_{\text{proj}}^2 \right)^{-\frac{1}{2}} \cdot \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{\Gamma(s+1)\Gamma(ms)}{\Gamma(s+1+ms)} \left( \frac{p}{1-\varepsilon_{\text{proj}}^2} \right)^{-s} ds. \tag{A.7}
\]

\[
f = \frac{1}{2} \sqrt{\pi} \left( 1 - \varepsilon_{\text{proj}}^2 \right)^{-\frac{1}{2}} H_{1,2}^{2,0} \left[ \frac{p}{1-\varepsilon_{\text{proj}}^2} \right] \left( \frac{1}{2}, m \right) \left( 0, m \right), (v, 1) \tag{A.8}
\]

Therefore, the oblate (prolate) eccentricity (second eccentricity) uniform angle probability density functions are:

\[
n(\varepsilon_{\text{proj}}) = \frac{2N_i}{\sqrt{\pi} \Gamma(v, p)} \left( 1 - \varepsilon_{\text{proj}}^2 \right)^{-\frac{1}{2}} H_{1,2}^{2,0} \left[ \frac{p}{1-\varepsilon_{\text{proj}}^2} \right] \left( \frac{1}{2}, m \right) \left( 0, m \right), (v, 1) \tag{A.9}
\]

\[
n(\varepsilon'_{\text{proj}}) = \frac{2N_i}{\sqrt{\pi} \Gamma(v, p')} \left( 1 + \varepsilon'_{\text{proj}}^2 \right)^{-\frac{1}{2}} H_{1,2}^{2,0} \left[ \frac{p'}{1+\varepsilon'_{\text{proj}}^2} \right] \left( 1 + \varepsilon'_{\text{proj}}^2 \right) \left( \frac{1}{2}, m \right), (v, 1) \tag{A.10}
\]

By substituting \( p = \varphi_{n}^{2m} \) and \( p' = \varphi_{n}^{-2m} \) and using properties 1.4 and 1.5 from Mathai et al. (2010), we can put the projected eccentricity probability density functions in a format that is similar to Equation (3.18):

\[
n(\varepsilon_{\text{proj}}) = \frac{N_i}{\sqrt{\pi} \Gamma(v, \varphi_{n}^{1-\frac{1}{m}})} \frac{1}{\varphi_{n}} \Phi_{\text{proj}}(\varepsilon_{\text{proj}}) \left[ \frac{\varphi_{n}}{\Phi_{\text{proj}}(\varepsilon_{\text{proj}})} \right] \left( \frac{1}{2}, \frac{1}{2} \right) \left( v + |\delta_{\epsilon} - 1|, |\delta_{\epsilon} - 1| \right) \tag{A.11a}
\]

\[
n(\varepsilon'_{\text{proj}}) = \frac{N_i}{\sqrt{\pi} \Gamma(v, \varphi_{n}^{-\frac{1}{m-1}})} \frac{1}{\varphi_{n}} \Phi_{\text{proj}}(\varepsilon'_{\text{proj}}) \left[ \frac{\varphi_{n}}{\Phi_{\text{proj}}(\varepsilon'_{\text{proj}})} \right] \left( 0, \frac{1}{2}, \frac{1}{2} \right) \left( -v - |\delta_{\epsilon} - 1|, |\delta_{\epsilon} - 1| \right) \tag{A.11b}
\]

To prove that these forms are correct, we reproduce the randomly oriented oblate distribution example from Figure 3.9 but with the inclusion of Equation (A.11a). For simplicity, we numerically integrate the Mellin-Barnes integral representation given in Equation (A.11a) and compare to our other numerical methods. All three methods are shown in Figure A1. Furthermore, if we assume that \(|\delta_{\epsilon} - 1|\) can be written as a ratio of integers, then
we can use methods shown in Marichev (1983) to write Equation (A.11a) as a two-series of Kummer’s confluent hypergeometric function. Otherwise, we can use method of residues directly on Equation (A.11a) to derive an infinite series representation.

\[ n(\varepsilon_{\text{proj}})_{\text{rand}} = \frac{N_i}{\sqrt{\pi}} \left(\frac{n}{\varepsilon_{\text{proj}}}^{\frac{3}{2}}\right)^{\nu-1} \Gamma \left(\frac{1}{2} + \frac{1}{2} s \right) \Gamma \left(\nu + \frac{1}{2} + |\delta_*| + \frac{1}{2} + |\delta_*| \right) ds \]

\[ N_i = 1.0 \]
\[ \nu = 4.0 \]
\[ \delta_* = 0.9 \]
\[ \varphi_n = 0.5 \]

**Figure A.1.** A comparison of three bulk projection distribution techniques.
A.2 Moments of eccentricity equations

For simplicity, this section derives the moments for $n(\varepsilon_{\text{ob}})$ but the method is the same for $n(\varepsilon_{\text{pro}})$.

