

Model for Roasting a Carrot

Jana Mudrock

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Caramelization reactions occur when sugars are heated at high temperatures (Vieira, 1996). Unlike Maillard Reactions, caramelization does not require an amino group to occur. Rather, heat causes the dehydration of a sugar which, through several steps and reactions, results in the formation of complex chemical compounds (Vieira, 1996). These compounds are brown or black and have unique flavors. One major compound formed in caramelization is caramelan (Vieira, 1996). The temperature at which caramelization occurs varies depending on the sugar. For sucrose, one of the main sugars in carrots, the temperature is 160°C (Vieira, 1996). Both Maillard and caramelization reactions can occur in foods of all moisture contents (Vieira, 1996).

In terms of texture, a roasted carrot is softer and dryer than a raw carrot. The softness is partially due to pectin hydrolysis. Pectin is a structural polysaccharide that is common in the cell walls of fruits and vegetables, including carrots (Vieira, 1996). The average raw carrot contains approximately 1% pectin by weight (Sharma, 2012). High roasting temperatures cause pectin to degrade by hydrolysis (Vieira, 1996). Hydrolysis of pectin occurs rapidly when the temperature is 115°C or higher (Vieira, 1996).

In addition, exposure to high temperatures causes water to vaporize and exit as steam, resulting in reduced moisture content and dryer texture. A raw carrot is mostly water, and a significant portion of the water is lost as steam when the carrot is roasted (Sharma, 2012). The amount of water lost due to boiling depends on environmental factors such as the moisture content of the air.

Finally, a raw carrot's color is bright orange, while a roasted carrot is duller and brown in some areas. The color change occurs on the surface of the carrot and is a result of the products formed by caramelization and Maillard browning, including caramelans and melanoidins (Vieira, 1996).

The purpose of this model is to predict the time it takes to roast carrots in an oven. The model quantitatively evaluates taste, texture, and color by modeling heat transfer and chemical reactions. Values are set for the amount of water vaporized, amount of sugar reacted, amount of pectin reacted, and extent of color change in a "done" carrot. The time to doneness is determined as the time when all of those minimum values have been met.

In order to accurately model a variety of situations, the user is able to input parameters that affect the output of the model. These include: oven temperature, initial sugar content, initial water content, initial carrot temperature, total mass, size, convection coefficient, and reaction rate constants. The model was validated by comparing the output to usual carrot cooking times.

- The exposed area on the top and bottom of the carrot is much greater than the exposed area on the sides, so heat transfer is one-dimensional.
- The temperature profile is determined as a function of position and time (distributed system).
- The carrot is on a pan. The bottom of the carrot rests on the pan, and the rest of the surface is exposed to hot oven air.
 - The pan has a very high thermal conductivity, so it immediately reaches a temperature very close to the temperature of the oven.
 - The temperature of the pan is constant.
- Because of convection, the temperature at the surface exposed to the air is not equal to the temperature of the oven. To determine the surface temperature as a function of time, a very small thickness at the surface (5% of the total mass) is examined and treated as a lumped parameter system.
- The time for the carrot to reach any given temperature is based on the time for the coldest point in the carrot to reach that temperature.
- Heat capacity and thermal conductivity change with temperature and composition.
 - The Choi-Okos equation is used to estimate heat capacity and thermal conductivity (Choi & Okos, 1986).
 - New values for heat capacity and thermal conductivity are calculated after vaporization of the water and after reaching Tph.

Assumptions related to water vaporization

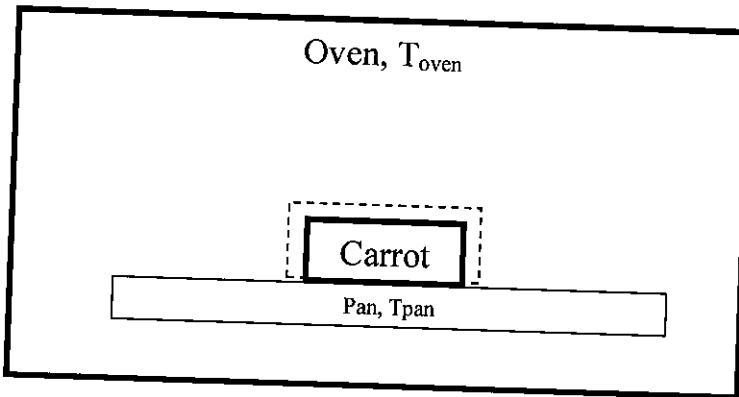
- The mass of water to be considered “done” is the mass of water that causes the concentration of water in the carrot to be equal to the concentration of water outside the carrot. This is set to a constant value.
- Once the system reaches T_{boil} , all of the water that will be vaporized (to reach equilibrium with the outside environment) is vaporized. There is no temperature change as the water is vaporized.
- After the water is vaporized, the temperature begins to increase again.
- The total mass of the system changes as the water vaporizes. The loss of total mass of the system is equal to the loss of water of the system.
- The total volume of the system changes as the water vaporizes. The loss of volume by the system is equal to the mass of water lost divided by the density of the water.
 - Therefore, the density of the system changes as the water vaporizes.
- The change in volume is related to system shrinkage (in height).
 - The change in the height of the carrot is assumed to be proportional to the change in volume.

Assumptions related to chemical reactions

- The reactions will not occur unless the temperature meets or exceeds the requirement; The Maillard and caramelization reactions begin at T_{carm} , and pectin hydrolyzation begins at T_{ph} (Viera, 1996).
- Pectin hydrolyzation begins before caramelization and Maillard reactions, since Tph is less than T_{carm} (Viera, 1996).

Final Model System Diagrams

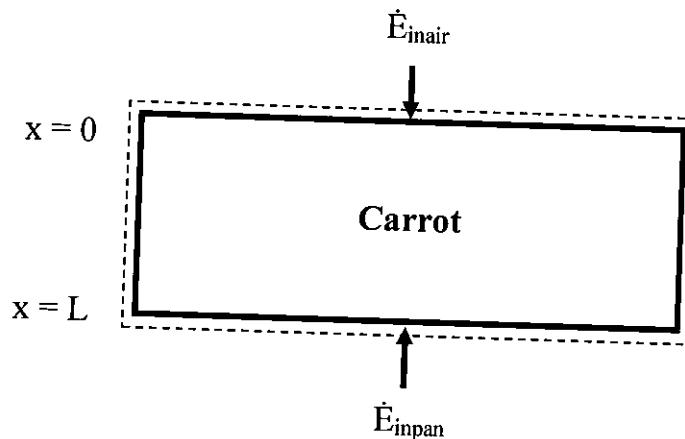
System Definition: Carrot Piece. System boundary is shown with a dotted line. Note that the pan is in contact with the carrot, but it is not inside the system boundary.



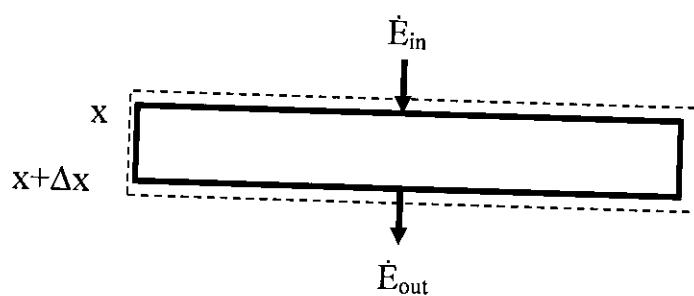
All of the following diagrams show only the carrot piece.

Phase 1: Temperature increases from $T_{carroti}$ to T_{boil} .

- There are no mass flows.
- The only energy flows are from the hot oven air and the hot pan to the carrot.

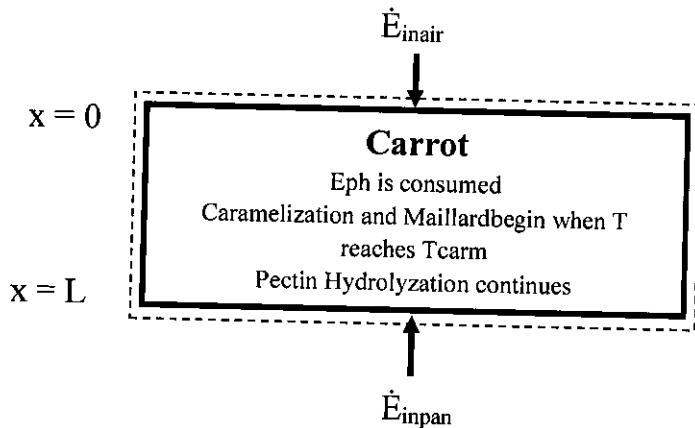


Differential Element, Phase 1

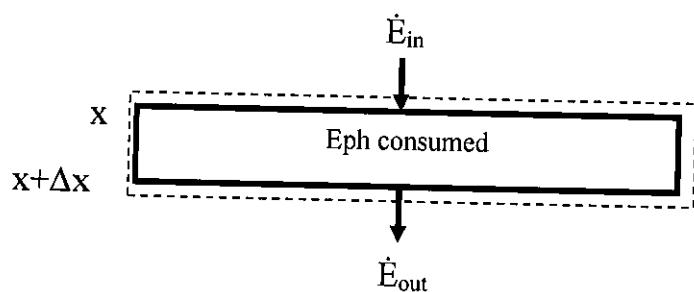


Phase 4: Temperature increases from T_{ph} to T_{carm} .

- There are no mass flows.
- There is an energy flow from the hot oven air and the hot pan to the carrot.
- Energy is consumed by the pectin hydrolyzation reaction.
- Caramelization begins at the end of this phase, once the temperature reaches T_{carm} . This would result in a consumption of energy as the temperature continues to increase.



