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Modeling Snow Aggregates and Their Single Scattering Properties: Implications to Snowfall Remote Sensing

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MODELING SNOW AGGREGATES AND THEIR SINGLE SCATTERING PROPERTIES: IMPLICATIONS TO SNOWFALL REMOTE SENSING

By

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ABSTRACT

Ice and snow particles have a great, yet poorly understood impact on the Earth's climate system. One of the difficulties of studying snow particles is their irregular shape. While spheres and even oblate spheroids backscatter radiation in a consistent manner, irregularly shaped objects do not. Due to the complexities of snowflakes, they are often assumed to be spherical for both satellite retrieval and modeling purposes. This can introduce error in many studies.

While there are several aggregate snowflake models in existence, many use spheres as a building block for the snowflake. This is inaccurate as most snowflakes are comprised of a combination of bullet rosettes, plates, columns, and dendritic snow crystals. Furthermore, most studies do not have constraints in place to make sure that snowflakes are of the correct size and density as observed from field studies. None of the theoretical models examined in this study analyze the single-scattering properties of the flakes.

In order to improve upon previous models, this study creates an aggregate snowflake using 200 μm and 400 μm 6-bullet rosette crystals. These crystals and resultant flakes are required to follow established size-density relationships obtained from numerous field studies. In addition, the flakes must also be of similar fractal dimension determined from other case studies. The single-scattering properties of these flakes are then determined from the discrete dipole approximation.
CHAPTER 1

INTRODUCTION

1.1 Importance of Research

Even with the technological advances over the last decade or so, there is much that is unknown about the Earth's climate system. Clouds, and their resultant precipitation, have appreciable impacts on the Earth's hydrologic cycle and radiative budget (Liou, 1986; Liu, 2008b). For instance, cloud ice and snow are more reflective of short-wave radiation and can act as an insulator of long-wave radiation both aloft and on the ground (Seo and Liu, 2005). While cloud radars on the ground can provide reflectivity data, the sparse ground coverage these radars have make them undesirable for use in numerical weather prediction (NWP) models or global circulation models (GCM) (Seo and Liu, 2005). NASA's CloudSat satellite, launched in 2006, is a better source for model input data as it provides frequent measurements over a wider area than the ground-based radars. CloudSat's Cloud Profiling Radar (CPR) operates at a frequency of 94-GHz and provides information of both the vertical structure of a cloud and its precipitation (CIRA, 2008).

Radar backscatter ($\sigma_{\text{bsc}}$) can be obtained by the CPR, which is used in determining an equivalent radar reflectivity versus snowfall rate ($Z_e$-S) (Liu, 2008b). This is akin to the Z-R relationship based on Marshall-Palmer (1948) size distribution for rainfall, although studies in relation to snowfall rate are fewer than those for rainfall (Sekhon and Srivastava, 1970). $Z$ (the radar reflectivity) is valid only when the drop size is smaller than the radar wavelength allowing for the application of Rayleigh theory for scattering (Nakamura and Inomata, 1991). When the radar wavelength is approximately the same size as the diameter of the target, as it is in the microwave region, scattering differs from Rayleigh theory. $Z_e$ (the equivalent radar reflectivity) is used in these cases as the scattering is much more complicated. The differences between $Z$ and $Z_e$ are further discussed in Chapter 2.3. Because $Z_e$ is used throughout this work, it will simply be referred to as the radar reflectivity.

Furthermore, $Z_e$-S relationships are less accurate than Z-R relationships due to the complexities of the snowflake shapes, densities and terminal fall velocities (Noh et al., 2006; Ishimoto, 2008). Determining the $Z_e$-S and Z-R relationships require knowledge of single-
scattering properties, such as the scattering cross-sections and phase function of the particles (Liu, 2008a and b).

In an effort to simplify these complexities, snowflakes are modeled as spheres or oblate spheroids (Maruyama and Fujiyoshi, 2005) despite in-situ ground studies suggesting that snowflakes are aggregates composed of many individual crystals (Brandes et al., 2007). The complex snowflake and crystal shapes make the determination of the single scattering properties difficult and cumbersome. In this study, a model is created that randomly generates aggregate snowflakes without modeling them as spheres or oblate spheroids. The single scattering properties are determined and a $Z_c$-S relationship is derived from the backscatter cross-section. These properties are crucial for radiative transfer modeling and satellite retrieval algorithms, although this is not examined here. This work is mainly concerned with the first step of generating more “realistic” flakes from which the scattering cross-sections can be determined and be available for future radiative transfer and retrieval work.

### 1.2 Previous Research

Liu (2004; 2008a and b) created a database of single-scattering properties in the microwave spectrum for several types of non-spherical ice crystal particles. Liu examined several different methods for calculating the scattering properties including the T-matrix method (Mishchenko and Travis, 1998), the finite-difference time domain method (Taflove, 1995; Yang and Liou, 1996, 1998) and the discrete dipole approximation (DDA) (Draine and Flatau, 1994). DDA is used in his database due to its flexibility to model irregularly shaped snowflakes without the added constraint in the T-matrix method imposes on the flake be rotationally symmetric and an aggregate of spheres (Liu, 2004; 2008a). This database does include dendritic snowflakes, but it does not include irregularly shaped aggregates.

In order to determine the scattering properties of snowflakes, aggregate snowflakes must be generated. Several different methods to generate these flakes have been attempted including a fractal method (Ishimoto, 2008) and a Monte Carlo method (Maruyama and Fujiyoshi, 2005). Both ways can include many different variables such as collision efficiencies, rotation and terminal velocity of constituent particles, but both use highly idealized flakes and do not calculate backscatter.
1.3 Objectives and Paper Organization

The intent of this study is to: 1) Create an aggregate snowflake generation program with snowflakes of adequate size and density; 2) Obtain and analyze the radar scattering cross-sections; 3) Determine a $Z_e$-S relationship. The background information is discussed in Chapter 2, while Chapter 3 discusses the generation of aggregate snowflakes employed in this study. Chapter 4 is a discussion of the single scattering properties determined from the generated flakes, including a $Z_e$-S relationship, with Chapter 5 being the conclusion.
CHAPTER 2

BACKGROUND

2.1 Snowflakes

While numerous studies and observations exist about the shape of snowflakes and how they are formed, their impacts on meteorological Earth processes are areas of ongoing research. Snowflakes and ice crystals are important elements in climate research for several reasons. Their presence in clouds, particularly cirrus and other high-level clouds, have important impacts on the Earth's radiation budget and hydrologic cycle (Liou, 1986; Stephens et al., 1990; Lynch et al., 2002; Liu, 2008b). Furthermore, snow on the ground not only cools daytime surface temperatures and increases the amount of shortwave radiation reflected from the Earth's surface (Strack et al., 2003), but it can have significant impact in the day-to-day life and be quite costly for areas experiencing heavy snowfall as ground conditions in these events are often quite poor and can have a costly impact on society (Lawson et al., 1998).

While ice crystals and snowflakes are parameterized in climate models in a variety of ways to simulate their impacts, the modeling is inadequate at best. Ice cloud processes, which can mark the beginning of snowfall formation, often introduce major uncertainty into GCMs (Heymsfield and Iaquinta, 2000). In order to improve forecasts, there must be a better understanding of the microphysical properties of ice crystals to not only improve the radiation budget modeling, but to improve retrieval techniques of cloud properties from satellite and ground sensors (Heymsfield and Miloshevich, 2003). Observations of particles and their resultant size distributions allow for improved microphysical parameterizations in NWP models which can produce better winter precipitation forecasts (Brandes et al., 2007). The following sections in this chapter detail the formation of snowflakes and crystals, the attempts to model snowflakes, and complications that arise from modeling and remote sensing of these objects.

2.1.1 Formation

Ice crystals are formed typically at the top of clouds. This temperature is cold enough to freeze liquid water or for water vapor to freeze to some kind of “seed” particle such as an ice
particle, dust, plant particulate matter or other aerosols. Jiusto (1973) identified three efficient nucleation conditions for generating ice crystals. The first method is for large ice particles to act as condensation nuclei. Ice crystals may form on the nuclei by condensation and crystallization processes. This means that after latent heat is released from the condensation of the water vapor to the seed particle, freezing will occur making the particle crystalline (Gravner and Griffeath, 2008).