The moments of Equation (3.20a) are represented by the integral:

$$E[n_{\text{ob}}] = \frac{1}{\int_{\varepsilon_{\text{ob}}=0}^{1} n(\varepsilon_{\text{ob}}) d\varepsilon_{\text{ob}}} \int_{\varepsilon_{\text{ob}}=0}^{1} n(\varepsilon_{\text{ob}}) d\varepsilon_{\text{ob}}$$

$$= \frac{2m}{\Gamma(n, \nu, m)} \int_{\varepsilon_{\text{ob}}=0}^{1} p^{\nu} \varepsilon_{\text{ob}}^{n+1} (1 - \varepsilon_{\text{ob}}^2)^{-vm-1} \exp \left[- \frac{p}{(1 - \varepsilon_{\text{ob}}^2)^m} \right] d\varepsilon_{\text{ob}}$$

$$= \frac{2m}{\Gamma(n, \nu, m)} f(n, \nu, m, p),$$

where $f(n, \nu, m, p)$ is the integral we are looking to evaluate.

Now Mellin-Transform of $f$ yields

$$\mathcal{M}[f] = \int_{p=0}^{\infty} \left\{ \int_{\varepsilon_{\text{ob}}=0}^{1} p^{\nu} \varepsilon_{\text{ob}}^{n+1} (1 - \varepsilon_{\text{ob}}^2)^{-vm-1} \exp \left[- \frac{p}{(1 - \varepsilon_{\text{ob}}^2)^m} \right] d\varepsilon_{\text{ob}} \right\} dp.$$  

(A.13)

It is assumed that $f$ convergences such that integral order can be swapped. This gives:

$$\mathcal{M}[f] = \int_{\varepsilon_{\text{ob}}=0}^{1} \left\{ \int_{p=0}^{\infty} p^{\nu} \varepsilon_{\text{ob}}^{n+1} (1 - \varepsilon_{\text{ob}}^2)^{-vm-1} \exp \left[- \frac{p}{(1 - \varepsilon_{\text{ob}}^2)^m} \right] dp \right\} d\varepsilon_{\text{ob}}.$$  

(A.14)

Notice that the integral expression in braces is just that of the gamma function. This allows
for the brace expression to evaluate as

\[
\mathcal{M} [f] = \int_{\varepsilon_{ob}=0}^{1} \varepsilon_{ob}^{n+1} (1 - \varepsilon_{ob}^2)^{-\nu m - 1} \left\{ (1 - \varepsilon_{ob}^2)^{\nu m + ms} \Gamma (\nu + s) \right\} d\varepsilon_{ob}.
\]  

(A.15)

Collecting terms and factoring out \(\Gamma (s)\) from the integral gives

\[
\mathcal{M}_s [f] = \Gamma (\nu + s) \int_{\varepsilon_{ob}=0}^{1} \varepsilon_{ob}^{n+1} (1 - \varepsilon_{ob}^2)^{ms - 1} d\varepsilon_{ob}.
\]  

(A.16)

The integral given in Equation (A.16) evaluates to a beta function using the substitution: \(t = \varepsilon_{ob}^2\). This puts the integral in a new form

\[
\mathcal{M}_s [f] = \frac{1}{2} \Gamma (\nu + s) \int_{t=0}^{1} t^{\frac{n}{2}} (1 - t)^{ms - 1} dt.
\]  

(A.17)

Therefore the Mellin-Transform of \(f\) can be represented in closed-form as:

\[
\mathcal{M}_s [f] = \frac{1}{2} \frac{\Gamma (\nu + s) \Gamma \left( \frac{n}{2} + 1 \right) \Gamma (ms)}{\Gamma \left( \frac{n}{2} + 1 + ms \right)}.
\]  

(A.18)

Finally, we can represent \(f\) in terms of Mellin-Barnes contour integral by taking the Inverse Mellin-Transform of Equation (A.18):

\[
f (n, \nu, m, p) = \mathcal{M}^{-1} [\mathcal{M}_s [f]] = \frac{1}{2} \Gamma \left( \frac{n}{2} + 1 \right) \int_{s=c-i\infty}^{c+i\infty} \frac{\Gamma (\nu + s) \Gamma (ms)}{\Gamma \left( \frac{n}{2} + 1 + ms \right)} p^{-s} ds.
\]  

(A.19)

\[f (n, \nu, m, p) = \frac{1}{2} \Gamma \left( \frac{n}{2} + 1 \right) H_{1,2}^{2,0} \left[ p \begin{pmatrix} \frac{n}{2} + 1, m \\ \nu, 1, 0, m \end{pmatrix} \right],
\]  

(A.20)