Differential Element, Phase 4



Parameters related to heat transfer

h	heat transfer coefficient of hot oven air	[kW/m ² K]
c_{pi}	initial heat capacity of carrot	[kJ/kgK]
c_{p2}	heat capacity of carrot after Phase 2	[kJ/kgK]
c_{p3}	heat capacity of carrot after Phase 3	[kJ/kgK]
c_{pw}	heat capacity of water	[kJ/kgK]
c_{pc}	heat capacity of carbohydrates (sugar)	[kJ/kgK]
c_{pf}	heat capacity of fiber (pectin)	[kJ/kgK]
c_{pp}	heat capacity of protein	[kJ/kgK]
k_i	initial thermal conductivity of carrot	[kW/mK]
k_2	thermal conductivity of carrot after Phase 2	[kW/mK]
k_3	thermal conductivity of carrot after Phase 3	[kW/mK]
k_w	thermal conductivity of water	[kW/mK]
k_c	thermal conductivity of carbohydrates (sugar)	[kW/mK]
k_f	thermal conductivity of fiber (pectin)	[kW/mK]
k_p	thermal conductivity of protein	[kW/mK]
α_i	initial thermal diffusivity of carrot	[m ² /s]
α_2	thermal diffusivity of carrot after Phase 2	[m ² /s]
α_3	thermal diffusivity of carrot after Phase 3	[m ² /s]
$m_{waterout}$	mass flow rate at which water leaves during Phase 2	[kg/s]
H_{vap}	water enthalpy of evaporation	[kJ/kg]
ρ_{carrot}	density of carrot	[kg/m ³]
$\rho_{carrot2}$	density of carrot after Phase 2	[kg/m ³]
ρ_w	density of water	[kg/m ³]
\dot{E}_{ph}	rate at which enthalpy is consumed by pectin hydrolyzation reaction	[kJ/s]

Geometrical Shape and Size Parameters

L	initial height of carrot	[m]
L_{new}	height of carrot after water has vaporized	[m]
A	cross sectional area of carrot	[m ²]
V	initial volume of system ($V=LA$)	[m ³]
V_{new}	volume of system after water has vaporized	[m ³]
S	total surface area of the carrot	[m ²]
$m_{surface}$	mass of thin surface layer of carrot	kg

Rate Constant Parameters

k_{carm}	rate constant for caramelization reaction	[1/s]
k_{ph}	rate constant for pectin hydrolyzation reaction	[m ³ /kmol.s]
k_{m0}	rate constant for Maillard reactions	[m ³ /kmol.s]
k_{m1}	rate constant for Maillard reactions	[m ³ /kmol.s]
k_{m2}	rate constant for Maillard reactions	[m ³ /kmol.s]
k_{m3}	rate constant for Maillard reactions	[1/s]
k_{m4}	rate constant for Maillard reactions	[1/s]
k_{m5}	rate constant for Maillard reactions	[m ³ /kmol.s]
k_{m6}	rate constant for Maillard reactions	[m ³ /kmol.s]

twater	total time to reach desired water content in carrot	[s]
tcarm	time to reach Tcarm after reaching Tph	[s]
tcarm2	time for caramelization reaction to occur after reaching Tcarm	[s]
tcarm	total time to reach desired sugar and brownness level	[s]
tph1	time to reach Tph after water is vaporized	[s]
tph2	time for pectin hydrolyzation reaction to occur after Tph is reached	[s]
tph	total time to reach desired pectin content in carrot	[s]
td	time to doneness	[s]

$L := 0.01$	m	height of carrot slice
$A := 0.002$	m^2	cross sectional area of carrot slice
$V := L \cdot A = 2 \times 10^{-5}$	m^3	initial volume of carrot
$\rho_{carrot} := \frac{m_{total}}{V} = 500$	kg/m^3	initial density of carrot
$S := .006$	m^2	surface area of carrot
$\rho_w := 1000$	kg/m^3	density of water

$k_{carm} := 0.0008$	1/s	caramelization rate constant
$k_{ph} := 0.85$	$m^3/kmol.s$	pectin hydrolyzation rate constant
$k_{m0} := 0.0001$	$m^3/kmol.s$	Maillard rate constant
$k_{m1} := 0.0005$	$m^3/kmol.s$	Maillard rate constant
$k_{m2} := 0.0001$	$m^3/kmol.s$	Maillard rate constant
$k_{m3} := 0.005$	1/s	Maillard rate constant
$k_{m4} := 0.005$	1/s	Maillard rate constant
$k_{m5} := 0.1$	$m^3/kmol.s$	Maillard rate constant
$k_{m6} := 0.2$	$m^3/kmol.s$	Maillard rate constant
$\beta_{carm} := 1 \cdot 10^{-7}$	1/s.K	Caramelization rate proportionality constant
$\beta_{ph} := 1 \cdot 10^{-4}$	$m^3/kmol.s.K$	Pectin Hydrolyzation rate proportionality constant
$\beta_{m0} := 1 \cdot 10^{-8}$	$m^3/kmol.s.K$	Maillard rate proportionality constant
$\beta_{m1} := 1 \cdot 10^{-7}$	$m^3/kmol.s.K$	Maillard rate proportionality constant
$\beta_{m2} := 1 \cdot 10^{-8}$	$m^3/kmol.s.K$	Maillard rate proportionality constant
$\beta_{m3} := 1 \cdot 10^{-7}$	1/s.K	Maillard rate proportionality constant
$\beta_{m4} := 1 \cdot 10^{-7}$	1/s.K	Maillard rate proportionality constant
$\beta_{m5} := 1 \cdot 10^{-5}$	$m^3/kmol.s.K$	Maillard rate proportionality constant
$\beta_{m6} := 1 \cdot 10^{-5}$	$m^3/kmol.s.K$	Maillard rate proportionality constant

Calculation of Molecular Weights of Reaction Products and Reactants

$mwP := 12 \cdot 12 + 18 \cdot 1 + 13 \cdot 16 = 370$	kg/kmol Pectin
$mwW := 2 \cdot 1 + 16 = 18$	kg/kmol Water
$mwGA := 6 \cdot 12 + 10 \cdot 1 + 7 \cdot 16 = 194$	kg/kmol Glucuronic Acid
$mwS := 12 \cdot 12 + 22 \cdot 1 + 11 \cdot 16 = 342$	kg/kmol Sucrose
$mwC := 24 \cdot 12 + 36 \cdot 1 + 18 \cdot 16 = 612$	kg/kmol Caramelan

$$cpfi := .001 [1845.9 + 1930.6 \cdot 10^{-3} \cdot (T_{carroti} - 273) - 4650.9 \cdot 10^{-6} \cdot (T_{carroti} - 273)^2] = 1.883 \text{ kJ/kgK}$$

initial heat capacity of fiber (pectin)

$$cippi := .001 [2008.2 + 1208.9 \cdot 10^{-3} \cdot (T_{carroti} - 273) - 1312.9 \cdot 10^{-6} \cdot (T_{carroti} - 273)^2] = 2.032 \text{ kJ/kgK}$$

initial heat capacity of protein

$$cpi := \frac{mwateli}{m_{totali}} \cdot cpwi + \frac{msugari}{m_{totali}} \cdot cpci + \frac{mpeptini}{m_{totali}} \cdot cpfi + \frac{mprotein}{m_{totali}} \cdot cippi = 4.014 \text{ kJ/kgK}$$

initial overall carrot heat capacity

$$\alpha_i := \frac{k_i}{cpi \cdot p_{carrot}} = 2.878 \times 10^{-7} \text{ m}^2/\text{s}$$

initial carrot thermal diffusivity

Phase 1: Raise Temperature to Tboil

Energy Balance to determine boundary condition at the interface with the hot air

Because of convection, the temperature at the surface of the carrot is not equal to the temperature of the oven. To determine the surface temperature, we will examine a very small thickness at the surface (5% of the total mass) and treat it as a lumped parameter system. This assumption is valid because the section is so small.

$$\frac{dE_{total}}{dt} := Ein$$

$$\frac{dE_{total}}{dt} := -msurface \cdot cp \cdot \frac{dT_s}{dt}$$

$$Ein := hA \cdot (T_s(t) - T_{oven})$$

$$\frac{dT_s}{dt} := \frac{-hA}{msurface \cdot cp} \cdot (T_s(t) - T_{oven})$$

Boundary Condition: at t=0, T=Tcarroti

$$T_s(t) := T_{oven} + (T_{carroti} - T_{oven}) \cdot \exp\left(\frac{-h \cdot A \cdot t}{msurface \cdot cp}\right)$$