In the second method, crystal formation occurs via thermophoretic or Brownian deposition providing that the particle is large enough for these mechanisms. Brownian deposition occurs when there is a colder particle, for example an ice particle, that creates a temperature gradient with the surrounding environment. This particle is referred to as the Brownian particle. Smaller, turbulent particles moving in this environment will move down gradient towards the colder particle where it can collide and/or join with the initial Brownian particle. The movement opposite of the temperature gradient is called thermophoretic movement.

In the third method, ice nuclei already encased in a water that have not yet reached their activation potential, or the temperature at which they freeze, may do so when they ascend to a colder environment. More water can condense around the newly formed particles, but usually the water in the cloud evaporates due to the pressure gradient so initial growth is dominated by vapor diffusion. Vapor diffusion is dependent on humidity and temperature in the environment and typically crystal formation of this type peaks in supersaturated environments around -15º C (Pruppacher and Klett, 1978; Lawson et al., 1998; Gravner and Griffeath, 2008). Pure snow crystals tend to grow by vapor diffusion alone and have predictable dimensional relationship patterns (Pruppacher and Klett, 1997).

Hydrometeors (e.g., ice particles) exist in many different shapes and sizes and can be anything from a pristine crystal to an aggregate consisting of many different crystal types (Matrosov et al., 1996). Magono and Lee (1966) developed a widely used crystal classification scheme of around 80 different crystal types. Crystal types, or habits, are dependent upon the temperature and humidity of the location of formation. As a crystal moves from one area to another, the habit type changes and adapts to the new environment (Pruppacher and Klett, 1997). This means that a crystal can start out as a dendrite, but then be transported to an area where the environment favors columnar crystal development creating an ice crystal with a mixture of
dendritic and columnar features. This leads to ice clouds containing a mix of different ice crystal types.

There have been numerous studies into the distribution of different ice crystal habits throughout a cloud layer in an effort to determine what environmental conditions are conducive to the growth of a certain crystal (Heysmfield et al., 2002; Field and Heymsfield, 2003; Woods et al., 2008). In Field and Heymsfield (2003), they analyzed data obtained data along a Lagrangian spiral descent from the Atmospheric Research Measurement (ARM) intensive observation period in Oklahoma on March 9, 2000. The flight started at -50º C (9,500 m) and descended to -28º C (6,600 m). Images from the cloud particle imager (CPI) aboard the aircraft revealed that most the ice particles larger than 100 μm were either bullet rosette crystals or aggregates of bullet rosettes. The CPI data is shown in Figure 1 with a characteristic bullet rosette image from the Magono and Lee classification in Figure 2. Bullet rosettes have between one to eight bullets and typically form in colder environments where temperatures are below -40º C (Heymsfield and Iaquinta, 2000; Heymsfield et al., 2002; Woods et al., 2008).

Using images from a Particle Measuring System (PMS) 2D-C imaging probe, Woods et al. (2008) found during the Improvement of Microphysical Parameterization through Observation Verification Experiment (IMPROVE) that bullet rosettes form below -40º C and sideplanes, sectors, bullets and their assemblages and aggregates below -18º C. In addition, data sets collected by M. Kajikawa at Mt. Hachimontai Observatory of Akita University showed that out of 45 different particle types observed in cirrus clouds, 39 of them were classifiable as bullet rosettes (Heymsfield et al., 2002). Magono and Lee (1966) wrote that bullets, along with plates, columns and needles, are the most common constituent in upper cirrus clouds with maximum dimensions usually larger than 10 μm yet no larger than 1 to 2 mm. Pruppacher and Klett (1997) found that bullet rosettes that typically form between -25º C to -60º C in cirrus clouds have a maximum dimension of 200 to 800 μm for a single crystal and 400 to 1,500 μm for an aggregate crystal. Since most researchers agree that bullet rosettes form in the cold upper regions of the atmosphere, authors such as Seo and Liu (2005) used bullet rosettes to mimic aggregates in ice clouds.
Figure 1. CPI images from March 9, 2000 ARM flight. Images are arranged in height with particle sizes less than 100 μm on the left, particles between 400 to 600 μm in the center and those 800 μm and above on the right (Field and Heymsfield, 2003).
Growth can continue through accretion of supercooled water droplets as long as favorable environmental conditions exist (Jiusto, 1973; Gravner and Grifféath, 2009) and the ice particle size distributions (PSD) are comprised of mostly smaller particles. As ice PSDs go from being mostly smaller to larger particles, the method of ice crystal growth also changes. Small ice crystals are grown by accretion while larger ice crystals are typically grown by aggregation with surrounding particles and crystals (Field and Heymsfield, 2003). Usually between the temperatures of -24°C and -7°C, aggregation is the primary growth mechanism for snow crystals (Woods et al., 2008). Numerous studies by Mitchell (1988, 1991, 1996) in which he developed an analytical-numerical 1D ice particle growth model with diffusional and aggregation particle growth, showed that very large snowflakes cannot be produced by diffusional growth alone (Lawson et al., 1998).

As ice particles grow and become heavier, they start to descend through the cloud and can ultimately reach the ground. Jiusto (1973) wrote of three different cloud systems that produce precipitation. The first system is a high-level cloud (e.g., cirrostratus or altostratus) that releases the crystals that can ultimately reach the ground. According to Heymsfield and Miloshevich (2003), during a highly active generation phase of cirrus clouds, the upper portion of the cloud can become highly supersaturated with respect to ice which results in an increase of ice nucleation and early particle development. This can lead to precipitation in support of Jiusto's theory. In the second case, the high level cloud can act as a seeder cloud to a lower level cloud (e.g., lower level stratus) producing precipitation. Third, there could be a shallow spender cloud (e.g., convective stratocumulus or cumulus) whose precipitation potential is not always released naturally but can be seeded from above.

When the particles are heavy enough to precipitate out of the cloud layer, they are usually irregularly shaped snowflakes created by the aggregation of ice crystals (Ishimoto, 2008). While snowflakes can be larger than several centimeters, most are no larger than 2 cm (Pruppacher and Klett, 1997). Large aggregate particles and heavy snowfall rates are typically seen at the surface.
in warmer temperatures. Heavy snowfalls of pristine ice crystals are not typically seen (Stewart, 1992; Lawson et al., 1998; Brandes et al., 2007; Brandes et al., 2008).

2.1.2 Previous Methods for Snowflake Generation

Snowflake shapes are often modeled as spheres or oblate spheroids to ease the complexity of calculations, despite the fact that they are typically aggregates of crystals. For improved accuracy in satellite remote sensing, it is important to model snowflakes as close to nature as possible. There are several existent techniques for generating aggregate snowflakes.

2.1.2.1 Fractal Method. Ishimoto (2008) explored modeling snowflakes as fractals, which are further explained in Section 3.2. Maruyama and Fujiyoshi (2005) concluded that when looking at detailed microphysics of the collision-coalescence process, the resultant flakes resembled fractals. Ishimoto determined the fractal dimension of particles by comparing the shape characteristics of different measured snowflakes. The fractal dimension \( d_f \) of large aggregate clusters is given by the equation \( m = l^{d_f} \) where \( m \) is the aggregate mass and \( l \) is the linear span. The variable \( d_f \) depends on the method of aggregation, given in the study as either diffusion-limited aggregation (DLA) or reaction-limited aggregation (RLA). In DLA, particles are given random walk trajectories where they move randomly each timestep and can form larger particles. In RLA, each crystal or crystal cluster has a “sticking probability” which depends on the mass of the clusters. If the “sticking probability” is not high, these particles simply won’t aggregate. Experimentally, \( d_f \) for DLA is 1.75 and for RLA is 2.07.

Specifically, the fractals are generated in the following manner. On a 3D grid space, two particles occupy neighboring points on the grid. The program then divides the grid space in half between the two particles and randomly places another particle in the newly created space that connects the original points. This process repeats for a given amount of iterations making sure that the points are joined together so no particles form separately. The number of lattice sites occupied in the grid can be written as \( N = \delta^4 \) where \( \delta \) is the grid interval. The illustration from Ishimoto is shown in Figure 3.

While this method does produce realistic looking snowflakes, it does not have constraints in place to ensure that these flakes follow an accurate size-density relationship. Several studies conducted on aggregate snowflakes have yielded a relationship between size of a flake and the predicted density. This relationship is discussed further in Section 3.3.
\[ d_f = 2.1 \quad N = 70240 \]

Figure 3. Sample of the generated snowflakes from Ishimoto (2008). \( d_f \) is the fractal dimension and \( N \) is the number of data points in the flake. The grid is 350 x 350 units for each figure.

