THOLIN AGGREGATION IN TITAN'S ATMOSPHERE: DEVELOPING A PROBABALISTIC MODEL.

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Introduction: Titan, the largest satellite of Saturn, is uniquely appealing to study due to its similarities and differences to Earth [1]. Titan has an atmosphere and a complex surface geomorphology that has many features in common with Earth but also many that are unique to Titan [2]. Titan's surface is composed of tectonic, cryovolcanic, and impact cratering features, but also shows evidence of "fluvial erosion" resulting from a hydrological cycle like Earth's but with liquid methane instead of water [2]. Much of Titan's weather is controlled by complex-organic aerosol particles, called tholins.

Titan's characteristic hazy reddish-orange appearance is due to high concentrations of tholin in the lower atmosphere. As tholin settles out of the formation zones in the upper atmosphere, it condenses into a thick layer above the surface where it dominates the atmospheric activity by filtering the incoming ultraviolet rays and controlling the atmospheric circulation. The methane clouds are influenced by the distribution of tholin concentrations. The production of tholin has been studied from many different perspectives including atmospheric dynamics, laboratory synthesis, climatology, optical properties, dusty plasma physics and theoretical models of tholin aggregation in Titan's atmosphere [3].

Due to the continuous influx of galactic cosmic radiation (GCR) and solar UV rays, the particles in Titan's atmosphere are charged and can be modeled as a complex plasma environment. The ion densities and temperatures for different sections of the atmosphere were measured on January 14, 2005, when the Huygens probe associated with the Cassini spacecraft descended through Titan's atmosphere to the surface [4].

The charging mechanisms differ on the day- and night sides of Titan. Photoionization by solar UV rays is the primary charging mechanism during the day, while electron/ion collisions created by the ambient plasma dominate nighttime charging. The charging of the grains is further complicated by the fact that the particles are irregular, fractal aggregates. The arrangement of charge on the irregular surface affects the orientation of colliding aggregates, changing the coagulation rate and the resultant morphology of the grains [5].

Most coagualation simulation models use a statistical approach to calculate the growth of particles at different heights in the atmosphere. Such analytical approaches can provide growth rates and particle sizes; however, collisions between particles must occur according to a specific set of rules designed to simplify the physics involved in these models. Usually the particles are approximated as spheres when calculating charge and coagulation probabilities. This approximation is contained in the coagulation kernel in the Smoluchowski equation, which gives the coagulation probability for particles with different masses [3]. Self-consistent N-body simulations are essential for properly modeling the dynamics of such interacting grains while also resolving collisions. This study is concerned with modeling the micro-physical processes which govern the aggregation, in particular the charge-dipole interactions. Statistical results from this study will be used to refine the coagulation kernel used in subsequent models of Titan's atmosphere.

Method: Tholin is a polycyclic aromatic hydrocarbon formed by photolysis in Titan's upper atmosphere and grows through coagulation of the nucleated embryos [6]. Following the model given by Bar-Nun [7], we consider the development of tholin with respect to altitude and the aggregate's mass. The formation of tholin molecules is presented in three primary generations based on the size of the aggregate as defined by the number of components contained in the aggregate [3], [7].

Aggregates were created by numerically modeling interactions between colliding particle pairs [5], [8]. Work was done in the center of mass (COM) frame of an initial seed particle; a second monomer or aggregate approaches a point slightly offset from the COM. The relative velocities between the grains are set assuming Brownian motion plus a velocity due to turbulence, dependent on the size and density of the particles. This added velocity was determined using a method that uses coupling times to turbulent eddies determined by atmospheric conditions [9].

Aggregates of increasing mass were built in several steps by specifying plasma parameters, velocities, and general particle characteristics at specific altitudes in Titan's atmosphere. The force acting on particle *i* from the electric field of particle *j* is calculated along with the torque induced by the dipole-dipole interactions. The torque induces a rotation of the aggregate altering its orientation during collision which can affect the resulting structure. Collisions are detected when monomers within each aggregate physically overlap. Colliding aggregates are assumed to stick at their point of contact with orientation being preserved. The charge and dipole moment of resultant aggregates are determined by the use of Orbital Motion Limited theory with a line of sight factor to determine unobstructed points on the aggregate [5].

The initial population of embryos were modeled as spheres with radius r = 40 – 50 nm. The charges on the particles were calculated for two cases: day-time charging, where UV photoionization is important, and night-time charging, where plasma (formed primarily by ionizing cosmic rays) is collected by the grains. The ion species in the atmosphere were mass-averaged and adjusted by the percent abundance in calculating the positive charging currents to a grain.

Aggregate populations were grown in three stages. First generation aggregates were created by addition of single monomers until the number of monomers reached N = 50. This growth is considered to take place at 270 km altitude and T = 175 K. As these particles settle lower in the atmosphere, the second generation forms at an altitude of 200 km and T = 158 K, and is grown to size N = 200 monomers through collisions between the first generation aggregates. The third generation is grown at an altitude of 100 km and T = 140 K up to a size N = 2500 monomers, through collisions between the second generation aggregates.

Collision data collected from aggregate formation include the number of monomers, maximum radius, charge, relative velocity, and compactness factor for each aggregate. Ultimately this data will be used to determine the coagulation kernel which gives the probability of coagulation for particles with masses m and m'.

Results: Sample data for the formation of first generation aggregates for each of the charging classes are shown in Figure 1, giving the probability that a monomer will collide with a certain size aggregate. Preliminary results indicate that the UV charged aggregates (daytime charging) have highly efficient collisions due to the less-negative surface charge, as compared to the aggregates charged during nighttime. Currently only single monomers are introduced as the incoming particles. The collision probability will be plotted against the aggregate size and the incoming particle size for second and third generations.

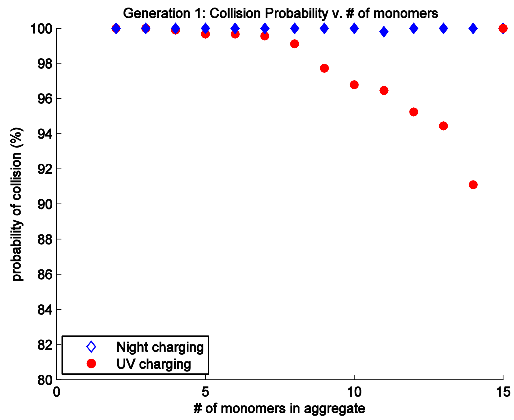

Figure 1. Collision probability as a function of aggregate size. Aggregation of aggregates charged under daytime conditions is highly efficient for the first generation.

Tholin is an interdisciplinary study in which further research must be done to understand the role it plays in the tropospheric activities of Titan. This study refines the simulation of the growth of tholin particles by including dipole-dipole interactions of the charged aggregates and determining the manner in which they affect coagulation rates. Statistical data including the radius, charge, and collision probability for aggregates with a given mass is being collected and analyzed for aggregate populations of the second and third generations. The first, second, and third generations of will be used to calculate the coagulation kernel in the Smoluchowsky coagulation equation.

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