Science in the Kitchen: Numerical Modeling of Diffusion and Phase Transitions in Heterogeneous Media

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Abstract

The science of cooking is crucial to human survival. Cooking enables us to change a normally inedible food and make it edible by adding heat to the food item and therefore changing the composition. In an egg, its raw state involves a high risk of Salmonella if eaten, but via the method of convection in a boiling pot of water, an egg can undergo denaturation and coagulation so that we can eat it. By having a basic understanding of how heat flows and temperature changes in the egg, it is possible to predict cooking times necessary to get a desired egg texture. The non-uniform conservative form of the heat equation analyzed in spherical coordinates and subject to radial symmetry is employed to develop such a model. Then using MATLAB, the PDE is analyzed and predicts cooking times based on the cooking temperature, water temperature, and the radius of the egg. The most interesting aspect of this problem is that the diffusivity is not uniform throughout the egg. Instead it differs between the yolk and albumen of the egg, in addition to at the interface. Once a discrete model is made of the physical situation of boiling an egg in water, the results are compared to experimental results and literature results. Upon completion of the mathematical modeling, our model slightly over-predicted the cooking times, but provided reasonable results that compared better to the experimental results than the literature results. Moreover, the model demonstrates the square relationship between the cooking times and egg radius.

1 Introduction

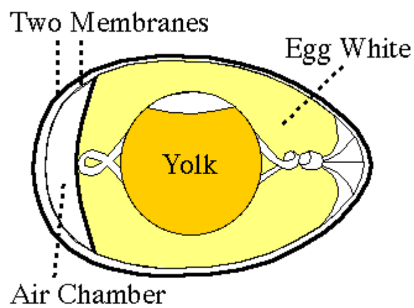
One of the most important necessities to sustaining life is the consumption of food. At the most microscopic level, there are dangers that hinder the consumption of all foods at the most raw state. Simply applying heat to the system can result in a change of state or texture allowing for the food that once a health hazard to become a savory dish. This is the foundation of the science of cooking.

In the case of an egg we run the risk of serving Salmonella if not cooked properly. Cooking utilizes the fundamentals of conduction, the process of transferring heat into any solid, and convection, the transfer of heat from a fluid to its surroundings. Yet how exactly does cooking work? A temperature gradient forms when two objects at different temperatures are placed close together. The heat flow causes the temperature to rise in the colder body and since the boiling water is constantly being supplied thermal energy from the stove, it will remain constant. Then thermal equilibrium is reached and no more heat flows [5].

By applying these methods we increase the range of foods we can eat and reduce the risk of food poisoning.This project entails developing a mathematical model of thermal diffusion within an egg being boiled. The issue with cooking the 'perfect boiled egg' is that everyone desires a certain texture; every egg is different so it also cooks differently and the equipment used varies [5]. Therefore the goal is to apply the model to predict phase transitions from a liquid to a solid state in the yolk and egg white and to predict phase transitions from liquid to solid in the yolk and no phase transition in the egg white.

Before creating a model, it is essential to learning what the parts which make up an egg are. An egg is composed of three primary parts: the shell, the albumen or egg white, and the yolk. Each of these parts has their own thermal diffusivity constant which is the measure of thermal inertia [7]. As heat is applied to the egg its proteins undergo the process known as denaturation [5]. Visually we see this as the albumen becoming opaque and once it has reached this phase transition we determine how well an egg is cooked [6]. By understanding the basics of the manner in which heat flows into a body, we can predict the cooking times for any situation to obtain a desired texture. From the literature, we expected that if our model was appropriately modeling the situation, we would get similar results from the literature equations and ours for the cooking times and also that there would be a square relationship between the mean radius of the dish and the cooking time [5].

