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

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Abstract

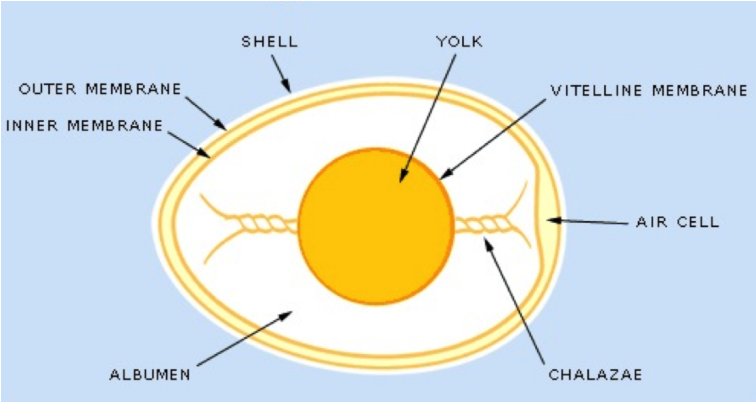
Boiling an egg in water is a common kitchen occurence throughout the world. As simple as the situation seems though, developing an accurate ad realistic model of the situation is not so simple. A discontinuous diffusion coefficient function due to the egg composition in addition to an undefined geometric egg shape provide the foremost problems in analysis of this situation. By making numerous assumptions, a very basic model can be developed of the egg which assumes a constant diffusion coefficient. Namely the heat equation from an introductory course on partial differential equations and a finite difference approximation of said equation were obtained as the foundamental, assumption-dominated model. However, removing the assumption of a constant diffusion coefficient, making it a piecewise function, and ignoring the discontinuity at the interface between the albumen and yolk, another partial differential equation is obtained along with a finite volume approximation equation. The aforementioned equations will be tested in an applied analysis lab to confirm the resulting equations. Ultimately the goal is to obtain a three-dimensional model of the egg boiling in the water and then attempt to cook the yolk of the egg without cooking the albumen.

1 Introduction

A mathematical model provides a description of a system using concepts and language from the field of mathematics. By mathematically modeling situations, predictions about the system's behavior can be ascertained in an efficient manner. Used in disciplines including engineering, natural sciences, business, and social sciences, mathematical modeling has a strong influence on the inner-workings of all society. Here, a mathematical model of science in the kitchen is applied to the seemingly simple situation of a boiling egg.

An egg is composed of three primary materials: the shell, the albumen, and the yolk. In general,the shell accounts for 9% to 12% of the total weight of the egg. The shell color, size, and strength primarily depend on the egg-producing animal's age and diet. Shells are porous solids that are sealed via a protective coating called a cuticle, which depends on the quality of the eggs and can be removed simply by washing the egg. Regardless of how the egg is produced though, shells are very thin and weak in comparison to the rest of the egg. The albumen is more commonly referred to as the egg white and makes up approximately 67% of the liquid weight of a standard hen's egg. As the egg itself ages, the white becomes thinner as the protein composition changes and it becomes more transparent with a lowering coagulate temperature range [3]. Coagulating refers to the change of a substance to a solid state [4]. Consequently, as an egg ages, it takes a shorter amount of time to boil that egg [4]. The remaining 33% of liquid weight that constitutes the total liquid weight of an egg is referred to as the yolk. The yolk is where all the fat resides in addition to approximately half the protein. It is composed of many substances and elements including phosphorus, iron, copper, calcium, vitamin D, etc. In contrast to the albumen, the coagulation occurs within the constant range of 65 to 70 degrees Celsius. Below is a picture of egg composition discussed above. Notice that there are thin membranes that separate the primary components of the egg in addition to the air cell and chalazae, which are an air space and anchors the yolk in the center of the egg respectively.

Figure 1.1 - Cross Section of an Egg



There are two general methods employed to boil an egg; soft-boiling and hard-boiling. Soft-boiling involves cooking the egg for a shorter amount of time than hard-boiling and refers to the firmness of the yolk upon conclusion of the cooking time frame. In both cases, there are two options within each method. One technique starts the egg in cold water, which is then brought to a boiling state, while the second involves boiling the water first and then inputting the egg. The manner in which the egg is cooked, whether it be soft-boiled or hard-boiled as an end result, is crucial to the modeling of this process [4].