Therefore, oblate distribution moments are represented in closed-form by combining
Equations (A.12) and (A.20)

\[
E[\varepsilon_{\text{ob}}^n] = \frac{\Gamma \left( \frac{n}{2} + 1 \right)}{\Gamma(v, p)} m H_{1,2}^{2,0} \left[ p \left| \left( \frac{n}{2} + 1, m \right) \right] (v, 1), (0, m) \right]. \tag{A.21}
\]

Similarly, the prolate second eccentricity moments are given by

\[
E[\varepsilon_{\text{pro}}^n] = \frac{\Gamma \left( \frac{n}{2} + 1 \right)}{\Gamma(v, p')} m H_{1,2}^{2,0} \left[ p' \left| \left( 1, m \right) \right] (v, 1), (-\frac{n}{2}, m) \right]. \tag{A.22}
\]

These equations simplify by employing various properties of the H-Function. Substituting the definitions of \(p\) and \(p'\) and using property 1.4 in Mathai et al. (2010) leads us to the following forms

\[
E[\varepsilon_{\text{ob}}^n] = \frac{1}{2} \frac{\Gamma \left( \frac{n}{2} + 1 \right)}{\Gamma(v, \varphi_n | \delta_s - 1|)} H_{1,2}^{2,0} \left[ \varphi_n^{-1} \left| \left( \frac{1}{2}, \frac{1}{2} \right) \right] (0, \frac{1}{2}), (v, |\delta_s - 1|) \right]. \tag{A.23}
\]

and

\[
E[\varepsilon_{\text{pro}}^n] = \frac{1}{2} \frac{\Gamma \left( \frac{n}{2} + 1 \right)}{\Gamma(v, \varphi_n | \delta_s - 1|)} H_{1,2}^{2,0} \left[ \varphi_n^{-1} \left| \left( \frac{1}{2}, \frac{1}{2} \right) \right] (v, |\delta_s - 1|), (-\frac{n}{2}, \frac{1}{2}) \right]. \tag{A.24}
\]

Finally, using property 1.3 from Mathai et al. (2010) on Equation (A.24) flips the argument \(\varphi_n\) into the numerator

\[
E[\varepsilon_{\text{pro}}^n] = \frac{1}{2} \frac{\Gamma \left( \frac{n}{2} + 1 \right)}{\Gamma(v, -\varphi_n | \delta_s - 1|)} H_{1,2}^{2,0} \left[ \varphi_n^{-1} \left| \left( 1 - v, |\delta_s - 1| \right) \left( \frac{n}{2} + 1, \frac{1}{2} \right) \right] (0, \frac{1}{2}) \right]. \tag{A.25}
\]

Note that if \(m = 1\) or equivalently, \(|\delta_s - 1| = \frac{1}{2} \implies \delta_s = 0.5\) or \(\delta_s = 1.5\) then each moment equation can be represented with the Meijer-G function (Meijer 1941; Mathai et al.
The corresponding moment equations for randomly oriented spheroids can be derived in the same way. The eccentricity moment equation for oblate spheroids is given by:

\[
E[\varepsilon'_n^\mathrm{ob}] = \frac{\Gamma\left(\frac{n}{2} + 1\right)}{\Gamma\left(\nu, \varphi_n\right)} G_{1,2}^{2,0} \left( \begin{array}{c} \frac{n}{2} + 1 \\ 0, \nu \end{array} \right).
\]  
\tag{A.26}

Similarly, the second eccentricity moment equation for prolate spheroids is given by:

\[
E[\varepsilon''_n^\mathrm{pro}] = \frac{\Gamma\left(\frac{n}{2} + 1\right)}{\Gamma\left(\nu, \varphi_n\right)} G_{1,2}^{0,2} \left( \begin{array}{c} \frac{n}{2} + 1 \\ 1, \nu \end{array} \right).
\]  
\tag{A.27}

Notice that taking the ratio of Equations (A.23) and (A.28) or Equations (A.24) and (A.29) produces the correct scaling factor from Table 3.2

\[
\frac{E[\varepsilon''_n^\mathrm{ob}]}{E[\varepsilon''_n^\mathrm{proj}]} = \frac{E[\varepsilon'_n^\mathrm{pro}]}{E[\varepsilon'_n^\mathrm{proj}]} = \sqrt{\pi} \frac{\Gamma\left(\frac{n}{2} + 1\right)}{\Gamma\left(\frac{n+1}{2}\right)} = \frac{\pi}{B\left(\frac{1}{2}, \frac{n}{2} + 1\right)}.
\]  
\tag{A.30}

Figure A.2 shows that this ratio is consistent with numerical integration of each moment equation for the oblate distribution example from Figure 3.9.
Figure A.2. Ratio of eccentricity moments to uniformly oriented, projected eccentricity moments.
A.3 Eccentricity normalization proof