Figure 1.1 - Egg Composition



2 Three Dimensional Heat Equation Derivation

Fortunately, modeling an egg does not require us to start from nothing. Instead, the fundamental partial differential equation known as the heat equation can be used to begin the modeling of an egg boiling in water. Although it is possible to just start with the heat equation, a quick derivation of the PDE helps us recognize that all the factors contributing to heat flow (specific heats, density, and thermal conductivity) all are included in the derivation even though the heat equation itself does not demonstrate their influence as noticeably. First, let us define the variables that will be used in the derivation as follows:

- c: specific heat
- ρ: density
- u(x,y,z,t): temperature of the material at location (x, y, z) at time t
- Q(x,y,z,t): amount of heat energy generated
- ϕ(x,y,z,t): heat energy flux
- K: thermal conductivity
- D: thermal diffusivity

By applying the Divergence Theorem to a material bounded by a surface S with unit normal vector n and occupying the three dimensional region R, we obtain the following:

$$\int\int_S F \cdot ndS = \int\int\int_R \nabla \cdot FdV \tag{1}$$

Considering the heat energy contained in region R at time t, the value is

$$\int\int\int_R c\rho udV \tag{2}$$

The heat energy then leaving R through S is given by

$$\int\int_S \phi \cdot ndS \tag{3}$$

Meanwhile, heat energy is being generated in region R and is quantified by the following:

$$\int\int\int_R QdV \tag{4}$$

Now by applying the conservation of heat energy law in region R, we see the following upon simplification.

$$0 = \int\int\int_R (Q - \nabla \cdot \phi - c\rho \frac{\partial u}{\partial t})dV \tag{5}$$

R is an arbitrary three-dimensional region, so from the conservation law we get

$$c\rho \frac{\partial u}{\partial t} + \nabla \cdot \phi - Q = 0 \tag{6}$$

Fourier's Law of Heat Conduction can then be stated as:

$$\phi = -K\nabla u \tag{7}$$

By performing substitutions and assuming no sources, we get this:

$$\frac{\partial u}{\partial t} = D\nabla^2 u \tag{8}$$

This is the heat equation seen in PDEs. Notice that despite only seeing temperature, time, and thermal diffusivity in the final result, the derivation of the equation utilized the most important factors when considering thermal diffusion. Therefore, it is appropriate to use as a basis for our model. Also, the thermal diffusivity in this equation is dependent on the conductivity, density, and specific heat.

$$D = \frac{K}{c\rho} \tag{9}$$

However, we need the general non-uniform conservative form of the heat equation. Therefore, the following equation is the one we want.

$$u_t = \nabla \cdot (Dgrad(u)) \tag{10}$$

The heat equation is generally expressed in Cartesian form, but since we are studying an egg, we want to analyze it in spherical coordinates. Therefore the following coordinate transformation equations can be applied to the Cartesian model to convert it into the spherical three-dimensional model.

$$x = \rho sin\theta cos\phi \tag{11}$$

$$y = \rho sin\theta sin\phi \tag{12}$$

$$z = \rho cos\theta \tag{13}$$

Once the equations above are applied, the following three dimensional spherical heat equation is observed.

$$\frac{\partial u}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}(Dr^2\frac{\partial u}{\partial r}) + \frac{1}{r^2 sin\theta}\frac{\partial}{\partial \theta}(Dsin\theta\frac{\partial u}{\partial \theta}) + \frac{1}{r^2 sin^2\theta}\frac{\partial}{\partial \phi}(D\frac{\partial u}{\partial \phi}) \tag{14}$$

From this equation we assume radial symmetry. Consequently the $\frac{\partial}{\partial \theta}$ and $\frac{\partial}{\partial \phi}$ partial derivatives are assumed to be zero. This simplifies the equation and yields the following PDE:

$$\frac{\partial u}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}(Dr^2\frac{\partial u}{\partial r}) \tag{15}$$

3 Finite-Volume Method

Though we have a governing equation for our situation, we do not actually want to 'solve' the PDE previously derived. Instead we developed a finite volume approximation of the heat equation stated above. There are three primary reasons that we do not want to solve the PDE.

