Mathematical Foundation

The formula displayed below is one that is very familiar to computational scientist, and it is a formula that is easy to solve by using various methods, whether by using a Fourier transform method or by using separation of variables and using eigenvalues and eigenfunctions. However, those methods are under the assumption that the boundary is constant as the variable $t$ increases indefinitely. In problems dealing with crystallization and dissolution, the boundary increases, or decreases respectively, and therefore the traditional methods are not effective.

$$\frac{\partial p}{\partial t} = k \Delta_x \rho$$

Another issue is that the crystal has to follow the laws of conservation. The equation displayed above is actually derived from an integral equation, which can be adapted to handle discontinuous solutions.

$$\int_\Omega \frac{\partial p}{\partial t} d\Omega = k \int_\Omega \Delta_x \rho d\Omega$$

There will be times when the solid we are integrating over changes over time as well. This will lead us to use several different integration concepts that derive from differential geometry and from the divergence theorem. The equation displayed below will give a relation between integration of a partial derivative of a function in respect to time over a solid that changes over time.

$$\int_{\Omega(t)} \frac{\partial p}{\partial t} d\Omega = \int_{\Omega(t)} \rho d\Omega - \int_{S(t)} C \rho dS$$

Where $S$ is the boundary of $\Omega$, and $C$ is the interface speed, or rate at which a point moves towards another point. This is dependent on time and the point in consideration.

$$k \int_{\Omega(t)} \Delta_x \rho d\Omega = k \int_{S(t)} \nabla_x \rho \cdot \vec{n} dS$$

Where $\vec{n}$ is the normal unit vector at a particular point on $S$. In the equations displayed above we arrive at a new equation, which will be displayed below.

$$\frac{d}{dt} \int_{\Omega(t)} \rho d\Omega - \int_{S(t)} C \rho dS = k \int_{S(t)} \nabla_x \rho \cdot \vec{n} dS$$

This equation not only applies to the whole solid, but also to partitions of this solid. Considering that the interior of the solid does not change, or propagate, but only the boundary, we will consider partitions of this solid that contains a portion of the boundary. Also, if we consider a crystal growth or dissolution instead a liquid, then we must model the "liquid" growth. Therefore, we model the mass at a particular time of the liquid and the solid. Therefore, we have a set of two equations, both pertaining to the mass of the liquid and the mass of the crystal. Below are some simulations that models the crystal growth and
dissolution in a liquid. Unless otherwise stated, all the simulations below all simulate the growth of the same crystal in the same liquid, but utilizes different computational methods. Also, each simulation ran in serial uses a 100 by 100 computational grid.