This proof will use the $H$-function representation for oblate eccentricities but the method is the same for prolate second eccentricities. The $H$-function representation of oblate eccentricity moments when $n = 0$ is given by

$$E[e_{ob}^n] = \frac{N_i}{2} \frac{1}{\Gamma\left(\nu, \phi_n^{\frac{1}{\delta_s-1}}\right)} H_{1,2}^{2,0} \left[ \phi_n \left| \frac{1}{2} \right. \left(1, \frac{1}{2}; 0, \frac{1}{\delta_s-1} \right), (\nu, 1) \right]. \quad (A.31)$$

Using Equation (2.17) puts Equation (A.31) into the following form

$$E[e_{ob}^n] = \frac{N_i}{2} \frac{1}{|\delta_s-1|} \frac{1}{\Gamma\left(\nu, \phi_n^{\frac{1}{\delta_s-1}}\right)} H_{1,2}^{2,0} \left[ \phi_n^{-\frac{1}{\delta_s-1}} \left| \frac{1}{2} \right. \left(1, \frac{1}{2\delta_s-1}; 0, \frac{1}{2\delta_s-1} \right), (\nu, 1) \right]. \quad (A.32)$$

Then from the definition of the $H$-function Equation (2.10)

$$E[e_{ob}^n] = \frac{N_i}{2} \frac{1}{|\delta_s-1|} \frac{1}{\Gamma\left(\nu, \phi_n^{\frac{1}{\delta_s-1}}\right)} \int_{c-i\infty}^{c+i\infty} \left(\phi_n^{\frac{1}{\delta_s-1}}\right)^{-s} \frac{\Gamma(\nu+s) \Gamma\left(\frac{1}{2|\delta_s-1|s}\right)}{\Gamma\left(1+\frac{1}{2|\delta_s-1|s}\right)} ds. \quad (A.33)$$

Now use the gamma function property: $\Gamma(1+x) = x\Gamma(x)$, for the denominator, canceling terms, multiplying the numerator and denominator by $\Gamma(s)$ and then reusing the same
gamma function property gives back the following \( H \)-function

\[
E[\varepsilon_{\text{ob}}^n] = \frac{N_i}{2} \left[ \frac{1}{\Gamma(\nu, \phi_n^{1/\delta_n-1})} \int_{s=c-i\infty}^{c+i\infty} (\phi_n^{1/\delta_n-1})^{-s} \frac{\Gamma(v+s)}{s} ds \right] \]

\[
= N_i \frac{1}{\Gamma(v, \phi_n^{1/\delta_n-1})} \int_{s=c-i\infty}^{c+i\infty} (\phi_n^{1/\delta_n-1})^{-s} \frac{\Gamma(v+s)}{s} \frac{\Gamma(s)}{\Gamma(1+s)} ds \]

\[
= N_i \frac{1}{\Gamma(v, \phi_n^{1/\delta_n-1})} H_{1.2}^{2.0} \left[ \begin{array}{c} (1, 1) \\ \phi_n^{1/\delta_n-1} \end{array} \right] \left( v, 1 \right) \left( 0, 1 \right) \]

The list of common \( H \)-function representations in Bodenschatz (1992) shows that the \( H \)-function in Equation (A.34) is that of the upper incomplete gamma function (page 68 in Bodenschatz (1992)). These two incomplete gamma functions cancel one another such that \( E[\varepsilon_{\text{ob}}^n] = N_i \).

### A.4 General Bin Projection Method

Bin microphysics models that use the microphysical method of moments (MMM) approach (Section 2.2 from Khain et al. 2015) predict either mass or mass and number for each mass bin. The size or mass distribution for each bin is generally approximated as a polynomial or linear function where the coefficients for each distribution is diagnosed through calculating integral moments. As an example for projecting bin distributions, we can use the linear distribution function given in Tzivion et al. (1987) as:

\[
n_i(m_i) = f_i \cdot \left( \frac{m_{i+1} - m}{m_i} \right) + \Psi_i \cdot \left( \frac{m - m_i}{m_i} \right), \quad m_i \leq m \leq m_{i+1} = pm_i, \quad (A.35)
\]
where \( f_i \) and \( \Psi_i \) are specified in Tzivion et al. (1987) as:

\[
f_i = 2 \frac{N_i}{m_i} \left( 2 - \frac{\bar{m}_i}{m_i} \right) \tag{A.36a}
\]

\[
\Psi_i = 2 \frac{N_i}{m_i} \left( \frac{\bar{m}_i}{m_i} - 1 \right) \tag{A.36b}
\]

and \( p = 2, 2^{1/2}, 2^{1/3}, \ldots \) dictates the bin scaling. Rearranging Equation (A.35) yields the concise form:

\[
n_i(m) = c_{i,1} + c_{i,2} m = \sum_{j=1}^{2} c_{i,j} m^{j-1} \quad m_i \leq m \leq p m_i, \tag{A.37}
\]