2.1.2.2 Monte Carlo Method. Maruyama and Fujiyoshi (2005) combined an aggregation model with the Monte Carlo method to randomly generate snowflakes. This method assumes that all constituent particles are spheres with the same low density which is unrealistic in nature. The authors factored in horizontal and vertical velocity differences, coalescence efficiency, which itself is dependent on the snow particle's cross-section, temperature and vapor pressure over ice, and rotational speed into the aggregation model.

The method produced very good results, images of which are given in Figure 4. Maruyama and Fujiyoshi were concerned not only with generating a snowflake, but with generating an accurate particle size distribution for snowflake creation for the initial crystals as previously discussed. For this, they included an aggregation model into their generation method. This model calculated collision probabilities between particles, the likelihood of the colliding particles to coalesce and the mass and rotation of each particle. After each time step, all these variables were recalculated.

The use of spheres makes these flakes difficult to use in other analysis methods. For example, a particular software package that uses discrete dipole approximation to calculate the single scattering properties of the flakes, DDSCAT, cannot use these flakes because it cannot model the individual constituent particles as “low density” spheres. DDSCAT requires that each base particle be a point or be comprised of single points. Making each sphere a collection of many single points is much too intensive for analysis. The aggregation model is so computationally daunting that Maruyama and Fujiyoshi's Monte Carlo method cannot be used as an input into a forecast model.
Figure 4. Generated snowflake from the Maruyama and Fujiyoshi (2005) Monte Carlo method study. This 3D snowflake image has 1760 particles with: (a) top view, (b) front view, and (c) side view. An actual snowflake image is given in (d) where the two lines in the background are separated by 5 mm.

2.2 Scattering by Non-Spherical Particles

The aerial expanse and quick sampling time satellite detection can provide makes remote sensing of ice particles and snowflakes highly desirable for data collection. The problem, however, is that snowflakes tend to have complex shapes that do not behave in a straightforward manner. Knowing the single scattering properties of irregularly shaped particles allows for development of an algorithm that converts observed radar reflectivity to ice water amount or snowfall rate. Analyzing each particle is something that is computationally inefficient and cannot be done repeatedly for a retrieval algorithm, so Liu (2004) analyzed many different
particle shapes and sizes in order to develop a database of the single scattering properties of ice particles and snowflakes.

The backscattering cross-section is one of the single scattering properties of particular interest. The radar backscatter cross section is used to determine the radar reflectivity which can ultimately be used in a $Z_e$-S relationship to determine the snowfall rate (Liu, 2008b). This cross-section is highly dependent on shape and orientation of the particle in microwave frequencies (Ishimoto, 2008).

Back-scattered energy can be measured in microwave frequencies by radars on the current CloudSat satellite and the future Global Precipitation Measuring (GPM) satellite. CloudSat, launched in April 2006, has the Cloud Profiling Radar (CPR) operating at 94 GHz (CIRA, 2008) on which is the first active, space-borne sensor that can estimate both the horizontal and vertical snowfalls distributions in an area. Previous attempts at studying scattering properties of snowflakes and ice crystals at microwave frequencies have been divided into two methods (Liu, 2004). The first is to treat ice particles as easily defined geometric shapes, such as columns and bullet rosettes. The second is to approximate ice particles as spheres with the same mass and apply Lorenz-Mie theory. Rayleigh scattering is also used to study smaller particles in place of Mie scattering when the size parameter is sufficiently large. The size parameter is given as:

$$\chi = \frac{2\pi a}{\lambda} \quad (1)$$

where $a$ is the radius of the particle and $\lambda$ is the wavelength. For Rayleigh scattering, $\chi$ must be less than 0.2 and between 0.2 to 2000 for Mie scattering (Petty, 2006). Another criteria is when $D/\lambda < 0.1$ for Rayleigh and $0.1 < D/\lambda <$ for Mie scattering, where $D$ is the diameter of the particle.

### 2.2.1 Mie Scattering

Mie scattering is a mathematical solution that determines scattering characteristics of a sphere assuming the sphere has dielectric properties. Radiation comes from excited oscillating dipoles which can emit partial electric or magnetic waves (Stephens, 1994). The backscatter Mie solution is an infinite series of sums that converge to a value dependent on $\chi$ and is determined by the equation:
\[\sigma_{bsc} = \frac{\pi a^2}{\lambda^2} \left| \sum_{n=1}^{\infty} (-1)^n (2n+1)(a_n - b_n) \right|^2 \]  

(2)

where \(a_n\) refers to the scattering arising from induced magnetic dipoles and \(b_n\) is scattering from the electric dipoles.

While helping to account for larger snowflakes, the problem is aggregate flakes do not reflect radiation as neatly as spheres. There are many irregularities in the shape of aggregate flakes that Mie scattering theory simply cannot account for. Overall, this is not a good method for large particles that are clearly non-spherical.

2.2.2 Rayleigh scattering

Rayleigh scattering considers the target particle as a single, small sphere with a single oscillating dipole. For this type of scattering, the particle size is much less than the wavelength of the incoming radiation. It is typically used to describe the way long-wave radiation interacts with cloud droplets, raindrops and atmospheric aerosols (Stephens, 1994). The electric field of the excited drop stays constant due to the object’s small size (Stephens, 1994). The backscatter cross-section for Rayleigh scattering is given by the equation:

\[\sigma_{bsc} = \frac{\pi^3 |K|^2 D^6}{\lambda^4}\]  

(3)

where \(K\) is a function of complex index of refraction of the material.

The problem, however, is that large ice particles and snowflakes are typically at or around the same size as the measuring microwave wavelength. For example, the CPR has a wavelength of 3.2 mm which makes Rayleigh approximations of snowflakes by equal volume spheres highly inaccurate (Matrosov, 2007; Liu, 2008b). In addition, large, irregularly shaped ice particles have greater reflectivities and greater orientation dependencies than their equal spherical counterparts (Matrosov, 2007). This leads to questionable validity for estimating irregular snowflakes as spheres under Rayleigh scattering.

2.2.3 Methods for Studying Scattering

Since modeling snowflakes as spheres leads to questionable results, several different techniques have been developed to model scattering of irregular objects. Three different methods are used in particular and are described below. While each have their caveats, these
methods are more applicable to calculate scattering by irregular particles than the spherical scattering methods described above.

2.2.3.1 Finite Difference Time Domain (FDTD). The FDTD method was used by Ishimoto (2008) for irregularly shaped ice particles. FDTD can be used for any inhomogenous and anisotropic shaped particles. Specifically, this method solves Maxwell's curl equation in differential form with scattering properties derived from Fourier transformations of the electromagnetic waves in the computational field. This particular method eliminates the problem of solving many linear equations by using a time-iterative solution.

2.2.3.2 T-Matrix Method. This method is applicable to any shape, but it is more practical to certain revolutions of a body (Mischenko and Travis, 1998). In contrast to the FDTD method, this method solves the whole Maxwell equations, not just the curl equation leading to fairly exact results. T-matrix assumes that light is scattered by a single-volume element containing many randomly oriented, rotationally symmetric scattering particles that are described by the average extinction ($C_{ext}$) and scattering ($C_{sca}$) cross-sections and the dimensionless Stokes scattering matrix (Mischenko and Travis, 1998). The main drawback to this method is that it is only good for certain rotations, not all possible rotations.