1. The homogeneous solution uses infinite series of Bessel functions which are rather complicated.
2. To solve the non-homogeneous PDE, we would need to 'stitch' two of the infinite series together.
3. MATLAB solves PDEs via numerical approximations and our ultimate plan is to code our model to predict cooking times and observe the behavior

The Finite Volume Method starts by taking our governing PDE and applying it to the discretized domain of the egg [2].

Since we are able to transform the volume integrals to surfaces integrals using the Divergence Theorem, we are able to evaluate each of these discrete terms as fluxes at their surfaces [2].

This simplifies the process of creating a computer model because it allows us to account for the change in diffusivity between the egg white and the egg yolk [2].

In this model, flux is a conserved quantity because the flux entering each volume is equal to the flux leaving the adjacent volume [2]. The resulting equation from this analysis is as follows:

$$\frac{\partial u}{\partial t}|_{r_i} = D(\frac{2}{r_i}\frac{u_{i+1} - u_{i-1}}{2\Delta r} + \frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta r)^2}) \tag{16}$$

4 Defining Diffusivity

The most interesting aspect of our problem is that an egg has a non-uniform diffusivity. As shown in the derivation of the heat equation, the thermal diffusivity constant is dependent on material properties such as specific heat, density, and thermal conductivity [1]. Therefore, the constant will be different between the yolk and the albumen.

By researching the thermal diffusivity constants of the yolk and albumen separately, we determined that D_w=0.37e-05 and D_y=1.66e-05 [3]. However the interface between the two is not a specified value. Instead we needed to analyze mathematically the interface between the yolk and albumen.

Consider the flux at r_i which is denoted by F_i. The flux must be continuous. So taking two points, r_i and r_{i+1}, in which the transition is supposed to occur in the middle, $r_{i+1/2}$. The flux at i+1/2 is then

$$F_{i+1/2} = D_{i+1/2}\frac{1}{r_{i+1/2}^2}\frac{\partial u}{\partial r}l_{i+1/2} \tag{17}$$

By employing the centered difference method, the above equation becomes

$$F_{i+1/2} = D_{i+1/2}\frac{1}{r_{i+1/2}^2}\frac{u_{i+1} - u_i}{\Delta r} \tag{18}$$

By considering the flux from the left and the right and then implementing the fundamental theorem of calculus, the flux at the interface then becomes

$$F_{i+1/2} = D_{i+1/2}\frac{1}{r_{i+1/2}^2}\int_i^{i+1}\frac{\partial u}{\partial r}dr \tag{19}$$

Applying the linearity principle to the left and right considerations of the above equation and solving the integrals and simplifying results in the following:

$$F_{i+1/2} = D_{i+1/2}(\frac{F_{i+1/2}^-}{2\alpha} + \frac{F_{i+1/2}^+}{2\beta}) \tag{20}$$

Since the fluxes are all equal, we can divide by $F_{i+1/2}$ and solve for $D_{i+1/2}$. This yields the following:

$$D_{i+1/2} = \frac{2\alpha\beta}{\alpha + \beta} \tag{21}$$

This result states that the diffusivity at the interface is equal to the harmonic mean of the yolk and albumen diffusion constants (α is the diffusivity constant in the albumen and *beta* is the diffusivity constant in the yolk). Therefore, the piecewise function for the diffusion constant is given by this:

$$D(r) = \begin{cases} D_y & r < 0.5r_{egg} \\ \frac{2D_wD_y}{D_w+D_y} & r = 0.5r_{egg} \\ D_w & r > 0.5r_{egg} \end{cases} \tag{22}$$

5 Code

Now we have a discrete finite volume approximation and have defined a continuous diffusivity coefficient, it is possible to code our model. Using MATLAB we developed a basic code. The theory behind the code is outlined as such:

1. Break the domain of the egg up into many infinitesimally small segments.
2. At a specificed time, calculate the temperature at each point in the egg using the equation from the finite volume approximation model.
3. Repeat the calculations at small time steps until the temperature at the center of the yolk is a specified temperature.

