THE MOLECULAR DIFFUSION OF ICE CRYSTALS OF VARIOUS SHAPES

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1. INTRODUCTION

Two main controlling factors of ice crystal growth are the heat and (gaseous) mass transfers, H&MT, as characterized by the Nusselt number (Nu) for heat and the Sherwood (Sh) number for mass. Nu and Sh express the increase of the molecular diffusions by the relative motions of the particles in air as characterized by the Reynolds number (Re). Traditionally Nu is assumed to be identical to Sh. Past laboratory measurements with various ice crystal shapes by the Toronto Cloud Physics Group involved Sh, thus this study will deal with Sh. The growth of a crystal depends on its size and shape, its fall speed (through Re) and the flux of water vapour from the surrounding air. It is controlled by the diffusion of heat which carries away the energy released on the crystal surface by deposition. Sh is a function of Re and was established by Schemenauer and List (1978) [S&L78] for snow crystals and graupel. Their study, however, did not address the case of pure diffusion (i.e. Re=0). Such values based on approximations have been available in the literature (McDonald, 1963 [Mc63], Jayaweera (1971)) only for a very limited number of shapes of crystals. Thus, it was decided to take a general approach to numerically calculate $Sh_{Re=0}$ for any ice crystal with a rectilinear shape. New values of $Sh_{Re=0}$ for additional shapes of crystals are addressed in this study along with the method developed for the computations.

The steady state diffusion is controlled by the Laplace equation. It was solved numerically with Dirichlet boundary conditions on a rectilinear 3 dimensional lattice system with variable lattice separation distances for hexagonal plates, hexagonal cylinders, stellar crystals, capped columns, and broad-branched crystals.

2. ELECTROSTATIC ANALOGY

The water vapour density field ($\rho$) around a stationary ice crystal growing under steady state diffusion obeys the Laplace equation

$$\nabla^2 \rho = 0$$

The initial growth of an ice crystal by the net deposition of water vapour in steady state diffusion, is controlled by the rate at which vapour diffuses to and from the crystal’s surface. The rate at which heat is released by the crystal is exactly the same as the rate at which heat is diffused from the surface. This balance leads to quasi constant value of crystal’s surface temperature, and this in turn leads to a constant local vapour density $\rho_0$ around the crystal. For a perfect capacitor that is geometrically similar to the crystal, the electrostatic potential $V$ in vacuum also obeys the Laplace equation, with the surface electrostatic potential $V_0$ constant as is the case for perfect capacitors. Identifying $V$ with $\rho$, the direct analogy between steady state diffusion and electrostatics is established. A capacitor that is geometrically similar to the crystal is then set in a rectangular box, a Faraday cage, sufficiently afar from its edges. The capacitor is then surrounded by the electrostatic potential obeying Laplace equation. The sides of the cage are set at potential zero to simulate “boundaries at infinity”. Since the water vapour tapers off to a constant value sufficiently far away from the crystal, imposing this Dirichlet boundary condition preserves the similarity. In this analogy, one uses Gauss’ flux law and Fick’s law of diffusion to establish that $Sh_{Re=0}$ is given by

$$Sh_{Re=0} = \frac{4\pi CL}{A}$$

where $A$, $L$, and $C$ are the surface area, characteristic length, and the crystal’s capacitance, respec-
3. FINITE LATTICES AND JACOBI’S
METHOD

To compute (2), a numerical scheme for finding the
capacitances for crystals of rectilinear shapes was
developed. “Rectilinear shapes” are those that can be
constructed with a finite number of straight edges.

A Cartesian grid system is established with a finite
number of lattice points within the Faraday cage, the
outer most points representing the edges of the cage
(box). Each side of the box is at least 20 times larger
than the respective sides of the crystal. The separation
between adjacent lattice points can be different
along different axis directions. Each of the lattice
points are labelled in terms of positive integer in-
formation between adjacent lattice points can be different
than the respective sides of the crystal. The separa-
tion by computing the difference (9) by

\[ \sum_{(i,j,k)} \delta V(i,j,k) < \epsilon \]  

where the sum in (9) is carried out for all grid points
in the box. It is well known from literatures in com-
putational physics that the number of iterations ‘r’
required to reduce the error given by the sum (9) by
a factor of \( 10^{-p} \) is

\[ r \sim O(pN^3) \]  

where N is the number of grid points in a NxNxN
cubic regular Cartesian grid system. At the end of
a run of this algorithm, values of all the V’s would
have been computed for each lattice point up to the
desired precision \( \epsilon \).

Some comments are in order at this stage. Al-
though no regular Cartesian grid system is used for
many of the crystal models studied here, the order of
convergence will be the same as (10). There
are other computational methods to solve Laplace’s
equation numerically, such as Gauss-Seidel and the
“simultaneous over-relaxation” (SOR) methods. The
SOR method has a convergence rate of \( O(N^2) \) for
3 dimensional Cartesian grid system.
Jacobi method, however, is one of the simplest algorithms that can be used for our study and is relatively free of the complications in implementation compared to the SOR method. It was thus selected for this study.

4. EXAMPLE: HEXAGONAL PLATE

The hexagonal plate was modelled using a non-regular rectangular grid system, with the proportionality factors $\alpha$ and $\beta$ not being equal. Only a finite number of grid points is available for “drawing” a hexagon to encapsulate the important features of the crystal, namely its vertices. Not all the vertices of the hexagon lie on lattice points if a regular ($\alpha = \beta$) Cartesian grid system is used. Hence a regular Cartesian coordinate system is not used for an optimal representation was achieved for other crystal shapes as investigated experimentally by S&L78 in a “liquid tunnel” (Schuepp and List, 1969).

