Name: **Nathan LeRoy**

| **Take home assignment (Individual): Building the model (Due beginning of class 9/27)** | |
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| **Please outline and describe how your model works in terms of computational structures. For each structure, please explain why the programming technique or process used was chosen. Include as much detail as possible, doing this for each computational structure within your model (groups of variables, loops, conditional statements, sets of equations etc).** | |
| Computational Structure: | How does it work? Why was it programmed this way?<br><br>**Commenting here on every single computational structure is WAY beyond the scope of this document as our source code is more than 600 lines. Each structure is outlined in incredible detail in the comments in my code. This is in addition to the fact that many structures are repeated.**<br><br>**However, I will highlight some large, repeating components.** |
| %CLEAR THE VARIABLE SPACE:<br>%This block of code (Lines 10-12) | is used to clear MATLAB of all variables<br>%and to close all currently open windows. This block of code does not<br>%represent anything physically in the model, it merely sets up the program<br>%for running this script. This block of code is included to prevent<br>%variable name mixups between scripts and to clean up the workspace. |
| %DEFINE THE PHYSICAL COMPOSITION OF OUR PUMPKIN PIE FILLING:<br>%This block of code (21-26) | initializes mass fractions for each food component.<br>%All data on physical composition was found on the USDA food database. This<br>%data is necesssary as it allows us to calculate the relevant thermodynamic<br>%properties of our food item. Without them, no analysis on the temperature<br>%profile of our food over time could be done |
| DEFINE INITIAL CONSTNATS AND CONDITIONS:<br>%This block of code (38-41) | serves to set and define the initial condtions of<br>%our system. This is essential for solving our system numerically. We must<br>%know the initial temperature profile of our can and the tempereautre of<br>%the steam in order to begin transient anaylsis. Hewre we will also define<br>%the time and size steps in both dimensions for numerical analysis. This<br>%code block will also serve to initialize our matrix that will store and<br>%iterate through our data. |

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| %INITIALIZE OUR DATA MATRIX:<br>%This block of code (59-75) | serves to initialize our matrix with the initial<br>%conditions of our system. Currently, the matrix is a zero matrix - we want<br>%to populate the entire thing with the initial temperature of our food<br>%product. Then, we want to initialize the outermost layer with our steam<br>%temeprature. This will serve as the starting point for the finite<br>%difference method.<br><br>%To optimize our code, it is necessary to predfine the size of our<br>%matrices. Otherwise, a large portion of our computational power is devoted<br>%to extending the memory of our matrices and can lead to sub-optimal<br>%performance when solving the finite difference method. We can do this by<br>%simply defining a zeros matrix that will be populated later. |
| %FINITE DIFFERENCE METHOD AND CALCULATION:<br>%This block of code (88-120) | is the meat and potatoes of our algorithm. This nested<br>%loop will iterate through each time step and each slice, calculating the<br>%chage in temperature in both space adn time dimensions. Theoutermost loop<br>%iterates through each time point. At each time, we get to the next loop<br>%with iterates through each slice. The finite difference equation from<br>%geankopolis is used to get the temeprature gradient. Notice that the inner<br>%loop decrements. This is becasue the largest n is our outer-most slice,<br>%while an n of 1 corresponds to the center. |
| %CALCULATE LOG REDUCTION IN CAN:<br>%This code (146-169) | allows us to calcualte the log reduction in the center of<br>%the can over time. It should be noted that we ASSUME a very long process,<br>%and then find the time-point where a 13.5 log reduction is achieved at the<br>%center. This time-point will be used as the heating process time and the<br>%temperature profile will be recalcualted. Without this recalculation, the<br>%cooling profile would be off and not accurate, as the material wuld be<br>%hotter than it is supposed to be. We choose to calculate the log-reduction<br>%here using the F0 method given our D250 value, and z-value. The units for<br>%this calculation are in seconds and Fahrenheit. |