2.2.3.3 Discrete Dipole Approximation (DDA) Method. Similar to those methods above, DDA is applicable to irregularly shaped particles, but does not have the bias towards certain revolutions like T-Matrix. DDA models approximate the target object as an array of polarizable points that are on a cubic lattice (e.g., 3D Cartesian grid space) (Liu, 2004). The polarizable points acquire dipole moments via their response to the local electric field (e.g., incoming electromagnetic wave) and the electric fields of surrounding points (Liu, 2004). This method requires that the spacing between dipoles must be sufficiently small compared to the interacting electromagnetic wavelength which can be determined from the following relationship:

$$|m|k \ d < 1$$

where $m$ is the complex index of refraction, $k$ is the angular wavenumber and $d$ is the dipole spacing (DDSCAT 7.0 User's Guide, 2008). Depending on the accuracy desired, the computation times can be quite long especially for larger particles with large grids.
2.3 $Z_e$-$S$ Relationship

Knowing the backscatter cross-section is necessary to determine a relationship between equivalent radar reflectivity and the liquid equivalent snowfall rate ($Z_e$ and $S$ respectively) if using remote sensing techniques. In addition, one must know the maximum dimension of the snowflake ($D$), particle size distribution ($N(D)$), the dielectric constant of liquid water at a given temperature ($K$), terminal velocity ($v_t$) and particle's mass ($m(D)$). The equations necessary to determine the $Z_e$-$S$ relationship are (Noh et al., 2006; Liu, 2008b):

\[ N(D) = N_0 \exp(-\Lambda D) \]  

(5)

\[ Z_e = \frac{\Lambda^4}{\pi^2 |K|^2} \int N(D) \sigma_{bsc}(D) dD \]  

(6)

\[ S = \int_D N(D) \frac{v(D)m(D)}{\rho_w} dD \]  

(7)

where $\Lambda$ is the slope and $N_0$ the zero intercept of the size distribution when plotted on a graph. Both $\Lambda$ and $N_0$ are functions of the snowfall rate (Noh et al., 2006). This differs from radar reflectivity ($Z$) given in Equation 8 (Nakamura and Inomata, 1991). When the wavelength of the radar is much larger than the diameter of the target object, scattering is defined by Rayleigh theory and Equation 8 may be used.

\[ Z = \int D^6 N(D) dD \]  

(8)

The high variability of particle shape, orientation and size distributions makes it difficult to determine an accurate $Z_e$-$S$ relationship. Size distributions are generally exponential in form where $\Lambda$ and $N_0$ can be determined from observations, such as those by Braham (1990) or from equation such as Sekhon and Srivastava (1970). In Braham's (1990) Table 4, he includes $\Lambda$ and $N_0$ values from several different observational studies. Liu (2008b) used this table, along with previous scattering studies (Liu, 2004) to determine other values in equations to derive a $Z_e$-$S$ relationship for rosettes, sectors and dendrites. His relationships are shown below in Figure 5 with $Z_e$ in mm$^6$m$^{-3}$ and $S$ in mm h$^{-1}$ which are the typical units.
2.4 Brightness Temperature

The intensity of scattered radiation is important for another variable: brightness temperature \( (T_B) \). According to Planck's function, there is a relationship between the intensity of emitted radiation from a blackbody and the blackbody's temperature. The Planck's function in terms of wavelength is:

\[
B_\lambda(T) = \frac{2hc^2}{\lambda^5 e^{\frac{(hc)}{k_B\lambda T}} - 1}
\]

where \( \lambda \) is the wavelength, \( h \) is Planck's constant, \( c \) is the speed of light, \( k_B \) is the Boltzmann's constant and \( T \) is the temperature of the blackbody or \( T_B \). To determine \( T_B \) from this equation, the Planck function is inversed:

\[
T_B = B_\lambda^{-1}(I_\lambda)
\]

For thermal IR wavelengths, the emissivity is close to one for most land and water surfaces. This means that \( T_B \) would be close to the actual surface temperature of these surfaces. In the microwave region, however, emissivity is usually less than one leading to \( T_B \)s that are less than the actual surface temperature (Petty, 2006). Despite this, \( T_B \) is still useful in the
microwave region for radiative transfer calculations in place of intensity as the intensity and temperature are proportional to one another.

As mentioned earlier, snowflakes are often treated as spheres in radiative transfer models and doing such results in imprecise radiation simulations. Benjamin Johnson, a researcher at NASA’s Goddard Space Flight Center, examined the $T_B$ differences between an aggregate snowflakes comprised of 5 and 10 dendritic snow crystals and equivalent volume spheres at a frequency of 89 GHz. $T_s$ differed by up to 12 K when the aggregate 5 and 10 dendritic snowflakes were compared to equivalent volume spheres. When the $T_{B,s}$ for the 5 and 10 dendritic crystal aggregates were compared against each other, the $T_B$ differences were around 3 K as shown in Figure 6 (Johnson, 2009). This difference would have a significant impact on any subsequent radiative transfer modeling.

![Figure 6](image)

Figure 6. $T_B$ differences at 89 GHz for equal-volume objects of different shapes (Johnson, 2009).
2.5 Chapter Summary

The parameterization of aggregate snowflakes as spheres, while they are actually aggregates comprised of many different crystals, can lead to many complications (Liu, 2004; Ishimoto, 2008). Bullet rosettes are commonly seen in cold, high level clouds and have been used by authors such as Seo and Liu (2005) to mimic aggregates. While there are many different methods to simulate the single scattering properties of irregularly shaped objects, DDA does not have the constraints and as much inaccuracies as the FDTD and the T-Matrix methods (Mischenko and Travis, 1998; Liu, 2004; Ishimoto, 2008). Single scattering properties can lead to better Z_e-S relationships and T_B calculations (Liu, 2008a and b; personal correspondence with Benjamin Johnson).
CHAPTER 3

GENERATION OF SNOWFLAKES

3.1 Generation Method

For this study, a new snowflake generation method is created. This model improves on previous studies as it has several different quality checks to ensure realistic results. As described in Chapter 2, many authors have found that bullet rosettes are the predominate crystal type in colder, upper layer cloud tops. This study's program generated aggregate snowflakes comprised of 6-bullet rosette crystals since this crystal type would be the starting component for snowflake formation in upper cloud layers. In the method, it is made sure that the particle size-density relationship and particle's fractal dimension follow what have been observed in field experiments.

3.1.1 Determination of rosette characteristics

The basic elements of snowflake aggregates are assumed to be 6-bullet rosettes in this study. In upper level cirrus clouds, bullet rosettes tend to have maximum dimensions between 200 to 800 μm (Pruppacher and Klett, 1997) and follow a range of size-density relationships whereby one can determine the density based off the snowflakes' maximum dimension. Due to the irregular shape of most aggregates, the radius or maximum diameter for the snowflake is defined as the minimum radius or diameter of a sphere that would encapsulate the flake. The density, however, is not the density of a solid sphere of ice, but rather a ratio of the solid ice rosette to the void space in the sphere. For the initial building of the flake, the starting components must be realistic; this is something that the previous studies by Ishimoto (2008) and Maruyama and Fujiyoshi (2005) did not do. The following method is devised to calculate the density of a solid ice rosette to determine what size(s) of bullet rosette to use in our model.

The 6-bullet rosette is thought to be made of equal sized cubes. For example, the volume of a single cube and the sphere surrounding that cube can be determined the following way:
In Figure 7, \( a \) is half the length of a cube face, \( x \) is the diagonal from the center of a cube face to a corner of the same cube face, and \( r \) is the length from the center to a corner of the cube. The equations for the length of \( x \) and \( r \) in terms of \( a \) are:

\[
x = \sqrt{2} a
\]

\[
r = \sqrt{a^2 + 2a^2} = \sqrt{3a^2} = \sqrt{3} a
\]

The volume of the cube and that of the surrounding sphere are:

\[
V_{\text{cube}} = 8a^3
\]

\[
V_{\text{sphere}} = \frac{4}{3} \pi (\sqrt{3} a)^3
\]

Dividing Equation 13 by 14 and multiplying by the density of ice, the density of the bullet rosette is determined.

\[
\rho_{\text{cube}} = \frac{6}{\pi^{3/2}} \cdot 0.916 \text{ g cm}^{-3}
\]
Here, the letter \( n \) represents the number of cubes in the column.