An egg is boiled and therefore cooked through a temperature gradient by a process known as thermal diffusion or thermodiffusion. Thermal diffusion is the process by which the temperature inside a substance is changed to reach an equilibrium state, which is defined at a constant temperature. Temperature changes occur more appropriately by energy transfer from a warmer region to a colder one, which is defined by heat. Therefore, heat and temperature are distinct yet interrelated scientific quantities. Once the temperatures are consistent between regions, heat ceases to flow and the equilibrium state is defined.

The rate of thermal diffusivity depends on material properties and hence changes based on substance composition [1]. The specific heat is, just as it sounds, unique to the substance it defines and refers to the amount of heat required to increase the temperature of one kilogram of said substance by one degree Celsius. It is this property that determines the rate at which temperature changes from the heat flow. The state of the substance is equally as important to the specific heat, though. Introductory chemistry concepts state that the temperature does not change when a substance is changing its state, i.e. going from liquid to solid. This is important to remember as the boiling of an egg is studied [3].

Furthermore, the rate of heat flow is dependent on how the bodies are in contact, the speed of heat flow in the objects, and the difference in the temperature of the two objects that create the temperature gradient and thus causes thermal diffusivity to occur. Since heat transfer is causing the temperature difference to shrink as the bodies reach equilibrium, intuitively it is known that the rate of heat flow decreases as the bodies reach that equilibrium state. Additionally, the thermal conductivity is crucial with respect to the thermal diffusion [1]. Thermal conductivity is defined as the rate at which heat will flow through a body and a perfect thermal conductor transmits the energy instantaneously and is impossible to observe in the real world. With that being said, a perfect thermal conductivity is a reasonable idealization to employ when developing some models of substances [3].

Convection is the method of heat transfer associated with the boiling of an egg and many other domestic heating applications. Simply stated, convection is the transfer of heat from a fluid, which may be a liquid or a gas, to its surroundings. This method of heat transfer consequently results in the temperature at any point in an object being heated to be dependent on both the time that the object has been placed in the surrounding fluid and on the position inside the object the temperature is being measured at. Designating that an object is cooked means that said object was placed at some high temperature for a specified time. Therefore, the heat from the surrounding fluid diffuses into the object being cooked.

2 Constant Diffusion Equation Derivation

Now that we know we are working with convection and thermodiffusion inside a egg being boiled, the next step is to develop a very simple equation that models the situation aforementioned. However, the egg presents a few immediate problems, which are as follows:

1. The egg is not an easily defined geometric shape.
2. The egg is composed of a shell, white, and yolk each consisting of a different thermal diffusivity constant.
3. The properties at which each part of the egg changes state depends on the elemental and protein composition of each part.
4. The boundaries will shift slightly as the state of the albumen and yolk solidify since solids are more compact then liquids.
5. The surrounding temperature can vary.

To account for these problems and aid the development of a simple model of the thermal diffusion in an egg, various assumptions were made.

1. Assume the egg is a perfectly spherical object.
2. Assume the shell is infinitesimally thin and a perfect thermal conductor.
3. Assume the diffusion coefficient in the albumen and yolk are equal.
4. Assume the effects of chemical variations in each primary part of the egg can be ignored.
5. Assume the boundaries are fixed.
6. Assume the surrounding temperature is constant.

For the sake of simplicity, a one-dimensional analysis is applied for the initial derivation of a model. Therefore, with the 1D analysis and assumptions stated above, a model can be developed. Stokes' Theorem permits the computation of flux through a surface. The flux is also the rate of change of temperature with respect to time. As a result, Stokes' Theorem unveils the following equation.

$$\frac{\delta u}{\delta t} = \int_{s\Omega} f \cdot \vec{n} ds\Omega = \int_{\Omega} \nabla f d\Omega \tag{1}$$

In this equation, u(x,t) is the temperature at position x after time t, sΩ is the Gaussian surface defining the egg, and f is the flux. From this, the goal is to find u(x,t) and how it changes with respect to time. Fick's First Law provides us a means of writing the flux in a different way. Fick's First Law relates the flux to the diffusion constant, D, and the temperature via this equation.

$$f = D\nabla u \tag{2}$$

By using equations 1 and 2 together, equation 3 is obtained. Equation 3 is important because it holds for every point in the egg.

$$\frac{\delta u}{\delta t} = \nabla \cdot [Dgrad(u)] \tag{3}$$

However, taking the one-dimensional analysis into consideration, equation 3 becomes the partial differential equation seen in equation 4.

$$\frac{\delta u}{\delta t} = \frac{dD}{dx}\frac{\delta u}{\delta x} + D\frac{\delta^2 u}{\delta x^2} \tag{4}$$