Within the code, the cooking temperature, water temperature, radius of the egg, and the diffusivity constants were fixed.

6 Experimentation

Using the code to predict the cooking times for the yolk to reach a desired temperature, our goal was to determine how reasonable the cooking times were in a real situation. Therefore we bought two dozen eggs from the store, one dozen being large eggs and the other dozen being extra large eggs. We then measured the circumference of the eggs and calculated the diameters to be 4.584 cm and 4.902 cm for the large and extra large egg respectively.

After bringing water to a boil in a pot on the stove, we placed an egg in the water from the refrigerator and used a stopwatch to cook the egg for the time specified by our code to reach the desired temperature. When the time was up, we quickly removed the egg and cut it in half. Then using a cooking thermometer, we measured the yolk temperature. This process was reached for multiple desired temperatures at different cooking times and for both egg sizes.

Once we completed the experiment to validate our model, we then used our model to compute the time it would take to cook an extra large egg so that the yolk solidified, but the white did not.

7 Results

After experimental procedures were taken using the code, the time values for the large and extra large egg were taken to observe its comparison to the literatures model [5]. Below is the table showing the temperature in the yolk to time relationship for a large egg and an extra-large egg.

Figure 7.1 - Cooking Times Predictions from MATLAB Code

LARGE EGG		EXTRA-LARGE EGG	
Temperature (°C)	Time (min)	Temperature (°C)	Time (min)
58	8.4	58	9.7
64	9.3	64	10.6
66	10.1	66	11.6
70	10.9	70	12.6
80	13.5	80	15.4

The chosen temperatures act as a marker for where the phase transitions would occur according to the literature. The table suggests that, naturally, the yolk in the extra-large egg takes longer to reach these temperature transition points. It is essential to refer back to the literature model to observe whether or not their equation yielded similar results [5]. Therefore, using the following literatures mode we plug in our own parameters [5]:

Figure 7.2 - Equation and Variables from Literature

$$t = 0.0015d^2 log_e[\frac{2(T_{water} - T_0)}{T_{water} - T_{yolk}}]$$

d: diameter of the egg (mm)
T_0: temperature of the egg before it was put into the water (C)

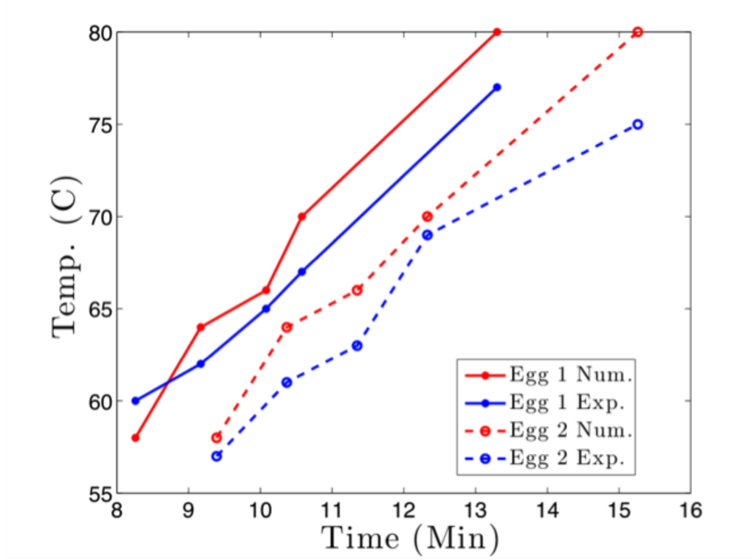
The following table shows the results using the literatures model [5].