The equations associated with Figure 8 for a column are:

\[
x = \sqrt{(n^2 + 1)a^2} 
\]

\[
r = \sqrt{(n^2 + 2)a^2} 
\]

\[
V_{\text{column}} = (n)8a^3 
\]

\[
V_{\text{sphere}} = \frac{4}{3}\pi[(n^2 + 2)a^2]^{3/2} 
\]

\[
\rho_{\text{column}} = \frac{6n}{\pi(n^2 + 2)^{3/2} \cdot 0.916 \ g \ cm^{-3}} 
\]

The density for a rosette comprised of 3 columns perpendicular to each other and all sharing a center cube can now be determined. The image of the rosette is given in Figure 9. This figure represents a symmetric, 6-bullet rosette crystal and is used as the basic building block of the snowflake generation program.
The variables $a$, $x$, $r$, and $n$ are defined the same way as in the column case, but the equations for the volume of the rosette and sphere, as well as the density differ. They are given by:

\[ V_{\text{rosette}} = (3n - 2)8a^3 \]  
\[ V_{\text{sphere}} = \frac{4}{3} \pi [(n^2 + 2)a^2]^{3/2} \]  
\[ \rho_{\text{rosette}} = \frac{6(3n - 2)}{\pi (n^2 + 2)^{3/2}} \cdot 0.916 \text{ g cm}^{-3} \]

The density of any rosette with $n$ number of blocks per column, assuming the blocks are an odd number thereby representing a symmetric rosette, can be calculated. The density of rosettes with $n = 3, 5, 7$ and $9$ are 0.336 g cm$^{-3}$, 0.162 g cm$^{-3}$, 0.0913 g cm$^{-3}$ and 0.058 g cm$^{-3}$ respectively. Figure 10 is a plot of these densities along with a size-density relationship for rosettes sampled in clouds from Heymsfield et al. (2002), given as Equation 24, determined from examining all the 5-bullet rosettes from a case study. While not a 6-bullet rosette, the size-
density relationship is not exact and can be extended in this study to a 6-bullet rosette. The density relationship is given as:

$$\rho_e = 0.0265D^{-0.46}$$  \hspace{1cm} (24)

where D is the diameter of the rosette in cm and density is g cm$^{-3}$.

As seen in Figure 10, from the density calculation in Equation 24, 200 μm and 400 μm rosettes satisfy both the theoretical density of a rosette in this study and the density determined from Heymsfield et al. (2002). The 200 μm rosette corresponds to each column being 5 units long with the 400 μm rosette being 7 units long. For the 200 μm and 400 μm rosettes, this corresponds to cube lengths of 40.0 μm and 57.1 μm respectively. Since it is assumed that each cube is solid ice, the mass for the cube unit in each rosette can be solved by finding the volume.
of the cube components of the rosette and multiplying by the density of ice as in Equations 25 and 26.

\[
\text{mass}_{200,\mu m} = (40.0 \cdot 10^{-4} \text{ cm})^3 \cdot 0.916 \text{ g cm}^{-3} = 5.86 \cdot 10^{-8} \text{ g} \tag{25}
\]

\[
\text{mass}_{400,\mu m} = (400.0/7) \cdot 10^{-4} \text{ cm}^{-3} \cdot 0.916 \text{ g cm}^{-3} = 1.71 \cdot 10^{-7} \text{ g} \tag{26}
\]

3.1.2 Generation of aggregate flakes

The method developed to generate aggregate flakes comprised of 6-bullet rosettes is similar to the Monte Carlo method of Maruyama and Fujiyoshi (2005). The method of this study does not contain an aggregation model, thereby eliminating much of the computationally intensive parts of the Maruyama and Fujiyoshi method. The method starts with a 3D grid of lattice points either 100 \times 100 \times 100 units or 200 \times 200 \times 200 units depending on the size of the desired flake. The center lattice point is set to be true. From this center point, either a 5-unit (200 \mu m) or 7-unit (400 \mu m) rosette is generated, depending on the model run. The model runs are homogenous, meaning that they are either comprised of all 5-unit rosettes or 7-unit rosettes; the size of the rosettes are not mixed nor do they vary. A 5-unit rosette that is generated off a true lattice point looks like Figure 11a and two 5-unit rosettes are shown in Figure 11b.

All the crystals of the rosette are touching. In the case of Figure 11b, the rosettes are touching each other, but they are not overlapping or sharing point locations. In the real world, the outer face of the crystals would touch each other, but individual crystals would not have lattice points in common with one another. Our model does not allow for rosettes to generate if they will share lattice points with a previously existing rosette.

Figure 11. Graphs of (a) A single, 5-unit rosette crystal. (b) Two, 5-unit rosette crystals.
Once the size of the 3D grid is determined and the origin point set to true, the method then randomly determines another true lattice point +/- 1 from the last valid point in the x,y,z directions or any combination of the 3 directions. This lattice point becomes the center of the next generated crystal. If the run is for the 200 μm (400 μm) rosette crystal, all points +/- 2 (+/- 3) in the x,y, and z directions are valid. If any of the points in the generated rosette are already true, the crystal is discarded and another point is chosen. If a boundary is reached, meaning that a valid data point results in a rosette laying beyond the valid lattice area, the valid data point is set back to the origin and generation begins again from the center.

Predetermined growth conditions are based on two parameters that control the desired size and density of the generated flake. These two parameters are referred to in the model as total rosette and central growth. Total rosette dictates the total number of rosettes possible for generation including rosettes that are determined to be invalid. The central growth helps control the shape of the flake. Its value is always equal to or less than the total rosette. When the remainder of the total rosette divided by the central growth is zero, the valid point is reset to the origin and growth begins again from this point.

For example, if total rosette is equal 500 and central growth is 250, this means that there are 500 total rosettes possible (including those discarded through boundary conditions), but that the flake can only grow outward by at most 250 rosettes (also including those rosettes discarded). When the total rosette is divided by the central growth, the remainder is zero and the next rosette origin lattice point will originate from the center of the lattice space instead of the last valid point. By setting the central growth to a low number, this creates a more blob-like, denser flake while making the central growth closer to the total rosette yields a lighter, more branched-like shape as the origin points for valid rosettes are less frequently set to the center. A lower central growth number is used for generating the smaller diameter flakes while higher central growth numbers are used for the larger, lighter flakes. These variables for each crystal size and for each snowflake diameter are chosen from trial and error making this particular area of the generation program time consuming. Figures 12 and 13 show the total rosette and central growth numbers for the 200 and 400 μm rosette crystal snowflakes respectively.
Figure 12. The total rosette and central rosette values to generate flakes from 200 μm rosettes. The approximate sizes of the flakes are labeled.

Figure 13. The total and central density values to generate flakes from 400 μm rosettes. The approximate sizes of the flakes are labeled.
Figure 14 is a flowchart illustrating our model. The growth conditions are different for each desired flake size and are chosen so that the resultant flakes are in good agreement with the size-density relationships discussed in Section 3.3. Similarly, the growth conditions for the same size flake are different between the 200 μm and the 400 μm rosettes due to their size difference.

While not as computer intensive as the other methods, individual snowflakes can take up to 4 hours to run to completion. The actual generation of the snowflake is under a minute, but the computation of the diameter of the snowflake is time-intensive as it compares all valid data points against each other to determine the largest distance across the flake. To cut down the computation time significantly, the diameter can be determined by doubling the largest radius from the origin to the furthest point since the Brandes et al. study of 2007 determined most aggregates 1 mm and above are close to spherical in overall shape. This method, however, is imprecise if the flakes do not grow equally around the center.
Figure 14. Flowchart of the aggregate snowflake generation model used in this study.
3.2 Aggregate Snowflakes

Since heavy snowfalls and large flakes are typically aggregates, several studies have been conducted to determine the size-density relationship of aggregate snowflakes. A summary of size-density relationships from various studies is given in Brandes et al. (2007) along with their own relation. The equations are shown in Figure 15 with equations given in Table 1. Note: the Brandes et al. (2007) relation is referred to as Equation 7 in Figure 15. There are noticeable differences between the relationships from different studies. This is believed to be a factor of how the maximum dimension of the snowflake is determined and what type of flake is included in the study (e.g., dry snowflakes versus studies that also included heavily rimed snowflakes). Particularly, Magono and Nakamura (1965) used the geometric mean of the particle's major and minor axes as seen from above, while Muramoto et al. (1995) determined the maximum dimension based off the maximum horizontal dimension. The Fabry and Szyrmer (1999) relation is off the equivalent volume diameter while Heymsfield et al. (2004) used the diameter of the minimum circumscribed circle (Brandes et al., 2007).

![Figure 15. Size-density relationships from Brandes et al. (2007). Included are the Brandes et al. relationship and that of several previous studies along with the Brandes' et al. observed data. Equations are given in Table 1.](image-url)
Table 1. Equations from Figure 15. D is the maximum diameter of the snowflake in mm with ρs in g cm\(^{-3}\) (Brandes et al., 2007).