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| %CALCUALTE AVERAGE TEMPERATURE:<br>%This block of code(391-408) | will calcualte the average temperature in our can for<br>%each time-point. This is done by weighting the temperature in each slice<br>%by its relative volume in the can as awhole, and then summing these<br>%temperatures up. It is the discrete version of the average value theorem.<br>%it also looks for and fidns the time the average temperature is the<br>%required exit temperature in our can. |
| %PLOT THE DATA:<br>%This section of code (541-593) | serves to only present the data visually to the user.<br>%This is imperitive to help the user visualize what is occuring inside our<br>%can over time and amake education decisions on what the optimized<br>%paramters and steps need to be. |

**Please describe any assumptions made during the modeling process and why those may have been good or appropriate assumptions?**

| Assumption(s): | Why did you make this assumption? | How does this impact how your model works? |
|---|---|---|
| **1. Thermal Resistance is limited to conduction within the can.** | This is actually a pretty good assumption for the heating process. Heated steam has a very high convective heat transfer coefficient. For the cooling water, the assumption of negligible convective resistance was again made as it allowed us to re-use the finite difference model developed for the heating. | For the cooling process, this will affect how quickly our can cools. In reality there is a finite amount resistance due to convection, and we may be underestimating the time required to cool the cans. |
| **2. Heat transfer is unsteady state and one dimensional** | To greatly simplify the finite difference model, we assume that heat transfer only occurs radially. This is actually a pretty good assumption as we can imagine stacking our cans on top of each other in the retort producing a pseudo-infinite cylinder. | Assuming one dimensional heat transfer assumes a perfectly insulated can on top and bottom. In reality, heat is being absorbed in all directions. Our simplification will cause us to over estimate the time required to both heat and cool. This may not be the worst assumption however, error on the side of over-heating is the safest option when it comes to sterilization. |

**What process parameters are you using for each of the food materials?**

**The following given process parameters are being used in the algorithm**
*Filling Temp.*
*Maximum Steam Temperature*
*Target Exit Temperature*
*Cooling Water Average Temperature*
*Moisture Content*
*Can #*
*Z-Value (organism and nutrients)*
*D250 Value (organism and nutrients)*

i. **What microorganism is your program targeting? All of them? Only one? Why?**

C. Botulinum as it is the most dangerous and lethal microorganism, and it also is the most difficult to kill with thermal processing. It has the highest $D_{250}$ value, indicating it takes the longest time to sterilize.

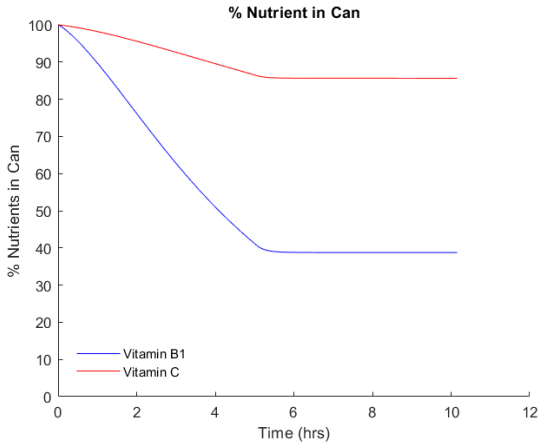
ii. **What is the new time needed to commercially sterilize the product, and the time needed to cool the product to the required average temperature?**

Out algorithm predicts that we can achieve a 13.58 log reduction in C. Botulinum activity after 2.53 hours of sterilization/heating with 250°F. Subsequently, it requires 1.42 hours of cooling at 55°F to achieve an average temperature of 100°F in the can.

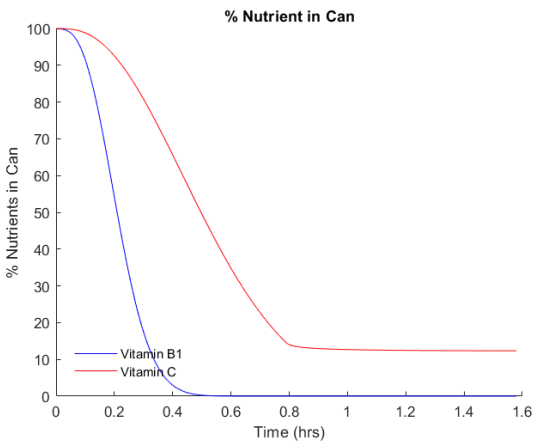
iii. **What optimum temperatures were used for sterilization to retain nutrients? How do you know this is the optimum? Compare the optimum between the original (200 fill temperature) with the alternate (180 fill temperature).**