where \( c_{i,1} = p f_i - \Psi_i \) and \( c_{i,2} = \frac{1}{m_i} (\Psi_i - f_i) \). If we perform a transformation of variables for \( m \mapsto \varepsilon_{\text{ob}} \) or \( m \mapsto \varepsilon'_{\text{pro}} \), then we can follow the same procedure as in Section 3.4 for calculating bulk projections for each bin. Projected distributions for both oblate and prolate particles for all bins are therefore given by:

\[
n(\varepsilon_{\text{proj}}) = \frac{1}{C} \sum_{i=1}^{n_{\text{bins}}} \sum_{j=1}^{2} c_{i,j} g_{i,j} \tag{A.38a}
\]

\[
n(\varepsilon'_{\text{proj}}) = \frac{1}{C'} \sum_{i=1}^{n_{\text{bins}}} \sum_{j=1}^{2} c'_{i,j} g'_{i,j} \tag{A.38b}
\]

where \( C \) and \( C' \) are normalization constants and

\[
g_{i,j} = \int_{\varepsilon_{\text{ob},i+1}}^{\varepsilon_{\text{ob},i+1}} (1 - \varepsilon_{\text{ob}}^2)^{r_j} \left( 1 - \frac{\varepsilon_{\text{proj}}^2}{\varepsilon_{\text{ob}}^2} \right)^{-\frac{1}{2}} \tilde{n}_i(\beta) \, d\varepsilon_{\text{ob}} \tag{A.39a}
\]

\[
g'_{i,j} = \int_{\varepsilon'_{\text{pro},i+1}}^{\varepsilon'_{\text{pro},i+1}} (1 - \varepsilon'_{\text{pro}}^2)^{r'_j} \left( 1 - \frac{\varepsilon'_{\text{proj}}^2}{\varepsilon'_{\text{pro}}^2} \right)^{-\frac{1}{2}} \tilde{n}_i(\beta) \, d\varepsilon'_{\text{pro}}. \tag{A.39b}
\]
Appendix B

H-function Evaluation and Applications

B.1 Series Evaluation of the H-function

The general approach for evaluating the H-function is to sum a finite number of the gamma function pole residues. The following is the formulation of Cook (1981) who developed a Fortran program for evaluating the H-function.

Assume \( r_k = 1, 2, 3, \ldots \) represents the order of each pole \( s_k \) for \( k = 1, 2, 3, \ldots \) NP where NP is the total number of evaluated poles. Similarly, assume \( r_{dk} \) is the number of singularities for \( s = s_k \) in the denominator of the H-function integrand. The evaluation of LHP is

\[
H(z) = \sum_k \frac{V^{(r_k-1)}(s_k)}{(r_k-1)!}, \tag{B.1}
\]

where

\[
r_k = 1: \quad V^{(0)}(s_k) = \prod_{i=1}^{p+q+1} f_i(s_k) = z^{-s_k} \frac{\prod_{i=1}^{m+n} F_i(s_k)}{\prod_{i=m+n+1}^{p+q} F_i(s_k)} \tag{B.2}
\]

\[
r_k = 2: \quad V^{(1)}(s_k) = V^{(0)}(s_k) \cdot W^{(0)}(s_k)
\]

\[
= V^{(0)}(s_k) \left[ \sum_{i=1}^{m+n} G_i^{(0)}(s_k) - \sum_{i=m+n+1}^{p+q} G_i^{(0)}(s_k) \right] \quad \tag{B.3}
\]

\[
r_k > 2: \quad V^{(r)}(s_k) = \sum_{r=0}^{t-1} \binom{t-1}{r} V^{(t-1-r)}(s_k) \cdot W^{(r)}(s_k) \tag{B.4}
\]
\[ W^{(r)}(s_k) = \sum_{i=1}^{m+n} G_i^{(r)}(s_k) - \sum_{i=m+n+1}^{p+q} G_i^{(r)}(s_k) \tag{B.5} \]

\[ F_i(s_k) = \begin{cases} \Gamma (c_i + d_i s_k), & \text{if } I_i = 0 \\ \left[ d_i (-1)^{J_{ik}} J_{ik}^{-1} \right], & \text{if } I_i = 1. \end{cases} \tag{B.6} \]

\[ G_i^{(0)}(s_k) = \begin{cases} d_i \psi (c_i + d_i s_k), & \text{if } I_i = 0 \\ d_i \psi (J_{ik} + 1), & \text{if } I_i = 1. \end{cases} \tag{B.7} \]

\[ G_i^{(r)}(s_k) = \begin{cases} d_i^{r+1} \psi^{(r)}(c_i + d_i s_k), & \text{if } I_i = 0 \\ d_i^{r+1} \left\{ \psi^{(r)}(1) + (-1)^r \left[ \psi^{(r)}(J_{ik} + 1) - \psi^{(r)}(1) \right] \right\}, & \text{if } I_i = 1. \end{cases} \tag{B.8} \]

\[ I_i = \begin{cases} 0, & c_i + d_i s_k \in \mathbb{Z}^+ \\ 1, & c_i + d_i s_k = -J_{ik} \in \mathbb{Z}^- \end{cases} \tag{B.9} \]

The above equations can be used to evaluate either LHP or RHP. When evaluating RHP, the negative of the final result is taken.