<table>
<thead>
<tr>
<th>Study</th>
<th>Relation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Magono and Nakamura (1965)</td>
<td>ρs = 2D(^{-2})</td>
</tr>
<tr>
<td>Holroyd (1971)</td>
<td>ρs(D) = 0.17D(^{-1})</td>
</tr>
<tr>
<td>Muramoto et al. (1995)</td>
<td>ρs(D) = 0.048D(^{0.406})</td>
</tr>
<tr>
<td>Fabry and Szyrmer (1999)</td>
<td>ρs(D) = 0.15D(^{-1})</td>
</tr>
<tr>
<td>Heymsfield et al. (2004)</td>
<td>ρs(D) = 0.104D(^{0.95})</td>
</tr>
<tr>
<td>Brandes et al. (2007) (Eq. 7 in Fig 15)</td>
<td>ρs(D) = 0.178D(^{0.922})</td>
</tr>
</tbody>
</table>

As can be seen from all the relationships included in Figure 15, density decreases with increasing particle size. Also given in the study is the aspect ratio, the ratio between the maximum vertical dimension divided by the maximum horizontal dimension, of aggregate snowflakes. It is almost a 1 to 1 ratio for larger flakes as shown in Figure 16. Magono and Nakamura (1965) similarly noted that larger aggregates tend to be spherical in overall shape.

![Figure 16](image.png)

Figure 16. Image and relationship of the aspect ratio of aggregate for particles less than 10 mm (Brandes et al., 2007).

The aggregate snowflakes made of 200 and 400 μm crystals are generated to closely follow the Brandes et al. (2007) diameter-density relationship given in Table 1. The flakes generated in this study and the relationships given in Table 1 are plotted in Figure 17. The aggregates of 200 μm rosette crystals are shown as yellow circles with the 400 μm aggregates
given as blue circles. These flakes are allowed to grow uniformly in all directions and resulted in fairly spherical flakes as suggested by Brandes et al. (2007). Figure 18 a-h is an example of the 200 μm aggregate flakes in both 2D and 3D views. 400 μm flakes are not shown as they are similar to the 200 μm flakes.

Figure 17. The size-density relationships from Brandes et al. (2007) with the 200 μm and 400 μm rosette aggregate flakes are shown on this graph with Diameter (mm) on the x-axis and density in g cm$^{-3}$ on the y-axis.
Figure 18 a-f. The flakes shown in this figure are examples of actual generated flakes comprised of 200 μm crystals. A 1.00 mm flake is shown in 2D (a) and 3D (b); 5.13 mm flake in 2D (c) and 3D (d) views; an 8.79 mm flake in 2D (e) and 3D (f) views.
The example flakes here are shown in 2D for two reasons: 1) When the flakes are graphed in 3D, the nuances of the structure are lost due to compression of the image, and 2) The 2D images, in the x-y plane, are used to calculate fractal dimension. There may be another plane that shows more interesting variation, but the x-y plane is used in all graphics for simplicity and to maintain uniformity amongst all analyzed flakes.

3.3 Fractals

3.3.1 Fractal Analysis

Researchers like Muramoto et al (1993), Maruyama and Fujiyoshi (2005) and Ishimoto (2008) studied the fractal dimension of snowflakes. Unlike a lot of other quantities, fractal dimension is only slightly affected by the angle of the camera and the particle's area (Maruyama and Fujiyoshi, 2005). While Mandelbrot helped spread the concept of fractal geometry to the scientific community, he had great difficulty determining the exact definition of a fractal (Mandelbrot, 1977; Feder, 1988). Previous definitions created by Mandelbrot often excluded fractals of scientific importance (Feder, 1988). In 1986, Mandelbrot settled on the vague definition of a fractal being an object that when broken down to smaller pieces, the smaller pieces resemble the whole object (Mandelbrot, 1977; Feder, 1988; Petigen et al., 1992).

3.3.1.1 Fractal Dimension Definition. Fractal dimension is a measure of how complex an object is by measuring how fast the length, area, volume, etc. change with respect to smaller and smaller scales (Petigen et al., 1992). While there are several different ways to measure the fractal dimension of an object, the one used by Maruyama and Fujiyoshi (2005) is the box-counting dimension. In the box-counting method, the object of interest is overlaid by a mesh grid of a given size $\delta$. Next, the number of the mesh boxes that contain part of the object, referred to as $N(\delta)$, is tallied. A graph of $\log(\delta)$ on the x-axis and $\log(N(\delta))$ on the y-axis is generated and the slope of the best-fit line between all data points is the fractal dimension (Falconer, 1990; Petigen et al., 1992). Different methods can result in different fractal dimensions, yet they are usually related to one another (Petigen et al., 1992).

3.3.1.2 Fractal Dimension Analysis. To analyze the fractal dimension of the generated flakes, the free software package ImageJ is used along with the free plugin FracLac. ImageJ is a public domain image processing and analysis software package built on a Java platform by
Wayne Rasband at the U.S. National Institute of Health (Rasband, 1997-2008). FracLac is a plugin for ImageJ used to analyze complex morphological features. It was developed and is maintained by the School of Community Health, Faculty of Science, Charles Sturt University in Australia (Karperien, 1999-2007).

The valid points of each flake are imported into MATLAB. Each image is graphed on an equal axis, meaning that the x and y-axes are proportionally equal yielding an unskewed image. Each valid data point is graphed as a filled square to reflect that the building block of each rosette is a cube as discussed in Section 3.1. The flake is a 2D image with just the x and y axes as shown in Figure 19a. The image is saved as a PNG to avoid problems JPEGs can have with being lossy and all of the files are imported into ImageJ. ImageJ has the ability to perform many different image manipulations, one of which is the ability to obtain the outline of the flake images from MATLAB. An example of the outline of the flake in Figure 19a is shown in Figure 19b.

![Figure 19. (a) is an example flake generated from MATLAB comprised of filled squares. (b) is the ImageJ generated outline of (a).](image)

Both the real 2D images and the outlines are analyzed with FracLac. This is done because Ishimoto (2008) analyzed real images while Maruyama and Fujiyoshi (2005) used the outline of images. The FracLac program uses the box-counting method to calculate fractal dimension and allows the user to define how many grid positions to use. For this work, the number of grid positions is set to 1, meaning that the overlaying grid of a given mesh size will start at (0,0). If the user chooses more than 1 grid position, the subsequent grids start at a randomly chosen point (x,y) within the image and all results are averaged together. Because all
generated images are in black and white, they are analyzed as binary files with the background color set to white for real images and black for outline images. The default box/mesh sizes are used with the minimum size set at 2 pixels and a maximum size of 45% of the size of the image. Figure 20 a-c gives an example of the different grid sizes that are used to calculate the fractal dimension. The ln-ln graph used to calculate fractal dimension is given in Figure 21 with natural log of the mesh size on the x-axis and natural log of the number of grids filled with the image/outline on the y-axis. The fractal dimension of this flake is 1.7224.

Figure 20 a-c. Illustration of the different grid calibers used in the FracLac box counting method.
Figure 21. The ln-ln analysis of the flake shown in Figure 19a. Each dot represent a different grid caliber calculated by FracLac. The slope of the trendline (e.g., the fractal dimension) is 1.7224.

### 3.3.2 Fractal Dimension

The 2D and outline PNG images from MATLAB are analyzed for fractal dimension and yield different results. The fractal dimension for the flakes calculated by the box-counting method are given in Table 2 and are broken down by flake constituent crystal and image type (the MATLAB 2D image or outline). The results are not exactly what is found in Maruyama and Fujiyoshi (2005). They studied 4 different flakes using 2 different views. The calculated dimensions in their study are between 1.10 and 1.19. While there is some variation between the top and side views they used, it is no more than 0.04 in any of the 4 cases. The dimension of the flakes in this study are greater than Maruyama and Fujiyoshi. This is most likely due to the difference in the calculation of the box-counting technique and less open space in this study's flake images due to lattice points being graphed as solid squares.
Table 2. The average fractal dimension for the 200 and 400 μm constituent flakes based on whether the 2D image was of the whole flake or the outline.