An optimum sterilization temperature is one that is as low as possible, that remains feasible in the time required to keep the process running economically. It is possible to "flash heat" the product, and this kills the bacteria very quickly and allows the process to be expedited. However, doing so seriously destroys the nutrient content inside of our can and drastically increases the energy requirement per can. A lower temperature allows us to preserve nutrient content while keeping energy costs low. See the nutrient graphs below. **A good temperature that didn't require an absurd heating time was between 110C and 120C.**

**Sterilize at 110 C for 5.08 hrs**

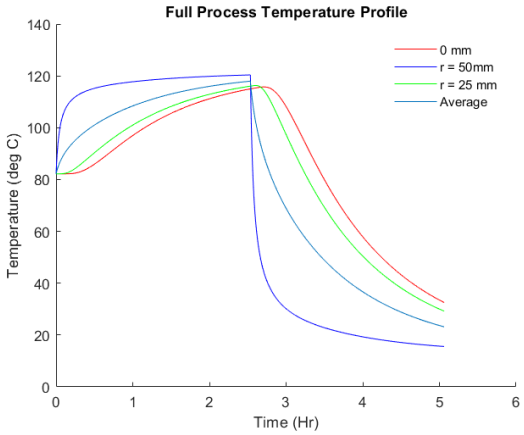



**Sterilize at 200C for 50 mins**

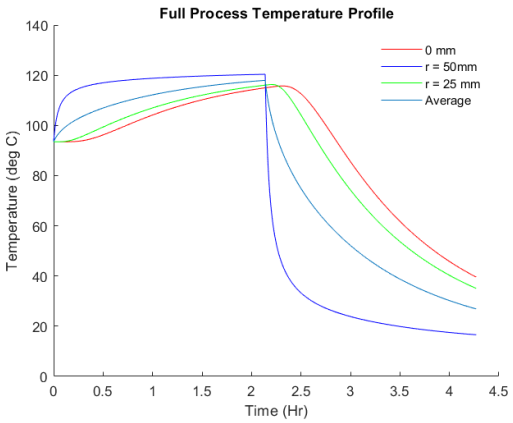



**iv. Insert graph of the heating and cooling profile of the center of the can during the process. How do specific physical properties of the food impact this graph?**

**Filling Temp = 180F**



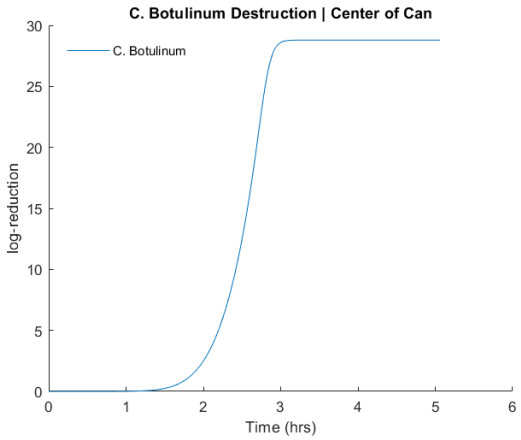

**Filling Temp = 200F**



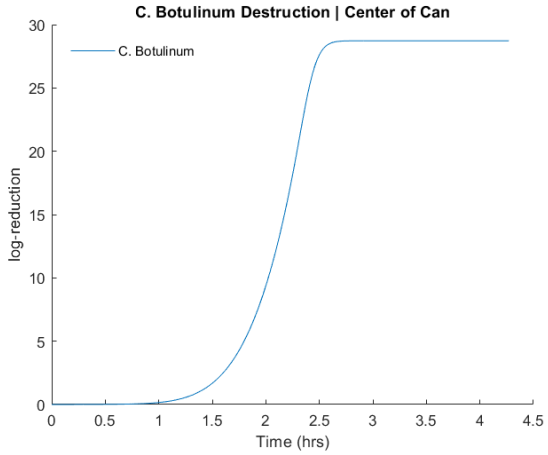

One can see that the lower filling temperature has an almost identical temperature profile throughout the can over time, however, the starting temperature is (obviously) lower. This is reflected in the fact that the heating process is longer for the 180F process (left), while the 200F process (right) reaches the required log-reduction more quickly.