**B.2 Incomplete Moments of the H-function distribution**

Integration of the H-function over a finite interval \(0 < a < b < \infty\) can be achieved using the approach of Marichev (1983). To do this, multiple Heaviside functions are used as multipliers in the H-function integral. The general result of this method is that definite moments of the H-function can be represented using a bivariate H-function. Alternatively,
the definite integral can be separated into two piecewise components

\[ E_t[x'] = \int_{x=x_{\min}}^{x_{\max}} x' H(x) \, dx \]

\[ = \int_{x=x_{\min}}^{\infty} x' H(x) \, dx - \int_{x=x_{\max}}^{\infty} x' H(x) \, dx. \]  

(B.10)

where \( R(x) \equiv x\theta(x) \) is the ramp function. Both integrals in Equation (B.10) can be represented in terms of H-functions using the Mellin convolution method and images given in Marichev (1983).

\[ E_t[x'] = H_{x_{\min}} - H_{x_{\max}}, \]  

(B.11)

where

\[ H_{r}(z) = H_{p+1,q+1}^{m+1,n} \left[ \begin{array}{c} (a_1,A_1) \\ (a_2,A_2) \\ \vdots \\ (a_p,A_p) \\ (r+1,1) \\ (b_1,B_1) \\ (b_2,B_2) \\ \vdots \\ (b_q,B_q) \end{array} \right]. \]  

(B.12)

For instance, the upper incomplete gamma function can be recovered if \( H(x) \) is represented by a 3-parameter gamma distribution, \( r = 0 \) and \( x_{\max} \to \infty \)

\[ \frac{E_t(x'^0)}{E(x'^0)} = \int_{x_{\min}}^{\infty} R \left( 1 - \frac{x_{\min}}{x} \cdot \frac{x_n}{x} \right) \left( \frac{x}{x_n} \right)^0 \left( \frac{x_{\min}}{x_n} \right)^{v-1} \exp \left( -\frac{x}{x_n} \right) d \left( \frac{x}{x_n} \right) \]

\[ = H_{1,2}^{2,0} \left[ \begin{array}{c} \frac{x_{\min}}{x_n} \\ (1,1) \\ (0,1) \end{array} \right] \]  

(B.13)

\[ = \Gamma \left( v, \frac{x_{\min}}{x_n} \right). \]
B.3 A General Approximate Analytical Solution to the Kinetic Collection Equation using the Hydrodynamic Kernel

The analytical solution technique used by Verlinde et al. (1990) can be generalized for all integer moments (i.e. Equation 3.1 in Drake 1972) if the number distribution functions of both collecting species are assumed to be H-functions. In fact, the solution given by Verlinde et al. (1990) represents a series of H-functions that are reduced to G-functions using properties of the gamma function and then to a series of generalized hypergeometric functions using Slater’s theorem (although Verlinde et al. (1990) does not mention either H- or G-functions in their explanation). Here, we derive the full analytical solution for arbitrary H-function number distributions.

The total set of kinetic collection equations is given in Drake (1972) as

\[
\frac{dM_0}{dt} = \frac{1}{2} \int_{x=0}^{\infty} \int_{y=0}^{\infty} K(x,y)n(x)n(y) dy dx
\]

\[
\frac{dM_1}{dt} = 0
\]

\[
r = 2, 3, 4 \ldots \frac{dM_r}{dt} = \frac{1}{2} \int_{x=0}^{\infty} \int_{y=0}^{\infty} [(x+y)^r - x^r - y^r] K(x,y)n(x)n(y) dy dx
\]

\[
= \frac{1}{2} \sum_{j=1}^{r-1} \binom{r}{j} \int_{x=0}^{\infty} \int_{y=0}^{\infty} x^j y^{r-j} K(x,y)n(x)n(y) dy dx.
\]