5. DISCRETE VERSION OF GAUSS’ FLUX LAW AND SCALING RULES

A simple method of numerically computing $S_{h0}$ using the potential $V$ for lattice points around the crystal involves computation of the capacitance $C$. This is done by applying Gauss’ law to compute the “surface charge” of the crystal, via $C = \frac{Q}{V_0}$, where $V_0$ is the surface potential assigned to the crystal at the onset of Jacobi’s method mentioned previously. The total electric flux of the crystal is obtained by first enclosing the crystal in a “rectangular cage”. The sides of this cage are just one lattice point away from the closest side of the crystal. Each side of this enclosure consists of its grid elements, which are called “area element grids”. These grids have the same respective lattice spacing as the grid for the Faraday box.

Each of the “area element” is associated with a set of integers $I$. Then the discrete approximation of Gauss’ flux law can be written as

$$\oint_S \vec{E} \cdot dA \approx \sum_I -\frac{\partial V(i,j,k)}{\delta \mu} \cdot A_i$$

which is just a sum of flux through each of the area elements. Note that in (11), the fact that on the surface of a perfect conductor, the electric field is always perpendicular to its surface, was utilized. The flux through an area element whose outward unit normal is in $\pm \hat{\mu}$ direction is approximated discretely by

$$F_{\pm \mu} = -\frac{V((i,j,k) \pm \hat{\mu}) - V(i,j,k)}{\delta \mu}(\delta \nu)(\delta \gamma)$$

where $\nu$ and $\gamma$ are the other two coordinates not equal to $\mu$. The main reason for placing our rectangular prism enclosure at most one lattice point away from sides of the crystal is that such a construction allows dealing only with $\frac{\partial V}{\partial \mu}$ rather than with the more complicated $\nabla V$, when computing the flux. It is worth discussing the consequence of (12) for a specific direction $\mu$. For the flux through a face with its unit normal in $\pm \hat{z}$ direction, the flux through this area element (12) reduces to

$$F_{\pm z} = \delta x \frac{\alpha}{\beta} [-V(i,j,k \pm 1) + V(i,j,k)]$$

The main feature of (13) is that the only unknown value is $\delta x$. The flux through a face in any of the other directions reduce to expressions of the form (13). In all of these expressions, the only term with unknown value and dimension is $\delta x$. For solving (8), it is not necessary to know the physical value of $\delta x$ since all the quantities, except for $V$, are in dimensionless form as proportionality constants $\alpha$ and $\beta$. Thus, the numerical evaluation of potential $V$ does not depend on the choice of length unit; $V$ can be in whatever unit one desires. But (13) draws attention to the actual physical value that $\delta x$ represents in the grid system. But note that $Q \sim \delta x$, and so $C \sim \delta x$. Thus, when computing $S_h$ via (2), it is seen that $S_h \sim (\delta x)^2 = 1$. In other words, although $\delta x$ is unknown throughout our calculations, all $\delta x$’s cancel out at the end because similarity numbers are
involved in our modelling. Only the relative proportions of shapes and boundary conditions are of importance. The actual physical length scales are irrelevant in computation of dimensionless numbers, Sh and Nu, and this is well demonstrated in our model. The total electric flux through the rectangular prism enclosure is calculated by summing the flux (12) through each of its area elements. From the net flux, the “surface charge” of crystal is computed, and thus its capacitance. The Sherwood number Sh at Re=0 is computed using (2), with δx carried throughout all these calculations but cancelling out at this last stage.

6. RESULTS AND DISCUSSION

The Sherwood number (Sh) for crystal shapes of interest in a cloud physics environment have been computed for zero convection (Re=0) using the methods outlined above. The results are listed in Table 1.

| Crystal Shape | Approximate Sh | Numerical Sh | Difference |
|---------------|---------------|--------------|------------|
| HP            | 2.74          | 2.84         | +3.64%     |
| HC            | 2.48          | 2.36         | -4.83%     |
| BB            | 4.02          | 3.88         | -3.48%     |
| SC            | 5.50          | 5.70         | -3.51%     |
| CC            | N/A           | 5.67         | N/A        |

Table 1: Present numerical calculations of dimensionless mass transfers (Sherwood numbers) of hexagonal plates HP, hexagonal columns HC, broad branched dendrites BB, stellar crystals SC, and capped columns CC; comparisons with previous values of Sh approximated by Mc63 (“Approximate Sh”) and extrapolations by S&L78, with differences.

The “approximate capacitances” which lead to the corresponding approximate Sh were given by Mc63. Using the analytical calculations of capacitances of spheres and thin circular disks of radius r to approximate the capacitances, Mc63, S&L78, and Jayaweera have given expressions for capacitance for the shapes listed in Table 1 (with the exception of CC).

In summary, the numerical methods developed and applied here provide convincing values of the molecular diffusion of water vapour to ice crystals of various shapes when compared with the values obtained by approximations and extrapolations (Mc63). It is also of interest to see that the Sherwood number for capped columns is not much different from the value for columns and that the ordering of the values for Re=0 is consistent with the measurements of S&L78 at higher Reynolds numbers.

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