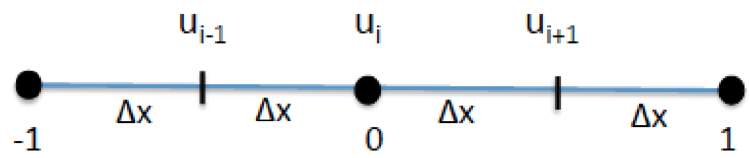
Equation 4 is the governing equation for a simplified model of an egg boiling in water. However, the objective is not to obtain a model subject to errors, but instead obtain the most exact model possible for this situation. As simple as this model is, applying the assumptions above simplifies it more and permits analysis of the model. Assuming the egg is centered on the x-axis so that the outer boundaries are at x=-1 and x=1 and taking the temperature at the boundaries to be the temperature of the constant water temperature provides the necessary boundary conditions. Additionally, an initial condition is necessary for analysis in which the state of the egg is given by f(x), which is initial heat distribution profile. Moreover, equation 4 simplifies to the following since we are assuming D is constant.

$$\frac{\delta u}{\delta t} = D\frac{\delta^2 u}{\delta x^2} \tag{5}$$

Equation 5 is an introductory partial differential equation known as the heat equation, and from a beginning course in partial differential equations, it is possible using the method of separation of variables and Fourier series to analyze equation 5. With that being said, the goal is to obtain a more complex and exact model, which starts by making a finite difference approximation of the heat equation.

Finite difference approximations call on the method of undetermined coefficients and visually are defined by figure 2.1 below. Equation 6 is the direct result from the approximations and Taylor series expansions of the neighboring temperatures demonstrate the error involved from the approximations [2].

Figure 2.1 - Finite Difference Approximation Visual



$$\frac{\delta u}{\delta t} = D\frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} \tag{6}$$

The error is demonstrated by equation 7.

$$\frac{\delta^2 u}{\delta x^2} + \frac{\Delta x^2}{4!}\frac{\delta^4}{\delta x^4} = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} \tag{7}$$

Obviously $\frac{\Delta x^2}{4!}\frac{\delta^4}{\delta x^4}$ is the term that accounts for the error resulting from the finite difference approximations. However, this error was acceptable for practical analysis of the situation for the assumptions made. Therefore, MatLab can be employed to visualize the results obtained with greater ease.

By using a simple code with fixed constants and setting a desired end temperature for the center of the egg to reach, it is obvious to understand the behavior of the thermal diffusivity of an egg boiling in constant-temperature water. Table 2.1 below shows results based on equations 5 and 6 implemented in a code. The table demonstrates that a fixed value of D, the diffusion constant, was selected and the equations used in MatLab produced different time values based on the diffusion constant value, as expected.

Table 2.1 - MatLab Time Results for Different D Values

Diffusion Coefficients	Time
$1x10^{-1}$	4.6
$1x\ 10^{-2}$	44.8

Some important parameters and variables distinguished in the code to result in the values obtained in table 2.1 are as follows:

Table 2.2 - Fixed Values for Code

Water Temperature	Desired Center Temperature	Time Step
100	60	1.6s

From this table, notice that it took about ten times longer to reach the desired temperature at the center of the egg, according to our model, when the diffusion constant was decreased by a factor of ten. This observation results from the direct relationship between the diffusion constant and the thermal diffusion rate with respect to time seen in equations 4 and 5 above. Now the diffusion constant is a material property, but it is obvious that a material with a higher diffusion constant will take a shorter time to reach thermal equilibrium.

Equally as important to observe, figures 2.1 through 2.3 below demonstrate the unique initial temperature distribution throughout the egg, the increased continuity of the curve as time progresses, and the final temperature distribution in the egg once the desired center temperature is reached.