The hydrodynamic kernel can be simplified as follows:
Using Equation (B.15) in Equation (B.14c) yields

\[
\frac{dM_r}{dt} = \frac{\pi}{8} \sum_{k=0}^{2r} \sum_{j=1}^{r-1} \left( \binom{2}{r} \binom{2-k}{k} \alpha_x^{2-k} \alpha_y^{-k} \right) \int_{x=0}^{\infty} \int_{y=0}^{\infty} \alpha_y^{2-k} \alpha_x^{-k} \alpha_y^{-k} \left( \alpha_x^{-\frac{1}{2k}} x^{\frac{1}{2k}} + \alpha_y^{-\frac{1}{2k}} y^{\frac{1}{2k}} \right)^2 |\alpha_x^{\beta_{x}} - \alpha_y^{\beta_{y}}| n(x) n(y) dy dx
\]

\[
= \frac{\pi}{8} \frac{\alpha_v}{\alpha_v} \sum_{k=0}^{2r} \sum_{j=1}^{r-1} \left( \binom{2}{r} \binom{2-k}{k} \alpha_x^{2-k} \alpha_y^{-k} \right) \int_{x=0}^{\infty} \int_{y=0}^{\infty} \alpha_y^{2-k} \alpha_x^{-k} \alpha_y^{-k} \left( \alpha_x^{-\frac{1}{2k}} x^{\frac{1}{2k}} + \alpha_y^{-\frac{1}{2k}} y^{\frac{1}{2k}} \right)^2 |\alpha_x^{\beta_{x}} - \alpha_y^{\beta_{y}}| n(x) n(y) dy dx
\]

\[
= \frac{\pi}{8} \frac{\alpha_v}{\alpha_v} \sum_{k=0}^{2r} \sum_{j=1}^{r-1} \left( \binom{2}{r} \binom{2-k}{k} \alpha_x^{2-k} \alpha_y^{-k} \right) \int_{x=0}^{\infty} \int_{y=0}^{\infty} \alpha_y^{2-k} \alpha_x^{-k} \alpha_y^{-k} \left( \alpha_x^{-\frac{1}{2k}} x^{\frac{1}{2k}} + \alpha_y^{-\frac{1}{2k}} y^{\frac{1}{2k}} \right)^2 |\alpha_x^{\beta_{x}} - \alpha_y^{\beta_{y}}| n(x) n(y) dy dx
\]

\[
= \frac{\pi}{8} \frac{\alpha_v}{\alpha_v} \sum_{k=0}^{2r} \sum_{j=1}^{r-1} \left( \binom{2}{r} \binom{2-k}{k} \alpha_x^{2-k} \alpha_y^{-k} \right) \int_{x=0}^{\infty} \int_{y=0}^{\infty} \alpha_y^{2-k} \alpha_x^{-k} \alpha_y^{-k} \left( \alpha_x^{-\frac{1}{2k}} x^{\frac{1}{2k}} + \alpha_y^{-\frac{1}{2k}} y^{\frac{1}{2k}} \right)^2 |\alpha_x^{\beta_{x}} - \alpha_y^{\beta_{y}}| n(x) n(y) dy dx.
\]

(B.16)

We now use the method of Verlinde et al. (1990) where we expand the integral in \( J_\ast \) by finding the mass at which particle fallspeeds are the same. This occurs when

\[
v_t = v_y \quad \Rightarrow \quad L_{xy} = f_{xy} g_{xy},
\]

where \( f_{xy} \equiv \left( \frac{\alpha_x}{\alpha_y} \right)^{1/p_{xy}} \) and \( g_{xy} \equiv \frac{\beta_{xy}}{2k} \).
Substituting Equation (B.17) in $J_{yx}(y,x)$ and splitting the second integral into two positive intervals gives

$$J_\ast(x) \equiv \int_{y=0}^{\infty} J_{yx}(y,x) \, dy = \int_{y=0}^{L_{xy}} J_{yx}(y,x) \, dy - \int_{y=L_{xy}}^{\infty} J_{yx}(y,x) \, dy$$

$$= \int_{y=0}^{L_{xy}} y^{-j + \frac{k}{\beta_{vy}}} \left[ 1 - \left( \frac{y}{L_{xy}} \right) ^{\beta_{vy}} \right] n(y) \, dy + \int_{y=L_{xy}}^{\infty} y^{-j + \frac{k}{\beta_{vy}}} \left[ \left( \frac{y}{L_{xy}} \right) ^{\beta_{vy}} - 1 \right] n(y) \, dy. \tag{B.18}$$

Both terms on the right hand side of Equation (B.18) can be represented as H-functions if Equation (B.18) is put in the form a Mellin convolution of the fallspeed term and the distribution function like in Equation 1.1 from Marichev (1983). A simple way to do this is with the substitution: $y_\ast \equiv \frac{L_{xy}}{y}$. Substituting this new variable into Equation (B.18) and performing some algebra gives the following Mellin convolution integrals

$$J_\ast(x) = \ldots$$

$$L_{xy}^{\beta_{vy}} \left\{ \int_{y_\ast=1}^{\infty} y_\ast^{-\beta_{vy} - \beta_{vy} \left( y_\ast - 1 \right)} n \left( \frac{L_{xy}}{y_\ast} \right) \frac{dy_\ast}{y_\ast} + \int_{y_\ast=0}^{1} y_\ast^{-\beta_{vy} - \beta_{vy} \left( 1 - y_\ast \right)} n \left( \frac{L_{xy}}{y_\ast} \right) \frac{dy_\ast}{y_\ast} \right\}, \tag{B.19}$$