<table>
<thead>
<tr>
<th>Constituent Particles</th>
<th>200 μm</th>
<th>400 μm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Image</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2D</td>
<td>1.75</td>
<td>1.74</td>
</tr>
<tr>
<td>Outline</td>
<td>1.28</td>
<td>1.29</td>
</tr>
</tbody>
</table>

Ishimoto (2008) generated flakes of different fractal dimensions with the method described in Section 2.1.2.1. He determined that using a DLA model, e.g., a random walk trajectory, yielded fractal dimensions typically around 1.75. This study's fractal dimension of the 2D images are in very good agreement with Ishimoto.
CHAPTER 4

SINGLE SCATTERING PROPERTIES OF SNOWFLAKES

4.1 DDSCAT

The single scattering properties of the flakes are computed using the discrete dipole approximation method (DDA). The program used in this study is DDSCAT, developed by Draine and Flatau (2008). DDSCAT is FORTRAN 90 based and can calculate the single scattering properties of arbitrary particles with complex refractive indices. DDSCAT allows for the adjustment of refractive indices for different materials and temperatures, even multiple materials in one particle. The particle shape can be chosen from a list of shapes already existent in the program (e.g., ellipsoid, rectangular solids, hexagonal prisms, etc.) or the user can upload a shape file that specifies the true lattice points in a shape.

The output contains total cross-sectional areas and the scattering efficiencies for absorption, scattering and extinction along with a 4x4 Mueller scattering intensity matrix. The aforementioned cross sections are normalized by $a_{\text{eff}}^2$ or:

$$Q_x = \frac{C_x}{\pi a_{\text{eff}}^2}$$  \hspace{1cm} (27)

where $Q$ is the output efficiency, the $x$ subscript represents absorption, scattering or extinction and $a_{\text{eff}}$ is the effective radius of the object assuming the object is a solid sphere of ice, not an irregularly shaped snowflake with ice and air pockets. Backscattering differs as it is given as the differential cross section normalized by $a_{\text{eff}}^2$.

$$Q_{\text{bsc}} = \frac{C_{\text{bsc}}}{4 \pi ^2 a_{\text{eff}}^2}$$  \hspace{1cm} (28)
The only limitation for the program is that dipole spacing must be small enough where \( d \) in Equation 4 is less than 0.5 and for the differential scattering cross-sections, \( \frac{dC_x}{d\Omega} \), to be within a few percent of the average differential scattering cross section, \( \frac{C_x}{4\pi} \).

For analysis in DDSCAT, the shape is user defined and all shape files are uploaded. Each flake is comprised of only one dielectric material, and the refractive index is for ice at 260 K. 260 K is chosen since, as mentioned in section 2.1.1, aggregation mainly occurs between -24° C and -7° C (249 K and 266 K) (Woods et al., 2008). A frequency of 94 GHz (3,191 μm) is used for all flakes as this is the frequency of the CPR aboard CloudSat (CIRA, 2008). An effective radius of each flake was determined by dividing the mass of the flake by the density of ice and determining the radius of an equal volume sphere of solid ice.

Three separate angles are used to define the orientation of the target. In Lab Frame, the incident radiation is forced to propagate in the \( +\hat{x} \) direction. The definition of a target requires two different unit vectors (\( \hat{a}_1 \) and \( \hat{a}_2 \)) that are fixed to the target object where \( \hat{a}_2 \) is orthogonal to \( \hat{a}_1 \). 3 angles, \( \beta \), \( \Theta \) and \( \Phi \), are used to describe the direction of \( \hat{a}_1 \) from the incident radiation. The angles are shown in Figure 22.

The incident radiation lies in the \( \hat{x} \) and \( \hat{y} \) plane when \( \Phi = 0 \). When \( \Phi \) is non-zero, it indicates that \( \hat{a}_1 \) is rotated around \( \hat{x} \). \( \Theta \) is the angle between \( \hat{a}_1 \) and \( \hat{x} \). For \( \beta \), when it is equal to zero, \( \hat{a}_2 \) is in the \( \hat{x} - \hat{a}_1 \) plane. Non-zero values adds a rotation of \( \hat{a}_2 \) around \( \hat{a}_1 \). In this study, we examine the single scattering properties of randomly-oriented flakes, which means the averaged properties over multiple particle orientations. The number of target rotations was set to \( N_\beta = 6, N_\Theta = 10 \) and \( N_\Phi = 6 \). For example, \( N_\beta \) equal to 6 means that it will divide the available interval of \( \beta \) into 6 uniform sampling intervals. Smaller rotations of \( N_\beta = 3, N_\Theta = 5 \) and \( N_\Phi = 3 \) were tried, but for flakes on the size order of 8 mm and larger, backscatter cross-sectional areas differed by up to 8%, so the higher number sampling set is used. Although it is suggested in the DDSCAT 7.0 User Guide that using an odd \( N_\Theta \) might be more precise than an even \( N_\Theta \) since an odd number allows for use of the Simpson method for averaging, the difference is minimal for this particular study. The value of \( N_\Theta = 10 \) also allows for more rotational views. In addition, all variables used in DDSCAT leads to \( mk|d| \) values well below the
acceptable threshold of 1, and is usually below 0.1. Among the output variables from DDSCAT are $Q_{\text{bsc}}$, $Q_{\text{sca}}$, $Q_{\text{abs}}$, and $Q_{\text{ext}}$.

4.2 Single Scatter Properties

Liu (2004, 2008a) used DDSCAT on a variety of snowflake shapes and sizes to try to determine an empirical relationship for single scattering properties and create a database from which these values could be obtained quickly. The database outputs the absorption cross section ($C_{\text{abs}}$) that describes how much incident radiation is absorbed by a particle, backscatter cross
section ($C_{bsc}$) describing the scattered energy that is opposite in direction of the incident radiation, asymmetry parameter ($g$) meaning the degree of symmetry of the scattered energy distributed with respect to the plane dividing forward and backward hemispheres, and the phase function ($P(\cos(\theta))$) describing the angular distribution of scattered energy, where $\theta$ is the angle between the incident wave and observing direction.

The user inputs particle shape, maximum dimension, temperature and wave frequency. The database provides information for 11 particle shapes (Figure 23) with maximum dimensions ranging from 50 to 12,500 μm for temperatures between 0°C and -40°C for incident electromagnetic wave frequencies of 15 to 340 GHz. While producing a lot of valuable information, this database only includes single, pristine crystals which are rarely found in nature.
The backscattering, extinction, absorption and scattering coefficients for snowflakes generated in this study are calculated by DDSCAT. For comparison, normalized coefficients are used. For scattering, absorption and extinction, the normalized coefficients are simply the outputs \( Q_{\text{sca}} \), \( Q_{\text{abs}} \), and \( Q_{\text{ext}} \) from DDSCAT as given in Equation 27. Since the normalized backscatter coefficient (\( Q_{\text{bsc}} \)) as given in Equation 28 is different than the other cross sections, it must be multiplied by \( 4\pi \) to be equivalent to the other normalized cross sections in Equation 27.

When \( Q_{\text{sca}} \), \( Q_{\text{abs}} \), and \( Q_{\text{ext}} \) are plotted against the effective radius of the analyzed flake, they exhibit similar patterns as shown in Figure 24 a-f. Given the effective radius or mass (as mass can readily be calculated from the effective radius), \( Q_{\text{sca}} \), \( Q_{\text{abs}} \), and \( Q_{\text{ext}} \) can roughly be determined as there is a fairly uniform relationship. \( Q_{\text{bsc}} \) is not so straightforward as there is not a uniform relationship between the effective radius and the \( Q_{\text{bsc}} \) as illustrated in Figure 25 a and b. The scattered nature of effective radius-\( Q_{\text{bsc}} \) relationship indicates that \( Q_{\text{bsc}} \) could be dependent upon the shape of the flake while the other normalized coefficients are not and appear to be only dependent on effective radius/mass. An increase of randomness by increasing the numbers of \( \beta \), \( \Theta \) and \( \Phi \) in DDSCAT did not vary these normalized coefficients by a significant amount.
Figure 24 a-f. The effective radius in μm and the normalized absorption (a) and normalized scattering (b) for 200 μm flakes.
Figure 24 a-f (continued). The effective radius in μm and the normalized extinction coefficients for 200 μm flakes (c) and the normalized absorption coefficient 400 μm flakes (d).
Figure 24 a-f. The effective radius in μm and the normalized scattering (e) and normalized extinction (f) coefficients for 400 μm flakes.
Figure 25. The effective radius ($\mu$m) of the generated flake on the x-axis plotted against the normalized backscatter coefficient on the y-axis for (a) 200 $\mu$m flakes and (b) 400 $\mu$m flakes.
4.3 \( Z_e - S \) Relationship

As one of the many applications of the single scattering properties of snowflakes, a \( Z_e - S \) relation is developed in this section. Solving Equations 6 and 7, \( Z_e \) and \( S \) values are calculated from different flake groupings and snowfall rates. \( N_0 \) and \( \Lambda \) in Equations 6 and 7 are calculated using relations from the 1970 Sekhon and Srivastava study and are given in Equations 29 and 30 with \( R \) being the precipitation rate in mm h\(^{-1}\) and the units being mm\(^{-1}\) m\(^{-3}\) and cm\(^{-1}\) respectively. The terminal velocity, \( v_t(D) \), is one of the terminal velocity equations from Brandes et al. (2008) and given in Equation 31.