Boundary condition for the temperature at the surface as a function of time

Energy Balance for the rest of the carrot

Examining a very small section of the carrot, from x to x+Δx:

$$\frac{dE_{total}}{dt} := Ein - Eout$$

$$\frac{dE_{total}}{dt} := -m_{totali} \cdot cp \cdot \frac{dT}{dt}$$

Given

$$T_t(x, t) = c\alpha \cdot T_{xx}(x, t)$$

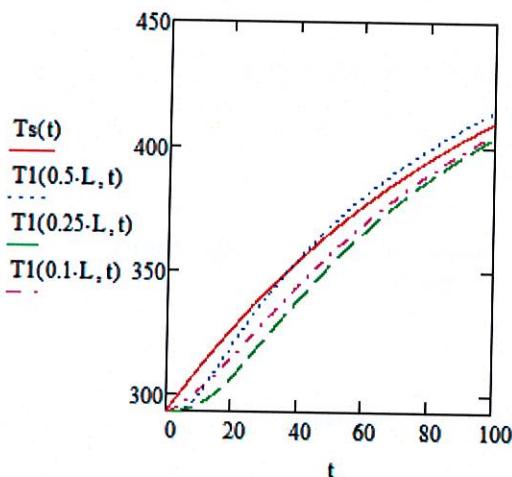
$$T(x, 0) = T_{carrot}$$

$$T(L, t) = T_{pan}$$

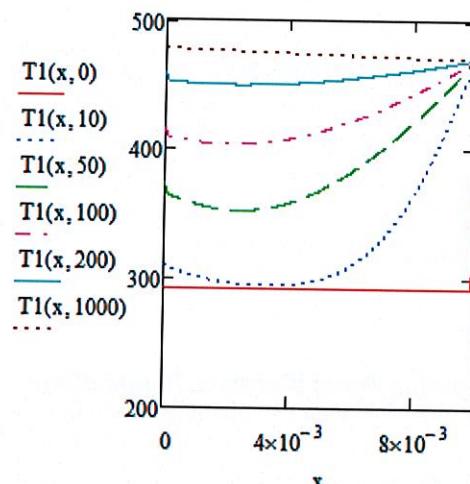
$$T(0, t) = T_s(t)$$

$$T1 := Pdesolve \left[T, x, \begin{pmatrix} 0 \\ L \end{pmatrix}, t, \begin{pmatrix} 0 \\ 1000 \end{pmatrix}, 100, 1000 \right]$$

temperature profile in phase 1 of cooking



Temperature profile as a function of time with position held constant, phase 1



Temperature profile as a function of position with time held constant, phase 1

Since we have assumed an even distribution of water, sugar, and pectin in the system, the entire carrot needs to reach T_{boil} in order for the required amount of water to be vaporized. We will determine t_{boil} by finding the time it takes for the coldest point of the carrot to reach T_{boil} .

From the graphs, it is clear that the coldest point in the carrot is not the center ($x=0.5*L$). Since the boundaries are at different temperatures, the location of the coldest point changes with time.

We will begin by solving for an approximate boiling time, using the center of the carrot as a guess for the coldest point. Then, we iterate twice to determine the actual coldest point in the carrot at this time and recalculate the true t_{boil} .

$$T_{boilapprox}(t) := T1(0.5 \cdot L, t) - T_{boil}$$

$$x := 100$$

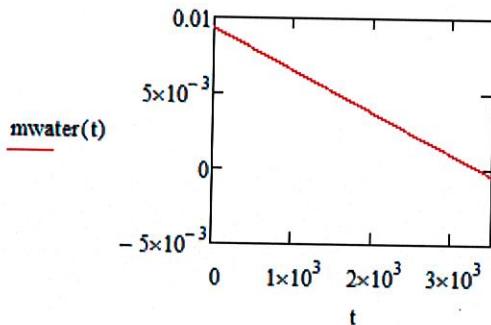
$$\frac{dm_{water}}{dt} := -m_{waterout}$$

$$\frac{dm_{water}}{dt} := \left[h \cdot S \cdot \frac{(T_{oven} - T_{boil})}{H_{steam}} \right]$$

Boundary Condition: At $t = 0$, $m_{water} = m_{wateri}$

$$m_{water}(t) := -h \cdot S \cdot \frac{(T_{oven} - T_{boil})}{H_{vap}} \cdot t + m_{wateri}$$

$$t := 0..3600$$



$$vap(t) := m_{water}(t) - m_{waterd}$$

$$x := 100$$

$$tvap := \text{root}(vap(x), x) = 1.005 \times 10^3$$

additional time for water to be vaporized once the system has reached t_{boil}

$$twater := t_{boil} + tvap = 1.072 \times 10^3$$

total time for required amount of water to be lost (s)

Calculation of new total mass and volume

We want to calculate the new total mass and volume to use in the calculations for the later phases. From the previous energy balance, we have

$$\frac{dm_{total}}{dt} := \frac{dm_{water}}{dt}$$

Boundary Condition: At $t=0$, $m_{total}=m_{totali}$

$$m_{total}(t) := -h \cdot S \cdot \frac{(T_{oven} - T_{boil})}{H_{vap}} \cdot t + m_{totali}$$

$$kf2 := .001 \left[.18331 + 1.2497 \cdot 10^{-3} \cdot (T_{boil} - 273) - 3.1683 \cdot 10^{-6} \cdot (T_{boil} - 273)^2 \right] = 2.766 \times 10^{-4}$$

thermal conductivity of fiber (pectin), phase 2
kW/mK

$$kp2 := .001 \left[.1788 + 1.1958 \cdot 10^{-3} \cdot (T_{boil} - 273) - 2.7178 \cdot 10^{-6} \cdot (T_{boil} - 273)^2 \right] = 2.712 \times 10^{-4}$$

thermal conductivity of protein, phase 2
kW/mK

$$k2 := \frac{mwated}{m_{totalnew}} \cdot kw2 + \frac{msugari}{m_{totalnew}} \cdot kc2 + \frac{mpectini}{m_{totalnew}} \cdot kf2 + \frac{mproteini}{m_{totalnew}} \cdot kp2 = 6.409 \times 10^{-4}$$

overall thermal conductivity of carrot, phase 2
kW/mK

Note that thermal conductivity increases slightly due to the water loss and rise in temperature.

Calculation of heat capacity, end of phase 2

$$cpw2 := .001 \left[4176.2 - 9.0862 \cdot 10^{-5} \cdot (T_{boil} - 273) + 5473.1 \cdot 10^{-6} \cdot (T_{boil} - 273)^2 \right] = 4.231$$

heat capacity of water, phase 2
kJ/kgK

$$cpc2 := .001 \left[1548.8 + 1962.5 \cdot 10^{-3} \cdot (T_{boil} - 273) - 5939.9 \cdot 10^{-6} \cdot (T_{boil} - 273)^2 \right] = 1.686$$

heat capacity of carbohydrates (sugar), phase 2
kJ/kgK

$$cpf2 := .001 \left[1845.9 + 1930.6 \cdot 10^{-3} \cdot (T_{boil} - 273) - 4650.9 \cdot 10^{-6} \cdot (T_{boil} - 273)^2 \right] = 1.992$$

heat capacity of fiber (pectin), phase 2
kJ/kgK

$$cpp2 := .001 \left[2008.2 + 1208.9 \cdot 10^{-3} \cdot (T_{boil} - 273) - 1312.9 \cdot 10^{-6} \cdot (T_{boil} - 273)^2 \right] = 2.116$$

heat capacity of protein, phase 2
kJ/kgK

$$cp2 := \frac{mwated}{m_{totalnew}} \cdot cpw2 + \frac{msugari}{m_{totalnew}} \cdot cpc2 + \frac{mpectini}{m_{totalnew}} \cdot cpf2 + \frac{mproteini}{m_{totalnew}} \cdot cpp2 = 4.007$$

overall heat capacity of carrot, phase 2
kJ/kgK

Note that the heat capacity decreases slightly due to the water loss and rise in temperature.

Calculation of thermal diffusivity, end of phase 2

$$\alpha2 := \frac{k2}{\rho_{carrot2} \cdot cp2} = 3.821 \times 10^{-7}$$

Given

$$T_t(x, t) = \alpha_2 \cdot T_{xx}(x, t)$$

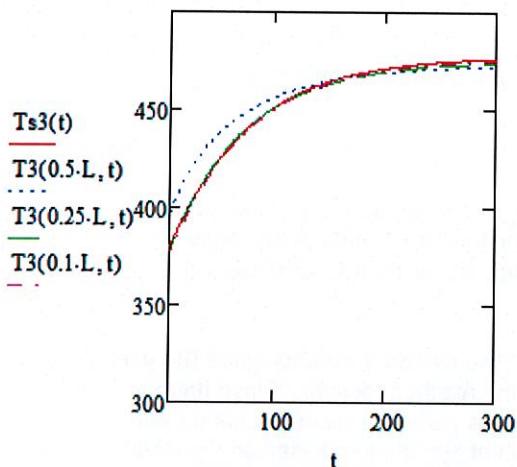
$$T(x, 0) = T_1(x, t_{boil})$$

$$T(L_{new}, t) = T_{pan}$$

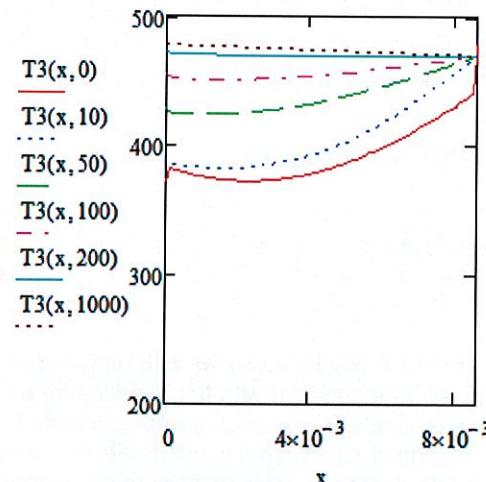
$$T(0, t) = T_{s3}(t)$$

$$T3 := Pdesolve\left[T, x, \begin{pmatrix} 0 \\ L_{new} \end{pmatrix}, t, \begin{pmatrix} 0 \\ 1000 \end{pmatrix}, 100, 1000\right] \quad \text{Temperature profile in phase 3 of cooking}$$

$x := 0, 0.0001.. 1$



Temperature profile as a function of time with position held constant, phase 3



Temperature profile as a function of position with time held constant, phase 3

Since we have assumed an even distribution of water, sugar, and pectin in the system, the entire carrot needs to reach T_{ph} in order for the required amount of pectin to be reacted. We will determine t_{ph} by finding the time it takes for the coldest point of the carrot to reach T_{ph} .