Figure 2.1

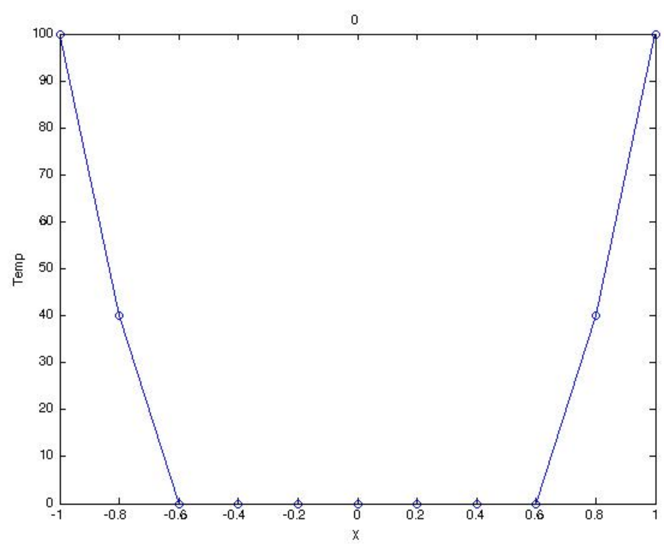


Figure 2.2

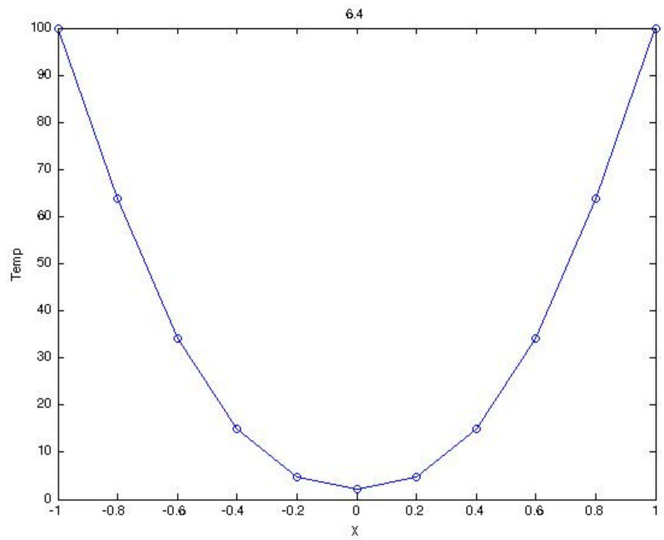
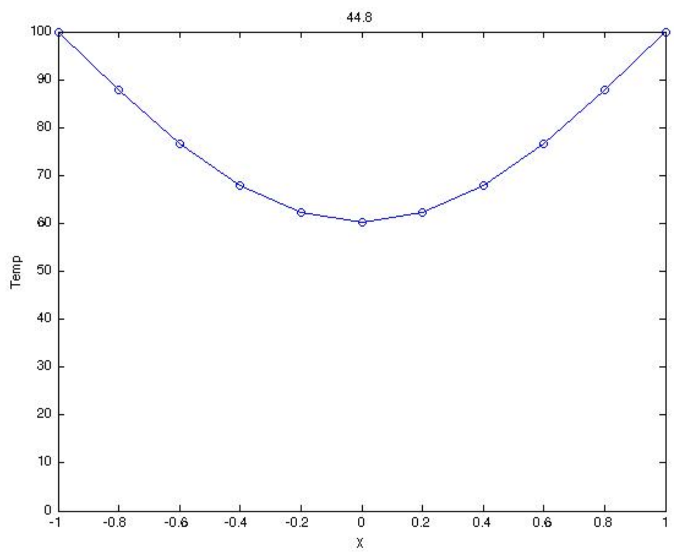


Figure 2.3



Though the equation derived and tested in MatLab provides expected information and results governing an egg boiling in water, it required various assumptions that are unrealistic. Ultimately, a mathematical model providing the most exact and realistic description of this situation is to obtained. From this simple model, a more complex model can be found by eliminating assumptions. The first assumption to be removed is that of a constant diffusion coefficient, D.

3 Varying Diffusion Equation Derivation

As aforementioned, the diffusion constant is a material property and therefore will differ values in each of the primary regions in an egg. Considering the diffusion coefficient in the yolk to be D_y and the diffusion coefficient in the albumen to be D_w, this problem presents a discontinuity at the interface between the two regions. From first-year calculus, it is known that derivatives only exist for continuous functions. Here the piecewise function is not differentiable, however for the sake of simplicity this problem is ignored. Equation 8 shows the diffusion function.

$$D(x) = \{ \begin{array}{cc} D_y - 0.5 & x \leq |0.5| \\ D_w & x > |0.5| \end{array} \tag{8}$$

Since the equation above confirms that the diffusion constant will vary according to the position x in the egg, equation 4 applies to this situation. The boundary conditions and initial condition are the same as before, but flux and the derivative of the flux must be computed yet again. Previously, finite difference approximations were applied to derive the constant diffusion coefficient equation. However, the same method cannot be applied here. Instead, finite volume approximations must be employed to find the previously ignored $\frac{dD}{dx}\frac{\delta u}{\delta x}$ term distinguishing equations 4 and 5 from each other.