**v. Insert graph of the biologic activity profile in the product at the center of the can versus time. Why would the center of the can make the most sense to monitor?**

**Filling Temp = 180F**



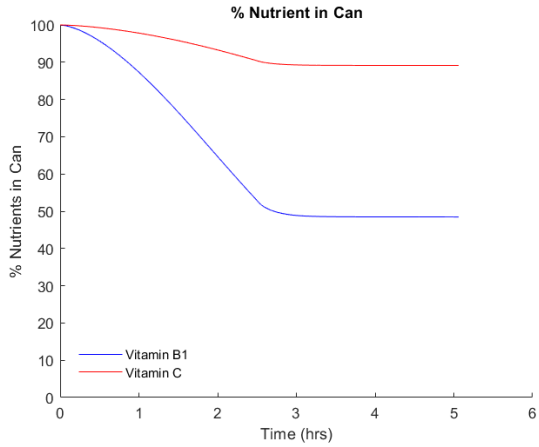

**Filling Temp = 200F**



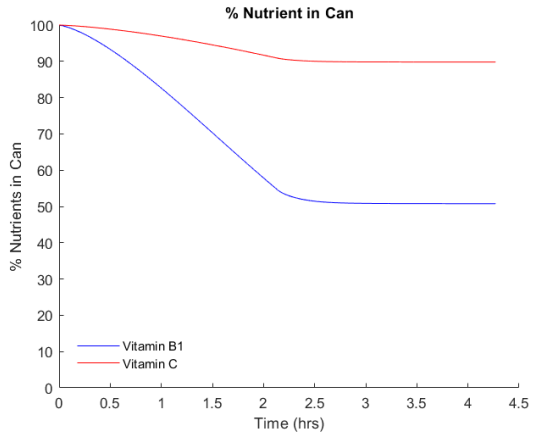

Again, the profiles of log-reduction at the center of the can look very similar, however, close inspection shows differences. The 180F filling temp doesn't hit a 5-log reduction until after 2 hours, while the 200F filling temperature reaches a 5-log reduction well-before the 2 hour point. Due to the incredibly large slope of our curves after this time-point however, the 13.5 log reduction remains close to 2.5 hrs. Specifically for 180F it requires 2.52 hrs of heating, while the 200F filling temperature requires 2.14 hrs. To maximize safety, we examine the center of the can as this is the most difficult part of our can to sterilize.

**vi. Insert graph of the average nutrient activity profile throughout the entire can versus time. Why would we use the average nutrient content across the can rather than at a single point?**

**Filling Temp = 180F**




**Filling Temp = 200F**




It is seen here that the average nutrient degradation in our can is the hardest to discern between the two filling temperatures. The 200F filling temperature produces a barely noticeable difference in nutrient degradation. The 180F filling temperature removes just over 50% of the vitamin B1, and just

under 10% of the vitamin C. Our 200F filling temperature is slightly more optimized removing just under 50% of the vitamin B1, and only about 8% of the vitamin C.

We are interested in the average nutrient content over the radius of our can's as we are not trying to maximize safety and look at the profile as a whole to determine how our product quality has been affected. This requires an average nutrient content at each time point to be assessed.

**How do parameters such as food composition, thermal properties of the food, geometry (can size) and processing parameters (times and temperatures) seem to impact the heating profile?**

**Food Composition and Thermal Properties:**
Higher moisture content makes it harder to heat the food item, and more energy input is required. The food composition directly affects the thermal properties of our food, which subsequently affects the heating and temperature profile.

**Geometry:**
Larger cans have a harder time being heated properly than smaller cans. This is a direct result of the fact that the heat transfer within our can is strictly governed by conduction through the material, and not convection. So, one can imagine that thicker cans radially would be more difficult to heat.

**Processing Parameters:**
In general, it is best to "flash heat" our product. At high temperatures, the associated degradation constant, k, is much larger for our bacteria than the vitamins, this indicates that to optimize and kill the most bacteria, while preserving the most vitamins, we should heat and cool for as long as possible. This is related to a higher filling temperature

**How did you test how these properties affected the heating profile?**

These properties were tested by altering the processing parameters manually within the MATLAB script. The general workflow is: perturb the parameter In the positive or negative direction (typically by a factor of 5 or 10), and then examine the output of the graph and the change.