From the graphs, it is clear that the coldest point in the carrot is no longer the center ($x=0.5*L$). Since the boundaries are at different temperatures, the location of the coldest point changes with time.

We will begin by solving for an approximate t_{ph1} , using the center of the carrot as a guess for the coldest point. Then, we can iterate twice to determine the actual coldest point in the carrot at this time and recalculate the true t_{ph1} .

Mass Balance:

$$V \frac{dC_p}{dt} := V \cdot -k_{ph} \cdot C_p \cdot C_w$$

Multiplying by volume converts concentrations to moles. Moles can be converted to mass by multiplying by the molecular weight conversion:

$$\frac{dm_{pectin}}{dt} := -k_{ph} \cdot m_{pectin} \cdot m_{water}$$

$$\frac{dm_{water}}{dt} := -k_{ph} \cdot m_{pectin} \cdot m_{water}$$

$$\frac{dm_{gacid}}{dt} := 2 \cdot k_{ph} \cdot m_{pectin} \cdot m_{water}$$

Given

$$\frac{d}{dt} P(t) = -k_{ph3}(t) \cdot P(t) \cdot W(t)$$

$$P(0) = \frac{m_{pectini}}{mwP}$$

$$\frac{d}{dt} W(t) = -k_{ph3}(t) \cdot P(t) \cdot W(t)$$

$$W(0) = \frac{m_{waterd}}{mwW}$$

$$\frac{d}{dt} GA(t) = 2 \cdot k_{ph3}(t) \cdot P(t) \cdot W(t)$$

$$GA(0) = 0$$

$$\begin{pmatrix} pectin \\ waterph \\ gacid \end{pmatrix} := \text{Odesolve} \left[\begin{pmatrix} P \\ W \\ GA \end{pmatrix}, t, 1000, 1000 \right]$$

Differential equation was solved in terms of moles; convert to kilograms:

$$m_{pectin}(t) := mwP \cdot pectin(t) \quad \text{mass of pectin as a function of time}$$

$$m_{waterph}(t) := mwW \cdot waterph(t) \quad \text{mass of water as a function of time, phase 3}$$

$$m_{gacid}(t) := mwGA \cdot gacid(t) \quad \text{mass of glucuronic acid as a function of time}$$

Calculation of heat capacity, end of phase 3

$$\text{cpp3} = .001 \cdot [2008.2 + 1208.9 \cdot 10^{-3} \cdot (\text{Tph} - 273) - 1312.9 \cdot 10^{-6} \cdot (\text{Tph} - 273)^2] = 2.132$$

heat capacity of protein, phase 3 kJ/kgK

Note that the heat capacity has increased slightly due to the rise in temperature.

Calculation of new value for thermal diffusivity

$p_{\text{carrot3}} := p_{\text{carrot2}}$ density of carrot, phase 3
(no change in density)

$$\alpha_3 = \frac{k_3}{\rho_{carrot}^3 \cdot c_p^3} = 3.832 \times 10^{-7}$$

Phase 4: Raise Temperature to T_{carm} and begin Caramelization and Maillard Reactions
In this phase, the time point t=0 corresponds to the end of the previous phase

Energy Balance to determine boundary condition at the interface with the hot open air

The energy balance is the same as in Phase 1. Only the Boundary Condition changes. See phase 1 for derivation of energy balance.

$$\frac{dT_s}{dt} := \frac{-hA}{msurface \cdot cp} \cdot (T_s(t) - T_{oven})$$

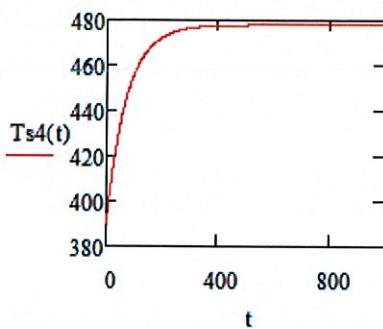
Boundary Condition: at $t=0$, $T=T_{ph}$

$$Ts4(t) := Toven + (Tph - Toven) \cdot \exp\left(\frac{-h \cdot A \cdot t}{msurface \cdot cp}\right)$$

Boundary condition for the temperature at the surface, phase 4

$$Ts4(t) := Toven + (Tph - Toven) \cdot \exp\left(\frac{-h \cdot A \cdot t}{msurface_{new} \cdot cp_3}\right)$$

Boundary condition for the temperature at the surface, phase 4



Given

$$T_t(x, t) = \alpha_3 \cdot T_{xx}(x, t) - \frac{Eph}{\rho \cdot c \cdot cp_3}$$

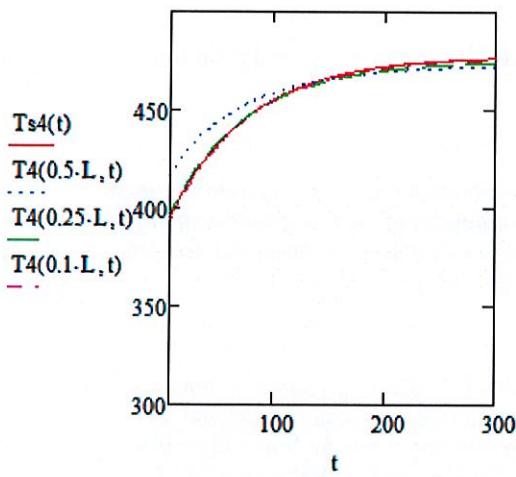
$$T(x, 0) = T3(x, t_{ph1})$$

$$T(L_{new}, t) = T_{pan}$$

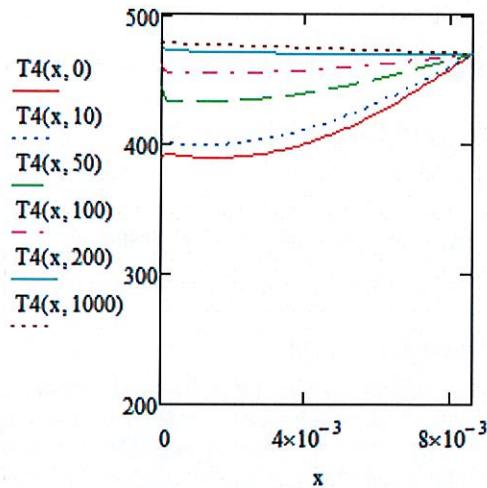
$$T(0, t) = Ts4(t)$$

$$T4 := Pdesolve\left[T, x, \begin{pmatrix} 0 \\ L_{new} \end{pmatrix}, t, \begin{pmatrix} 0 \\ 1000 \end{pmatrix}, 100, 1000\right] \text{ Temperature profile in phase 4 of cooking}$$

$$x := 0, 0.0001..1$$



Temperature profile as a function of time with position held constant, phase 4



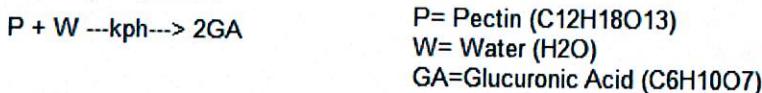
Temperature profile as a function of position with time held constant, phase 4

The user can change the β values as they desire or set them equal to zero if he or she does not want the rate constant to vary with temperature. Giving this option makes the program more flexible.

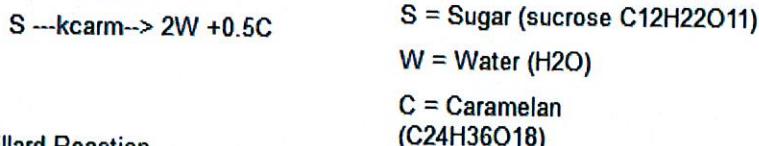
$$\begin{aligned}
 kph4(t) &:= kph3(tcam1) + \beta ph \cdot T4(coldpt2, t + tcam1) \\
 kcam1(t) &:= kcam + \beta cam \cdot T4(coldpt2, t + tcam1) \\
 km0(t) &:= km0 + \beta m0 \cdot T4(coldpt2, t + tcam1) \\
 km1(t) &:= km1 + \beta m1 \cdot T4(coldpt2, t + tcam1) \\
 km2(t) &:= km2 + \beta m2 \cdot T4(coldpt2, t + tcam1) \\
 km3(t) &:= km3 + \beta m3 \cdot T4(coldpt2, t + tcam1) \\
 km4(t) &:= km4 + \beta m4 \cdot T4(coldpt2, t + tcam1) \\
 km5(t) &:= km5 + \beta m5 \cdot T4(coldpt2, t + tcam1) \\
 km6(t) &:= km6 + \beta m6 \cdot T4(coldpt2, t + tcam1)
 \end{aligned}$$

We will consider the pectin hydrolyzation in the reaction network, since the reaction is still continuing from the previous phase. For the intitial values, we will use the value from our previous models at time tcam.