The flux for the varying diffusion problem is as follows:

$$f_{i+1/2} = D_{i+1/2}\frac{u_{i+1} - u_i}{\Delta x} \tag{9}$$

Equation 9 is differentiable and by taking the derivative equation 10 is obtained.

$$\frac{\delta}{\delta x} f_{i+1/2} = \frac{f_{i+1/2} - f_{i-1/2}}{\Delta x} \tag{10}$$

Putting the results from equations 9 and 10 together, an equation for the rate of change of temperature with respect to time is discovered. Equation 11 below is the varying diffusion constant equation for an egg being boiled in water developed via finite volume approximations. Just as in proceeding section, the error involved by applying this method to the generalized model can be seen using Taylor Series Approximations and a similar error value would result.

$$\frac{\delta u}{\delta t} = \frac{D_{i+1/2}(u_{i+1} - u_i) - D_{i-1/2}(u_i - u_{i-1})}{\Delta x^2} \tag{11}$$

Notice that if the diffusion constant does not vary, then equation 6 is obtained again. Equation 11 is approximately equivalent to the more involved partial differential equation found previously and denoted by equation 4. Despite this visually more complex equation, recall that there were numerous assumptions constraining the accuracy of the equation. Reference section 0.2 to see the assumptions again.

4 Conclusion and Next Steps

To summarize, studying the thermal diffusion in an egg boiling at constant temperature in water is an interesting and deceivingly complex situation to study. Composed of three primary parts and not easily defined by a standard geometrical figure, the egg is difficult to develop a mathematical model for. By removing assumptions systematically, more realistic models can be obtained to aid analysis of this everyday situation. Beginning with equations 5 and 6, a model distinguished by the constant diffusion assumption, which were obtained as described in section 2 provide a fundamental and basic model of the aforementioned situation. Acknowledging that the diffusion constant is a material property and that the egg is composed of three distinct materials essentially, a piecewise function for the diffusion coefficient was implemented in section 4. Consequently equations 11 and 4 model an egg with two diffusion constants boiling in water. Though the latter two equations are more complex, they are still heavily dependent on various assumptions and require further development to get a more realistic model.

At this point, there is a lot of analysis still possible. Prior to proceeding however, the goal is to validate the behavior described by our equations to confirm their reliability at this point. From the equations, there is an obvious relationship that the rate of thermal diffusion is directly related to the diffusion constant, as expected. Moreover, there is an important and intriguing relationship occurring with respect to the position inside the egg. However, other characteristics of the egg may also be significant but not described in the current mathematical model. For example, varying the width and even type may change the rate of thermal diffusion. For these reasons, an applied analysis lab will provide an opportunity to test the current equations. In the tests, different chicken eggs will be tested along with an ostrich egg to visualize the scenario more fully.

Upon confirmation of the results obtained here, the next step is to develop a three-dimensional model of the egg. This is an important step towards obtaining a realistic model simply because an egg is a three-dimensional figure and not spherical or even easily defined geometrically speaking. Notice that again, our process is to systematically eliminate assumptions stated in section 2. The assumptions made were of an ideal and impossible egg-boiling situation. Hence, by decreasing the number of assumptions, the model becomes more real. Once the three dimensional model is developed, again it will be put to the test in an applied analysis lab. To test the model, the goal will be to cook the yolk of the egg without cooking the albumen. Through a clear understanding and model of the diffusion rate in each part of the egg, cooking the yolk to be solid while the albumen remains liquid should be possible. At a glance, proceeding from this point will result in the following three dimensional and spherical model of the egg:

$$\frac{\delta u}{\delta t} = \frac{1}{r^2}\frac{\delta}{\delta r}(Dr^2\frac{\delta u}{\delta r}) + \frac{1}{rsin\theta}\frac{\delta}{\delta\theta}(Dsin\theta\frac{\delta u}{\delta\theta}) + \frac{1}{r^2sin^2\theta}\frac{\delta}{\delta\psi}(D\frac{\delta u}{\delta\psi}) \tag{12}$$

This equation will be derived and developed extensively moving forward. By developing a code, using the simple results obtained above, and further studying equation 12, a more applicable and significant mathematical model will result permitting us to make attempts at goals previously stated.

5 References

[1] Aslamazov, L. G., A. A. Varlamov, and A. A. Abrikosov. The Wonders of Physics. Singapore: World Scientific, 2001. 37-52. Print.

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