where $\beta_{vy} \equiv r - j + \frac{k}{\beta_{vy}} + 1$. The nice aspect of these integrals is that the distribution function $n_\ast$ has the same form for each integral whereas the fallspeed term flips LHP to RHP and vice versa. The H-function representation for each integral can therefore be derived from multiplying the images of each function. The images for each fallspeed terms are given in 2(3) and 2(6) in Marichev (1983) whereas the image of each distribution function is given in section 2. Alternatively, notice that each integral represents Euler transforms of the H-function which are given in Mathai et al. (2010) equations 2.53 and 2.54. Therefore, $J_\ast(x)$ can be evaluated as

$$J_\ast(x) = \frac{k_{vy} L_{xy}^{\beta_{vy} \ast}}{\beta_{vy} \ast} \sum_{i=0}^{1} H_{p_{vy}+1,q_{vy}+1}^{m_{vy}+i,n_{vy}+1-i} \left[ c_{vy} L_{xy}(x) \left( a_{vy} p_{vy}^{q_{vy}} B_{vy}^{q_{vy}+1} \right) \right]. \tag{B.20}$$
where

\[
\begin{align*}
i = 0 &: \quad (a_{yp0}, A_{yp0}) = \left( 1 - \frac{\beta_{xs}}{\beta_{vy}}, \frac{1}{\beta_{vy}} \right) (a_{yp}, A_{yp}) \\
&\quad (b_{yq0}, B_{yq0}) = (b_{yq}, B_{yq}) \left( -1 - \frac{\beta_{xs}}{\beta_{vy}}, \frac{1}{\beta_{vy}} \right) \\
\end{align*}
\]

(B.21a)

\[
\begin{align*}
i = 1 &: \quad (a_{yp1}, A_{yp1}) = (a_{yp}, A_{yp}) \left( 1 - \frac{\beta_{xs}}{\beta_{vy}} \right) \\
&\quad (b_{yq1}, B_{yq1}) = \left( -1 - \frac{\beta_{xs}}{\beta_{vy}}, \frac{1}{\beta_{vy}} \right) (b_{yq}, B_{yq}) \\
\end{align*}
\]

(B.21b)

Putting Equation (B.20) in Equation (B.16) gives

\[
\begin{align*}
\frac{dM_r}{dt} &= \frac{\pi}{8} \alpha_{vy} k_x k_y f_{xy} \cdots \\
&\quad \left( \frac{2}{r} \right) \left( \frac{2}{k} \right) \alpha_x^{2-k} \alpha_y^{-k} \int_0^\infty x^{\beta_x-1} H_x\left(c_x x\right) H_{p+y+1,q+y+1}^{m+y+i,n+y+1-i} \left( c_y f_{xy} x^{q_y} \right) dx, \\
\end{align*}
\]

(B.22)

where \( \beta_{xs} = \frac{2-k}{\beta_x} + \beta_{vx} + 2 + j + g_{xy} \). The form of the integral in Equation (B.22) is also a Mellin convolution of two H-functions which can be represented as a single H-function (see section 2.3 in Mathai et al. 2010). This puts the hydrodynamic kernel kinetic collection equation into a final form

\[
\frac{dM_r}{dt} = \frac{\pi}{8} \alpha_{vy} k_x k_y f_{xy} \sum_{k=0}^2 \sum_{j=0}^1 \left( \frac{2}{r} \right) \left( \frac{2}{k} \right) \alpha_x^{2-k} \alpha_y^{-k} c_x^{-\beta_x} H_{p+y,q+y}^{m+y,n+y} \left( c_y f_{xy} x^{q_y} \right), \\
\]

(B.23)

where \( m_{yx} = m_x + n_x + i, n_{yx} = n_y + m_x + 1 - i, p_{yx} = p_y + q_x + 1, q_{yx} = q_y + p_x + 1 \), and

\[
\begin{align*}
H\left(c_y f_{xy} x^{-q_y}\right) &= H_{p+y,q+y}^{m+y,n+y} \left[ c_y f_{xy} x^{-q_y} \right] \\
&\quad (1 - b_{yx} - B_y, g_{xy}, B_{yq}) \left( a_{yp}, A_{yp} \right) \\
&\quad (b_{ym}, B_{ym}) \left( 1 - a_{xp} - B_x, g_{xy}, A_{xp} \right) \left( b_{ym+1}, B_{ym+1} \right) \cdots \left( b_{yq}, B_{yq} \right), \\
\end{align*}
\]

(B.24)
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