Pectin Hydrolyzation

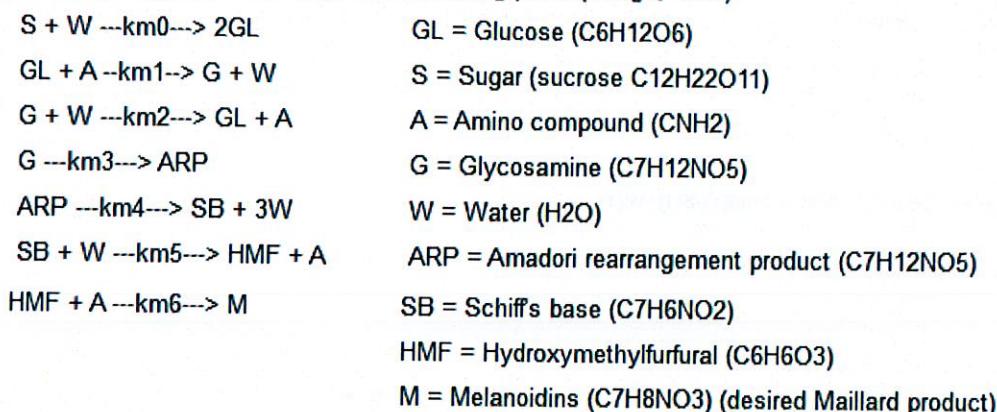


Caramelization Reaction



Maillard Reaction

Based on the diagram from Hodge and assuming pH<7 (Hodge, 1953)



$$W(0) = \frac{mw_{\text{waterph}}(\text{tcam1})}{mw_W}$$

$$\frac{d}{dt} C(t) = 0.5 k_{\text{cam}}(t) \cdot S(t)$$

$$C(0) = 0$$

$$\frac{d}{dt} GL(t) = 2km0(t) \cdot S(t) \cdot W(t) - km1(t) \cdot GL(t) \cdot A(t) + km2(t) \cdot G(t) \cdot W(t)$$

$$GL(0) = 0$$

$$\frac{d}{dt} A(t) = -km1(t) \cdot GL(t) \cdot A(t) + km2(t) \cdot G(t) \cdot W(t) + km5(t) \cdot SB(t) \cdot W(t) - km6(t) \cdot HMF(t) \cdot A(t)$$

$$A(0) = \frac{m_{\text{protein}}}{mw_A}$$

$$\frac{d}{dt} G(t) = km1(t) \cdot GL(t) \cdot A(t) - km2(t) \cdot G(t) \cdot W(t) - km3(t) \cdot G(t)$$

$$G(0) = 0$$

$$\frac{d}{dt} ARP(t) = km3(t) \cdot G(t) - km4(t) \cdot ARP(t)$$

$$ARP(0) = 0$$

$$\frac{d}{dt} SB(t) = km4(t) \cdot ARP(t) - km5(t) \cdot SB(t) \cdot W(t)$$

$$SB(0) = 0$$

$$\frac{d}{dt} HMF(t) = km5(t) \cdot SB(t) \cdot W(t) - km6(t) \cdot HMF(t) \cdot A(t)$$

$$HMF(0) = 0$$

$$\frac{d}{dt} M(t) = km6(t) \cdot HMF(t) \cdot A(t)$$

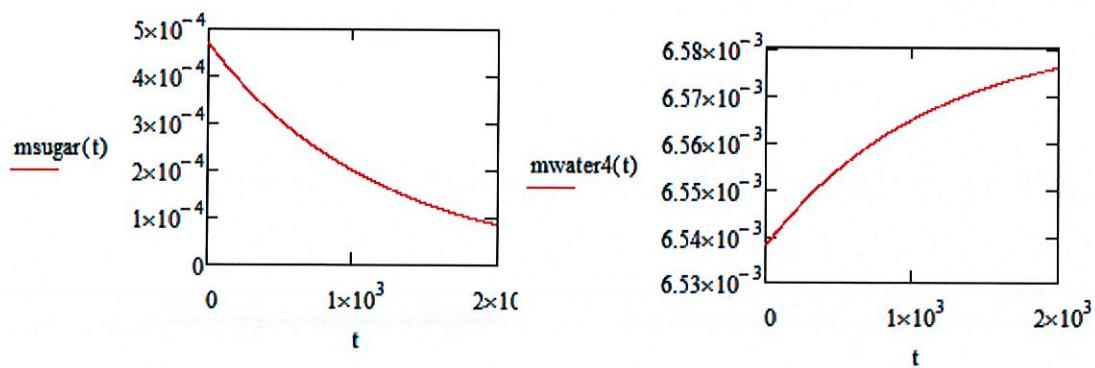
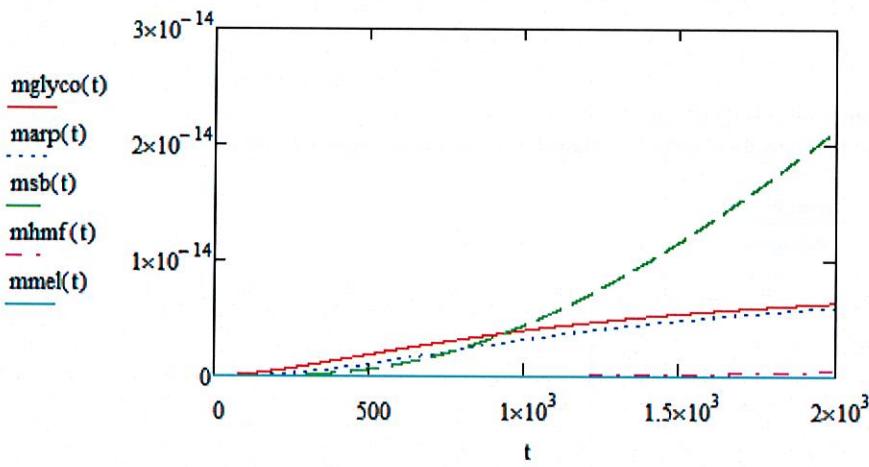
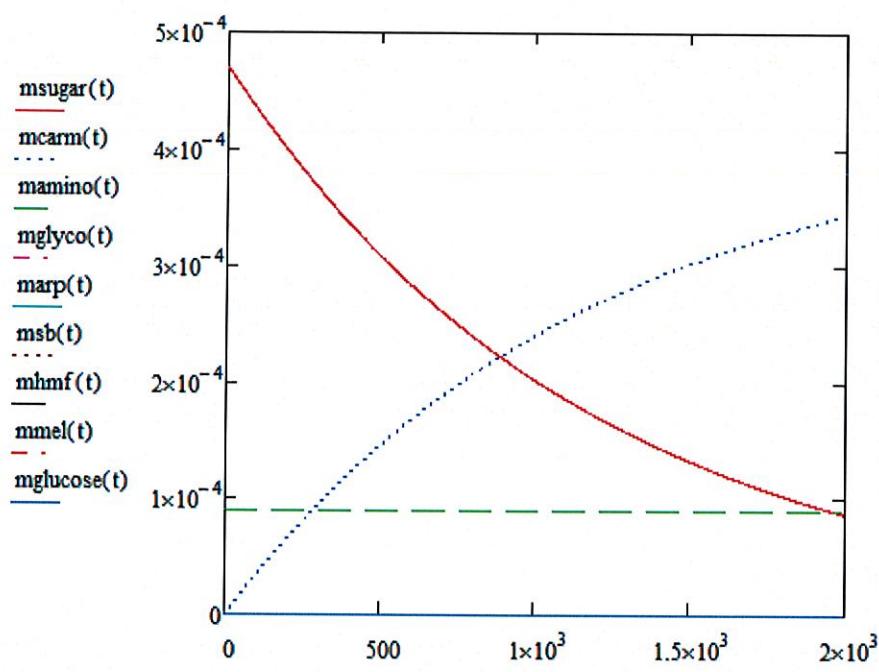
$$M(0) = 0$$

$$\frac{d}{dt} P(t) = -k_{\text{ph4}}(t) \cdot P(t) \cdot W(t)$$

$$P(0) = \frac{m_{\text{pectin}}(\text{tcam1})}{mw_P}$$

$$\frac{d}{dt} GA(t) = 2 \cdot k_{\text{ph4}}(t) \cdot P(t) \cdot W(t)$$

$$GA(0) = \frac{m_{\text{gacid}}(\text{tcam1})}{mw_{GA}}$$



$$tcarm := tcaml + tcamm2 + tph1 + twater = 1.956 \times 10^3$$

Total time for required amount of sugar
to be reacted (s)

$$tcammmin := \frac{tcarm}{60} = 32.592 \quad \text{minutes}$$

$$tph2a(t) := mpectin4(t) - mpectind$$

$$x := 100$$

$$tph2a := \text{root}(tph2a(x), x) = 994.088$$

Additional time for pectin to be
reacted once the system reaches
Tcarm (s)

We need to check that the required amount of pectin was not reached prior to the start of the caramelization/Maillard reactions; if so, it is not the limiting factor for the time to doneness.

$$tph2 := \text{if}(mpectin(tcaml) < mpectind, 0, tph2a) = 994.088$$

$$tph := tph2 + tcaml + tph1 + twater = 2.132 \times 10^3$$

Total time for required amount of
pectin to be reacted (s)

$$tphmin := \frac{tph}{60} = 35.527 \quad \text{minutes}$$

Determination of Done time

$$td := \text{if}(tcarm > tph, tcarm, tph)$$

$$td = 2.132 \times 10^3 \quad \text{seconds} \quad \text{total time to doneness}$$

$$tdmin := \frac{td}{60} = 35.527 \quad \text{minutes} \quad \text{total time to doneness}$$

Model Output: The time to doneness is 2132 seconds (35.5 minutes).