The \( Z_e - S \) relationships include over 100 different groupings of the original 300+ snowflakes. In determining \( Z_e \) and \( S \), only snowfall rates up to 2 mm h\(^{-1}\) are used. Above 2 mm h\(^{-1}\), the \( Z_e - S \) relationship starts to curl in on itself rather than increase as expected (Figure 26). In Figure 26, each dot represents a different snow rate. The snow rate increases by 0.001 mm h\(^{-1}\) between 0.01 and 0.1 mm h\(^{-1}\), then it increases by 0.1 between 0.1 and 5.0 mm h\(^{-1}\).

\[
N_0 = 2500R^{-0.94} \quad \text{(29)}
\]
\[
\Lambda = 22.9R^{-0.45} \quad \text{(30)}
\]
\[
v_t(D) = 0.67D^{0.25} \quad \text{(31)}
\]

As the snow rate increases, the size distribution changes and puts more weight on larger flakes as illustrated in Figure 27. In this figure, several different snow rates are plotted against the number of particles the size distribution dictates should be present for a snowflake of a given melted diameter. By holding all other variables constant except the snow rate, the larger the snow rate, the less smaller flakes count and the more larger flakes have an impact. Figure 28 illustrates how changing snow rate changes the size distribution by using a single grouping of flakes. This shows a similar trend as in Figure 27. In Figure 28, by 5 mm h\(^{-1}\) all the flakes start to be weighted similarly. From this, it can be inferred that due to the limitations of the flakes only being 10 mm and less in size in this study before melting, as the snow rate increases there are not enough large flakes to influence \( Z_e \) and \( S \). This can lead to the curl seen in Figure 26. In light of this, only snowfall rates up to and including 2 mm h\(^{-1}\) are used.
Figure 26. The impact of increasing snow rate on the Ze-S relationship due to size distribution. Each dot represents a different snow rate of between 0.01-0.1 mm h\(^{-1}\) and 0.2-5.0 mm h\(^{-1}\).

Figure 27. A log-log plot of the impact of snow rate on size distribution. The x-axis is the log of the melted diameter of a flake and the y-axis is the log of the number of particles that particular size would have in the size distribution. Shown are snow rates of 0.5, 1.0, 1.5 and 2.0 mm h\(^{-1}\).
Figure 28. This figure illustrates how the size distribution of a given flake changes with increasing snow rate. The diameters are given in legend.

After plotting the \( Z_e - S \) points, a relationship from the data is:

\[
Z_e = 7.39S^{0.98} \tag{32}
\]

A plot of the data points is shown in Figure 29 with 200 \( \mu \text{m} \) constituent flakes as open circles and 400 \( \mu \text{m} \) as asterisks. Also plotted are Equations 32, 33 (Matrosov, 2007) and 34 (Liu, 2008b).

\[
Z_e = 10S^{0.8} \tag{33}
\]

\[
Z_e = 11.5S^{1.25} \tag{34}
\]

While the first number in Equation 32 (7.39) is lower than Equations 33 and 34, this is most likely due to smaller flakes in the data set meaning there is a smaller spread of flakes. The exponent is the most important part as that determines the rate of growth of the relationship. The
exponent of Equation 32 is in between those of Equations 33 and 34 lending validity to the result of this study.

Figure 29. \(Z_e-S\) relationship of the study data graphed with Equations 32, 33 and 34.
CHAPTER 5

SUMMARY AND CONCLUSIONS

5.1 Snowflake Generation

A new approach that generates more realistic aggregate snowflakes is developed for this study. Previous studies, such as Ishimoto (2008) and Maruyama and Fujiyoshi (2005), while utilizing parameterizations such as collision efficiencies, revolutions, gravity, etc., do not have constraints in place to make sure the flakes are of correct size or density. Furthermore, the Maruyama and Fujiyoshi (2005) study models each flake constituent as a sphere making it impossible to compute its scattering properties using discrete dipole approximation. This study generates flakes comprised of either 200 μm or 400 μm 6-bullet rosette crystals.

This study improves upon previous modeling techniques. As a quality control measure to insure realistic size and density of the flakes, the Brandes et al. (2007) size-density relationship is used. All generated flakes are designed to be close to this relationship. If a grouping of flakes is too far off, bounds are reset and the group is rerun. The resultant flakes are therefore of correct size and density thus improving on the shortcoming in previous studies.

To further validate the findings of this study, the fractal dimension of the flakes are calculated. Using the FracLac plugin for ImageJ, 2D images of the flakes in the x-y plane are analyzed both as a 2D image and an image of just the outline of the flake. In the case of the actual image, the fractal dimension is 1.74 and 1.75 for 200 and 400 μm constituent flakes. This result is in very good agreement with Ishimoto's (2008) DLA flakes, which had a fractal dimension of 1.75. When the outlines are analyzed, the fractal dimensions are 1.28 and 1.29 for the 200 and 400 μm flakes. This is greater than the results from Maruyama and Fujiyoshi (2005), which are between 1.10 to 1.19 depending on the analyzed flake.

5.2 Scattering Relations

Most of the 300+ flakes are run in DDSCAT to determine backscattering, scattering, absorption and extinction coefficients. Random groupings of flakes are chosen from the total data set of analyzed flakes to calculate a $Z_e$-$S$ relationship. The $Z_e$-$S$ relationship for this study is
\[ Z_e = 7.39S^{0.98} \]. When compared to the previous studies of Matrosov (2007) and Liu (2008b), this result is inline with their relations.

One of the most important parts of this study is the scattering relationships of the aggregate snowflakes. The backscattering coefficient of irregularly shaped aggregate snowflakes comprised of 'realistic' crystal types has hardly been examined. The normalized extinction, scattering and absorption cross sections, when graphed with effective radius, have uniform relationships. With mass or effective radius known, these cross sections can be determined fairly easily. The normalized backscattering coefficient does not have a uniform relationship with the effective radius suggesting that backscattering is dependent not only on the effective radius, but also the shape of the flake.

### 5.3 Future Work

In the future, the snowflake generation model should undergo further refining. The additions of real-world processes, such as collision efficiency, rotation, turbulence, etc. used in the Maruyama and Fujiyoshi study, would be an improvement. Furthermore, the addition of other crystal types and even heterogeneous flakes comprised of multiple crystals would be closer to nature.

Ultimately, these results need to be included into Liu's scattering database. This would greatly benefit the scientific community. For inclusion, however, many more snowflakes need to be generated with a larger size range. Furthermore, multiple DDSCAT measurements would have to be run on each flake for numerous temperatures and frequencies. For normalized backscatter cross section, many flakes of the same effective radii must be run to obtain an average backscatter coefficient for flakes of that particular size. Once this is done for all the effective radii, a quantitative relationship for effective radii and normalized backscatter coefficients can be calculated.
LIST OF REFERENCES


BIOGRAPHICAL SKETCH

Holly Kreutzer Nowell was born Holly Ann Kreutzer on December 12, 1981, in Wichita, Kansas, to her parents Barney and Lorraine. She has an older sister Debra. She grew up in Wichita, Kansas, until she attended Washington University in St. Louis in 2000. She received her B.A. in Earth and Planetary Sciences in May 2004. During this time, she held a summer internship with the National Weather Service Office in Wichita, Kansas, from 1997-2001, and in 2002, held a summer internship at NASA's Goddard Space Flight Center working under Kristi Arsenault.

Upon graduation from Washington University, she worked at the University of Southern Mississippi's iTech department until attending Florida State University in the fall of 2007 to obtain her Masters in Meteorology. She married Robert Nowell, Jr., on July 27, 2007, in Tallahassee, Florida. She is working on snowfall remote sensing issues with Dr. Guosheng Liu of Florida State University and will be pursuing her PhD. She is currently living in Tallahassee with her husband Robert and their dog Clyde.