Figure 7.3 - Cooking Time Comparisons between Literature and MATLAB Code

LARGE EGG			**EXTRA-LARGE EGG**		
Temperature (°C)	**Literature Time (min)**	**MATLAB Time (min)**	**Temperature (°C)**	**Literature Time (min)**	**MATLAB Time (min)**
58	4.9	8.4	58	5.5	9.7
64	5.3	9.3	64	6.1	10.6
66	5.5	10.1	66	6.3	11.6
70	5.9	10.9	70	6.7	12.6
80	7.2	13.5	80	8.1	15.4

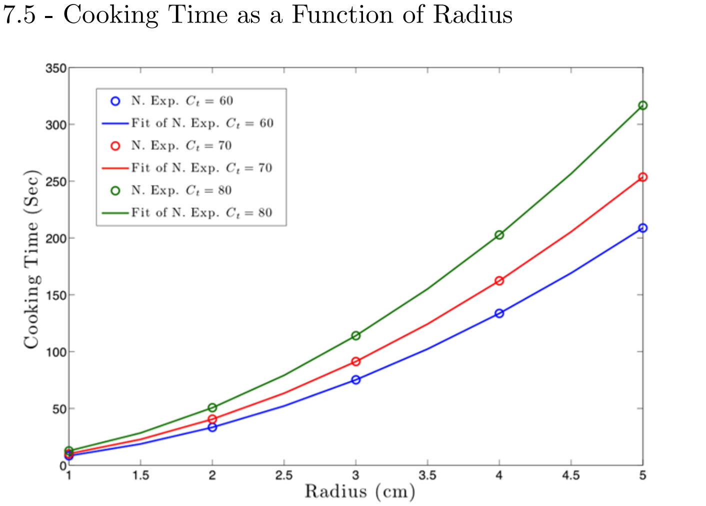
At first glance there are prevalent gaps shown between the literatures model and this projects code. The literatures model falls short of real-life application because realistically it takes more time to cook an egg so this is clearly an under prediction. In our case, the coded model makes a slight over prediction in comparison to the experimentally calculated time to temperature transition point as shown in the figure below.

Figure 7.4 - MATLAB Results vs Experimental Results



Lastly, once the analysis of the results we found that the cooking time depends on the square of the radius of the egg and by cooking the egg at a lower temperature, we were able to cook the yolk so that it is solid without solidifying the egg white. Thus, a square relation was calculated such that it suggests a consistent correlation displayed by the figure below.

Figure 7.5 - Cooking Time as a Function of Radius



The previous figure shows that even when the radius of the egg is manipulated, it has a consistent square relation.

Below are some pictures taken during experimentation. Figures 7.6 and Figure 7.7 shows a side-by-side progression of the phase transition in the egg for the cooking times developed by our MATLAB code. The difference between the two figures is the Figure 7.6 corresponds to the experiment conducted using the large egg and Figure 7.7 corresponds to the experiment conducted using the extra large egg.

Figure 7.6 - Large Egg At Different Cooking Times

Figure 7.7 -Extra Large Egg At Different Cooking Times

Figure 7.8 on the other hand demonstrates that it is possible to cook the yolk so that it solidifies while the egg white remains liquid-like.

Figure 7.8 - Large Egg At Different Cooking Times

8 Conclusion

In relation to the literature approach, one can see that this finite volume approximated use into MATLAB yielded much more realistic results [5]. This model fit well for our goals because we predicted some variation of a square relation to still hold in reference to the dish being heated [5]. It is true that our model did not yield similar results to that of the literatures model, yet it is our model which has shown superior results when measured again experimentally determined data.

Although the numerical method slightly over predicts the experimental relation, it satisfies the purpose of serving safe food. This model can be applied to get the desired texture of a dish and it estimates an effective cooking time. By use of convection from the boiling water to the egg our model used the spherical heat equation to then be transformed into code that could more easily solve the partial differential equations through finite volume approximation. Creating the connection between this approximation and the harmonic mean meant that the varying diffusion s could be defined. Allowing for the different diffusions meant that the numerical analysis could be applied to initiate experimental procedures using the literature model and our MATLAB code.

The result is an understanding of the behavior of boiling eggs at various times and temperatures and a stronger foundation on range of foods that can be consumed when the right amount of heat is applied and when the right amount of time is applied. Our model successfully provided the numerical approximations necessary to produce an egg that predicts phase transitions in the egg.

9 References

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