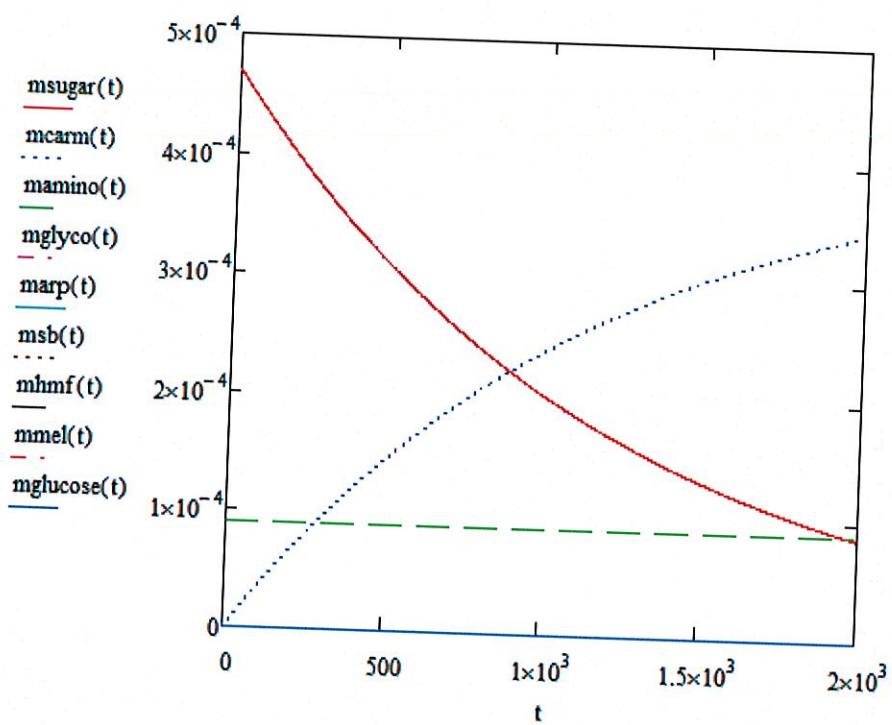


Figure 4: Summary of product and reactant masses (kg) versus time (s) for phase 4 reaction network, larger scale

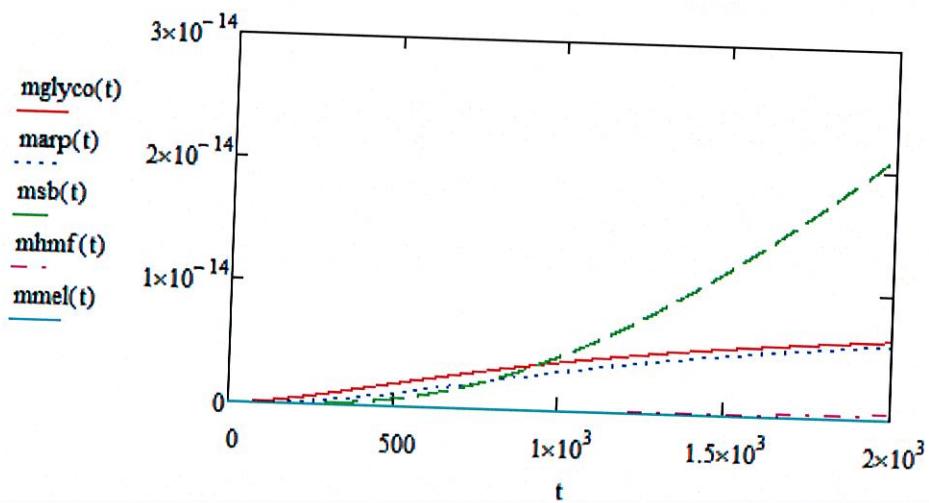


Figure 5: Summary of product and reactant masses (kg) versus time (s) for phase 4 reaction network, smaller scale

Analysis of Model and Conclusions

Please refer to the sample computational model given in the previous section. Reasonable input parameters were assumed, and the model output for time to doneness was 35.5 minutes. The total time for the water to vaporize was 17.9 minutes. The total time for the pectin hydrolyzation to occur was 35.5 minutes. The total time for the caramelization and Maillard reactions to occur was 32.6 minutes.

Reasonability of output

Based on general knowledge of cooking times, the time to doneness should be in the range of 10 to 60 minutes. The final output of 35.5 minutes falls in the middle of this acceptable range, which is a good validation of the overall model.

Examining the times for each process more closely, it can be noted that the times to increase the temperature were relatively short compared to the time required to vaporize the water and complete the reactions. Pectin hydrolyzation was the limiting factor to doneness because it took the longest to occur. This might be due to the low initial pectin concentration and because pectin is only broken down by one reaction, while sugar is depleted by two reactions. However, the total pectin hydrolyzation time was comparable to the total caramelization and Maillard reaction time (a difference of 2.9 minutes). This is also good validation of accuracy of the model and the input parameters used; from real life experience, it is known that a roasted carrot reaches the desired texture, taste, and color at approximately the same time.

The graphs produced in the model are consistent with the expected behavior as well. The temperature plots given in Figure 3 show that temperature increases with time and that the rate slows as the carrot gets closer to the oven temperature. The reaction network plots given in Figures 4, 5, and 6 show that sugar and pectin decrease over time and glucuronic acid, caramelans, and Maillard intermediate products increase with time, which is also consistent with actual behavior.

Limitations

Although the model produces a reasonable output, there are some limitations and ways that it could be improved. Many of these changes would require a greater level of knowledge and more sophisticated numerical methods.

One improvement would be to model heat transfer in multiple dimensions instead of one. The model does not apply as well to an entire carrot as it does to a carrot slice because of the different geometry. A model with cylindrical coordinates would be more suited to a whole carrot. The assumption that the pan is at constant temperature is reasonable as long as the pan is metal. For example, a glass baking dish is slower to heat up, so the assumption would not be valid.

In addition, the assumption that the entire carrot needs to reach a given temperature for a reaction to occur is also not completely accurate; in reality, the reactions would start at an earlier time in the warmer parts of the carrot. However, since the carrot is so small, the additional time for the coldest point to reach a certain temperature is also small. This assumption is very close to reality, and it results in much simpler calculations.

Appendix: Model Development

This section will display the development of the model, starting with a simple model based on fundamental principles and showing how the assumptions and model improved over several iterations. Rather than showing each iteration in its entirety, each section will highlight the changes and improvements made from the previous iteration. Note that the initial iterations are different than those presented in previous deliverables because certain assumptions were found to be inaccurate.

Assumptions Applying to All Iterations

Cooking is divided in four distinct phases:

- Phase 1: The temperature increases from T_{carrot} to T_{boil} .
- Phase 2: The water vaporizes. There is no change in temperature.
- Phase 3: The temperature increases from T_{boil} to T_{ph} . Once T_{ph} is reached, pectin hydrolyzation begins.
- Phase 4: The temperature increases from T_{ph} to T_{carm} . Once T_{carm} is reached, caramelization and Maillard Reactions (in later iterations) begin.

Assumptions related to heat transfer

- The shape of the carrot is a flat plate. (Picture a single flat slice from a larger carrot.)
- Heating the carrot does not cause the oven to cool down. The temperature remains constant at T_{oven} .

Assumptions related to water vaporization

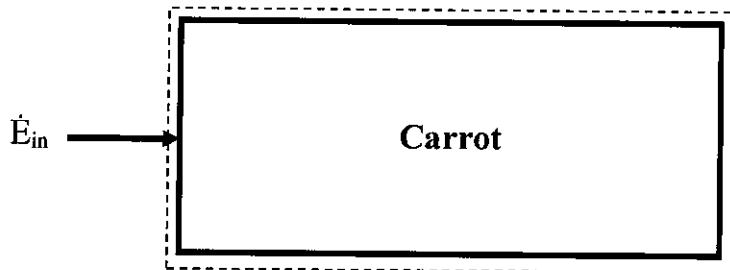
- The mass of water to be considered “done” is the mass of water that causes the concentration of water in the carrot to be equal to the concentration of water outside the carrot. This is set to a constant value.
- Once the system reaches T_{boil} , all of the water that will be vaporized (to reach equilibrium with the outside environment) is vaporized. There is no temperature change as the water is vaporized.
- After the water is vaporized, the temperature begins to increase again.

Assumptions related to chemical reactions

- There is an even distribution of water, sugar, and pectin throughout the carrot.
- The reactions will not occur unless the temperature meets or exceeds the requirement (T_{carm} or T_{ph}). Caramelization reactions begin at T_{carm} , and pectin hydrolyzation begins at T_{ph} (Viera, 1996).
- Pectin hydrolyzation begins before caramelization and Maillard reactions, since T_{ph} is less than T_{carm} (Viera, 1996).
- The degree of brownness on the outer surface is directly related to extent of caramelization reaction (i.e. $x_{brown} = 1 - (m_{sugar} / m_{sugar,i})$)
- Information could not be found for the rate constants, so educated guesses were used. These values can easily be changed by the user if more information becomes available.

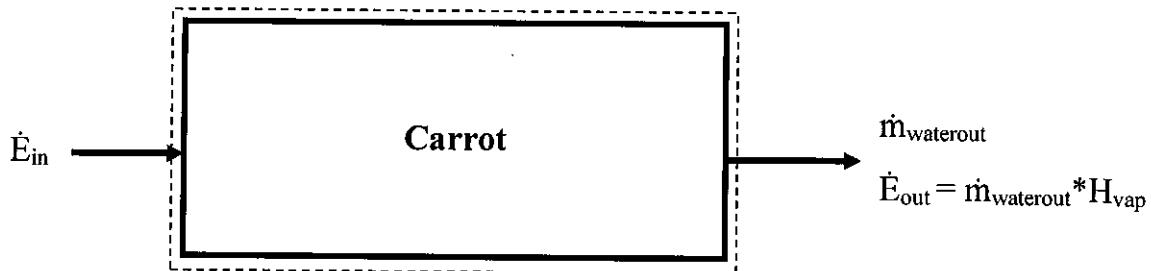
Phase 1: Temperature increases from T_{carrot} to T_{boil} .

- There are no mass flows.
- The only energy flow is from the hot oven air to the carrot.