**For your process, how are Vitamin B1 and Vitamin C affected? How much of these Vitamins remain? How much more Vitamin loss is there in the new process (180 degree fill temp, than the original 200 degree fill temp?)**

**(Please see graphs from section vi.)** I go over all of this in section vi, but to reiterate:
There is not a huge difference between the two filling temperatures. Vitamin B1 experiences ~50% reduction in total nutrient composition. While Vitamin C experiences a reduction og only ~10%. This is due in most part to the large D250 value for both and the large z-values.

There are slight differences between the 200F filling temp and the 180F temp. It is mostly a result of the increased heating time required for the 180F filling temperature that increases the degradation – although it is almost negligibly larger.
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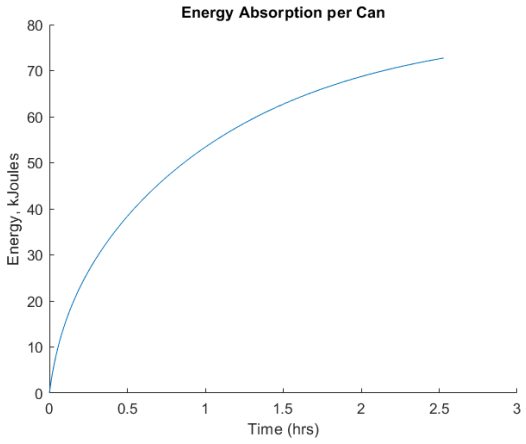
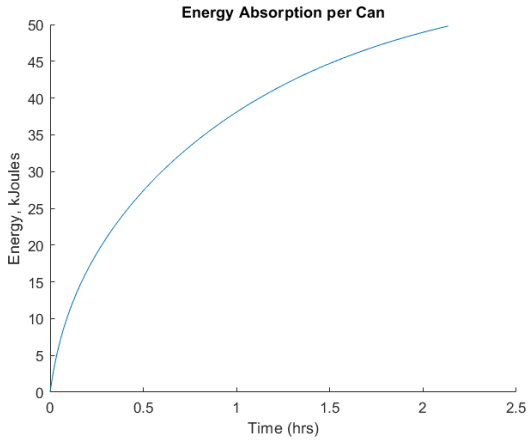
**What is your estimate of additional energy and time costs due to the impacted filling temperature for your product?**

**Filling Temp. = 180F**




**Filling Temp. = 200F**




As with all other parameters, one can see that the overall profile shape of both curves is very similar. This makes sense, since all parameters are identical except the initial filling temperature. Upon inspection, one can see that the maximal energy absorption during heating for the 180 Fill temperature is about 75 kJ/can, while the 200F filling temperature maxes out at 50 kJ/can. This makes sense as it requires less heating time and a smaller temperature change. We used macroscopic energy changes based on the average temperature difference within a can at each time-point. That is, the following equation:

$$\Delta q = mc_{\mathrm{p}}\left(\mathrm{T}_{\mathrm{avg}}(t) - \mathrm{T}_{\mathrm{fill}}\right)$$

Normalizing for total time, the 180F filling temp absorbs 29.76 kJ/hr/can while the 200F filling temperature absorbs 23.36 kJ/hr/can. Even after the end of the process, it can be seen that the 200F filling temperature is more optimal than the current operating conditions.

In summary, it seems as though in additional 5-6 kJ/hr/can is required with the new conditions. If the process is running at a high throughput, this could hurt expenses and budgetary requirements.

| **What recommendations would you make to the systems engineer, R&D, and microbiology to improve costs and efficiencies on this line moving forward?** |
| --- |
| I would recommend keeping the filling temperature as high as possible without risking damaging the product: 200 and 220 F. This saves costs on energy and speeds up the sterilization time. In addition, to preserve product quality, I would recommend sterilizing at a lower temperature. This requires more time, but provides significant improvements in the overall nutrient content of our filling as the amount of filling is orders of magnitude larger than with a “flash heat” system. |