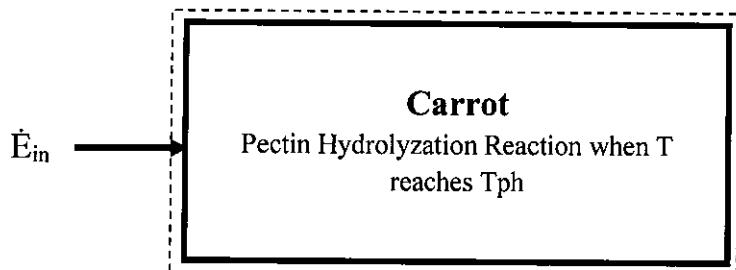
Phase 2: The water is vaporized.

- There is no accumulation of energy, so the temperature is constant at T_{boil} .
- All of the energy entering the system is used to vaporize the water.
- The only mass flow is the water exiting the system.



Phase 3: Temperature increases from T_{boil} to T_{ph} .

- There are no mass flows.
- There is an energy flow from the hot oven air to the carrot.
- Pectin hydrolyzation begins at the end of this phase, once the temperature reaches T_{ph}



Phase 4: Temperature increases from T_{ph} to T_{carm} .

- There are no mass flows.
- There is an energy flow from the hot oven air to the carrot.

Energy Balance

Since the temperature is constant, there is no energy accumulated

$$Ein - Eout = 0$$

$$Ein := h \cdot S \cdot (T_{oven} - T_{boil})$$

$$Eout := m_{waterout} \cdot Hvap$$

$$h \cdot S \cdot (T_{oven} - T_{boil}) = m_{waterout} \cdot Hvap$$

$$m_{waterout} := h \cdot S \cdot \frac{(T_{oven} - T_{boil})}{H_{steam}}$$

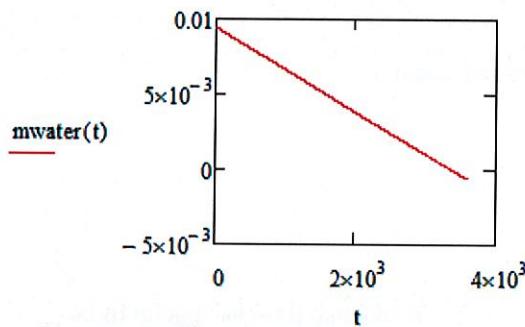
$$\frac{dm_{water}}{dt} = -m_{waterout}$$

$$\frac{dm_{water}}{dt} = -\left[h \cdot S \cdot \frac{(T_{oven} - T_{boil})}{H_{steam}} \right]$$

Boundary Condition: At $t=0$, $m_{water}=m_{wateri}$

$$m_{water}(t) := -h \cdot S \cdot \frac{(T_{oven} - T_{boil})}{Hvap} \cdot t + m_{wateri}$$

$$t := 0..3600$$



$$vap(t) := m_{water}(t) - m_{waterd}$$

$$x = 100$$

$$tvap := \text{root}(vap(x), x) = 1.015 \times 10^3$$

Additional time for water to be vaporized once the system has reached t_{boil} .

$$twater := t_{boil} + tvap = 1.375 \times 10^3$$

Total time for required amount of water to be lost (s)

Phase 3: Raise Temperature to T_{ph} and begin Pectin Hydrolyzation- In this phase, the time point $t=0$ corresponds to the end of the previous phase

Energy Balance

$$\frac{dE_{total}}{dt} := Ein$$

$$\frac{dE_{total}}{dt} := -m_{total} \cdot cp \cdot \frac{dT}{dt}$$

$$Ein := hS \cdot (T(t) - Toven)$$

$$\frac{dT}{dt} := \frac{-hS}{m_{total} \cdot cp} \cdot (T(t) - Toven)$$

Boundary Condition: at t=0, T=Tph

$$T(t) := Toven + (Tph - Toven) \cdot \exp\left(\frac{-h \cdot S \cdot t}{m_{total} \cdot cp}\right)$$

$$t := \ln\left(\frac{T(t) - Toven}{Tph - Toven}\right) \cdot \left(\frac{-m_{total} \cdot cp}{h \cdot S}\right)$$

$$t_{carm1} := \ln\left(\frac{T_{carm} - Toven}{Tph - Toven}\right) \cdot \left(\frac{-m_{total} \cdot cp}{h \cdot S}\right) = 425.878$$

Additional time for the system to reach caramelization temperature once Tph has been reached (s)

Reaction Derivation

$$\frac{dCsugar}{dt} := kcarm \cdot Csugar$$

Initial Condition: at t=0, Csugar=Csgari

$$Csugar(t) := Csgari \cdot \exp(-kph \cdot t)$$

Same volume, so we multiply by volume on both sides and obtain:

$$msugar(t) := msugari \cdot \exp(-kcarm \cdot t)$$

$$t := \frac{\ln\left(\frac{msugar(t)}{msugari}\right)}{-kcarm}$$

$$t_{carm2} := \frac{\ln\left(\frac{msugard}{msugari}\right)}{-kcarm} = 693.147$$

Additional time for sugar to be reacted once the system reaches Tcarm (s)

$$t_{carm} := t_{carm1} + t_{carm2} + tph1 + twater = 2.606 \times 10^3$$

Total time for required amount of sugar to be reacted (s)

Determination of Done time

$$td := \text{if}(t_{carm} > tph, t_{carm}, tph)$$

$$td = 2.606 \times 10^3$$

$$tdmin := \frac{td}{60} = 43.428$$

Model Output: The time to doneness is 2606 seconds (43.4 minutes).

$$E_{in} := hS \cdot (T(t) - T_{oven})$$

$$E_{ext} := Eph$$

$$\frac{dT}{dt} := \frac{-hS}{m_{total} \cdot cp} \cdot (T(t) - T_{oven}) + \frac{Eph}{m_{total} \cdot cp}$$

Boundary Condition: at t=0, T=Tph

$$C1 := \frac{-h \cdot S}{m_{total} \cdot cp}$$

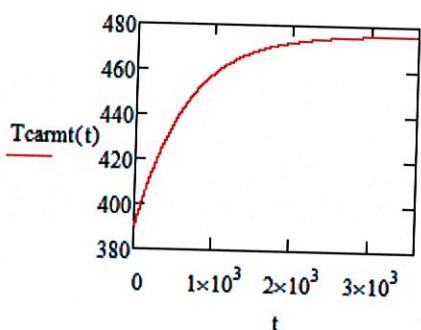
$$C2 := \frac{T_{oven} \cdot h \cdot S}{m_{total} \cdot cp} + \frac{-Eph}{m_{total} \cdot cp}$$

$$T_{carm}(t) := \left(Tph + \frac{C2}{C1} \right) \cdot \exp(C1 \cdot t) - \frac{C2}{C1}$$

$$tcarm1(t) := T_{carm} - T_{carm}(t)$$

$$x := 100$$

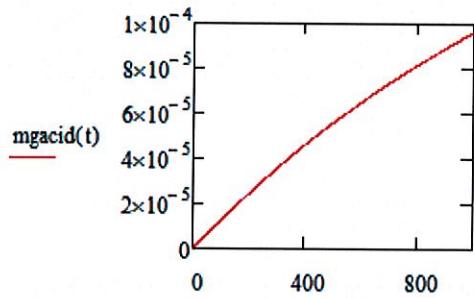
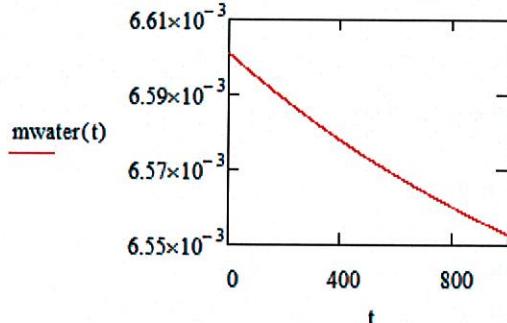
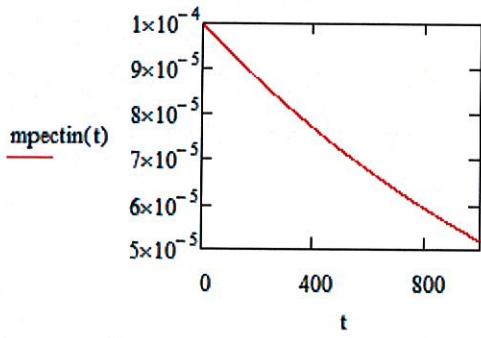
$$tcarm1 := \text{root}(tcarm1(x), x) = 437.701$$



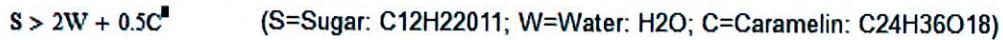
Additional time for the system to reach caramelization temperature once Tph has been reached (s)

$$GA(0) = 0$$

$$\begin{pmatrix} m_{pectin} \\ m_{water} \\ m_{gacid} \end{pmatrix} := \text{Odesolve} \left[\begin{pmatrix} P \\ W \\ GA \end{pmatrix}, t, 1000, 1000 \right]$$



Reaction Derivation



Mass Balance:

$$V \frac{dCs}{dt} := V \cdot -k_{camm} \cdot Cs$$

Multiplying by volume converts concentrations to masses.

$$\frac{dm_{sugar}}{dt} := -k_{camm} \cdot m_{sugar}$$

$$\frac{dm_{water}}{dt} := 2 \cdot k_{camm} \cdot m_{sugar}$$

$$\frac{dm_{gacid}}{dt} := 0.5 \cdot k_{camm} \cdot m_{sugar}$$

ITERATION 4

Iteration 4 Assumptions

All assumptions from Iteration 3 apply, except the ones given below:

- The total mass of the system changes with time. The loss of total mass of the system is equal to the loss of water of the system.
- The total volume of the system changes with time. The loss of volume by the system is equal to the mass of water lost divided by the density.
- Therefore, the density of the system changes with time.

Iteration 4 Model Output: 41.0 minutes

Iteration 4 System Diagrams: Refer to Iteration 1 and 2.

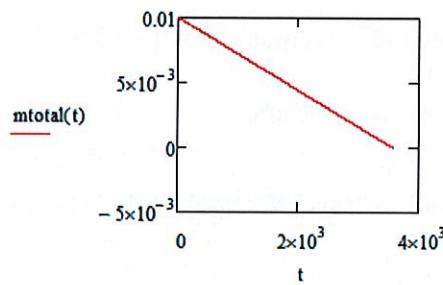
Iteration 4 Computational Model: Only the sections different from Iteration 3 are displayed.

We want to calculate the new total mass and volume to use in the calculations for the later phases. From energy balance, we have

$$\frac{dm_{total}}{dt} := \frac{dm_{water}}{dt}$$

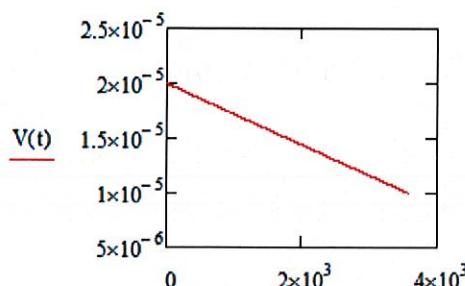
Boundary Condition: At $t=0$, $m_{total}=m_{totali}$

$$m_{total}(t) := -h \cdot S \cdot \frac{(T_{oven} - T_{boil})}{H_{vap}} \cdot t + m_{totali}$$



$$m_{totalnew} := m_{total}(tvap) = 7.171 \times 10^{-3}$$

$$V(t) := V - \frac{1}{\rho_w} \cdot (m_{wateri} - m_{water}(t))$$



$$V_{new} := V(tvap) = 1.717 \times 10^{-5}$$

$$\frac{d}{dt} CPC(t) = .001 \left[1962.5 \cdot 10^{-3} - 5939.9 \cdot 10^{-6} \cdot 2 \cdot (T1(t) - 273) \cdot \left[\frac{d}{dt} (T1(t)) \right] \right]$$

$$CPC(0) = cpc_i$$

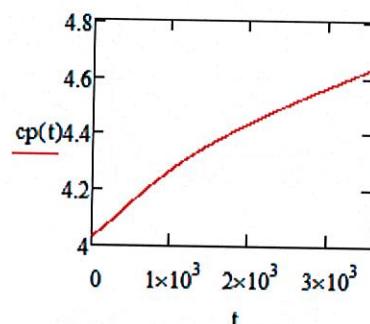
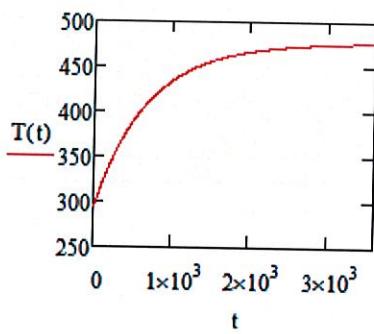
$$\frac{d}{dt} CPF(t) = .001 \left[1930.6 \cdot 10^{-3} - 4650.9 \cdot 10^{-6} \cdot 2 \cdot (T1(t) - 273) \cdot \left[\frac{d}{dt} (T1(t)) \right] \right]$$

$$CPF(0) = cpf_i$$

$$\frac{d}{dt} CP(t) = \frac{mwateni}{mtotali} \cdot \left(\frac{d}{dt} CPW(t) \right) + \frac{msugani}{mtotali} \cdot \left(\frac{d}{dt} CPC(t) \right) + \frac{mpectini}{mtotali} \cdot \left(\frac{d}{dt} CPF(t) \right)$$

$$CP(0) = cpi$$

$$\begin{pmatrix} T_{\text{nw}} \\ cpw \\ cpc \\ cpf \\ cp \end{pmatrix} = \text{Odesolve} \left[\begin{pmatrix} T1 \\ CPW \\ CPC \\ CPF \\ CP \end{pmatrix}, t, 3600, 3600 \right]$$



Given

$$\frac{d}{dt} T1(t) = \frac{-h \cdot S}{mtotali \cdot CP(t)} \cdot (T1(t) - T_{oven})$$

$$T1(0) = T_{boil}$$

$$\frac{d}{dt} CPW(t) = .001 \left[-9.0862 \cdot 10^{-5} + 5473.1 \cdot 10^{-6} \cdot 2 \cdot (T1(t) - 273) \cdot \left[\frac{d}{dt} (T1(t)) \right] \right]$$

$$CPW(0) = cpw(t_{boil})$$

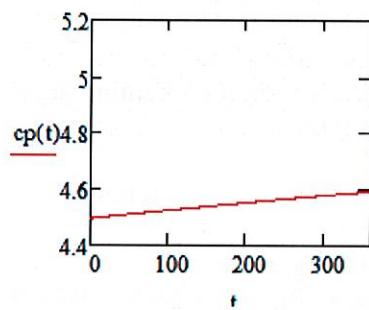
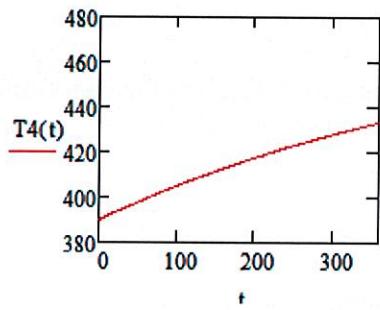
$$\frac{d}{dt} CPC(t) = .001 \left[1962.5 \cdot 10^{-3} - 5939.9 \cdot 10^{-6} \cdot 2 \cdot (T1(t) - 273) \cdot \left[\frac{d}{dt} (T1(t)) \right] \right]$$

$$CPC(0) = cpc(t_{boil})$$

$$\frac{d}{dt} CP(t) = \frac{mwateri}{mtotali} \cdot \left(\frac{d}{dt} CPW(t) \right) + \frac{msugari}{mtotali} \cdot \left(\frac{d}{dt} CPC(t) \right) + \frac{mpectini}{mtotali} \cdot \left(\frac{d}{dt} CPF(t) \right)$$

$$CP(0) = cp(tph)$$

$$\begin{pmatrix} T4 \\ CPW \\ CPC \\ CPF \\ CP \end{pmatrix} := \text{Odesolve} \left[\begin{pmatrix} T1 \\ CPW \\ CPC \\ CPF \\ CP \end{pmatrix}, t, 3600, 3600 \right]$$



Iteration 6 Computational Model

Only the sections that are different from Iteration 5 are displayed.

Equation for Heat Capacity based on the Choi-Okos Equation (1987)

$$cpwi := .001 \left[4176.2 - 9.0862 \cdot 10^{-5} \cdot (T_{carroti} - 273) + 5473.1 \cdot 10^{-6} \cdot (T_{carroti} - 273)^2 \right] = 4.178$$

$$cpci := .001 \left[1548.8 + 1962.5 \cdot 10^{-3} \cdot (T_{carroti} - 273) - 5939.9 \cdot 10^{-6} \cdot (T_{carroti} - 273)^2 \right] = 1.586$$

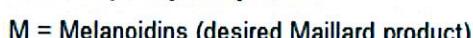
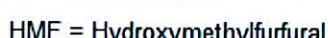
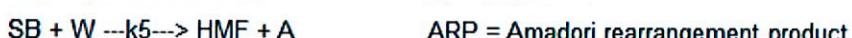
$$cpfi := .001 \left[1845.9 + 1930.6 \cdot 10^{-3} \cdot (T_{carroti} - 273) - 4650.9 \cdot 10^{-6} \cdot (T_{carroti} - 273)^2 \right] = 1.883$$

$$cppi := .001 \left[2008.2 + 1208.9 \cdot 10^{-3} \cdot (T_{carroti} - 273) - 1312.9 \cdot 10^{-6} \cdot (T_{carroti} - 273)^2 \right] = 2.032$$

$$cpi := \frac{mwatert}{mtotali} \cdot cpwi + \frac{msugari}{mtotali} \cdot cpci + \frac{mpectini}{mtotali} \cdot cpfi + \frac{mprotein}{mtotali} \cdot cppi = 4.014 \text{ kJ/kgK}$$

Maillard Reaction

Maillard Reaction Network: Based on the diagram from Hodge, 1953 and assuming pH<7



Assume Caramelization and Maillard Reaction occur in the same network because they begin at the same time

Mass Balance on Sugar:

$$V \frac{dCS}{dt} := V \cdot -k_{carm} \cdot CS - V \cdot k1 \cdot CS \cdot CA + V \cdot k2 \cdot CG \cdot CW$$

Multiplying by volume converts concentrations to masses.

$$\frac{dS}{dt} := -k_{carm} \cdot S - km1 \cdot S \cdot A + k2 \cdot G \cdot W$$

$$\frac{dW}{dt} := 2 \cdot k_{carm} \cdot S + km1 \cdot S \cdot A - km2 \cdot G \cdot W + 3 \cdot km4 \cdot ARP - km5 \cdot SB \cdot W$$

$$\frac{dC}{dt} := 0.5 \cdot k_{carm} \cdot S$$

$$\frac{d}{dt} SB(t) = km4 \cdot ARP(t) - km5 \cdot SB(t) \cdot W(t)$$

$$SB(0) = 0$$

$$\frac{d}{dt} HMF(t) = km5 \cdot SB(t) \cdot W(t) - km6 \cdot HMF(t) \cdot A(t)$$

$$HMF(0) = 0$$

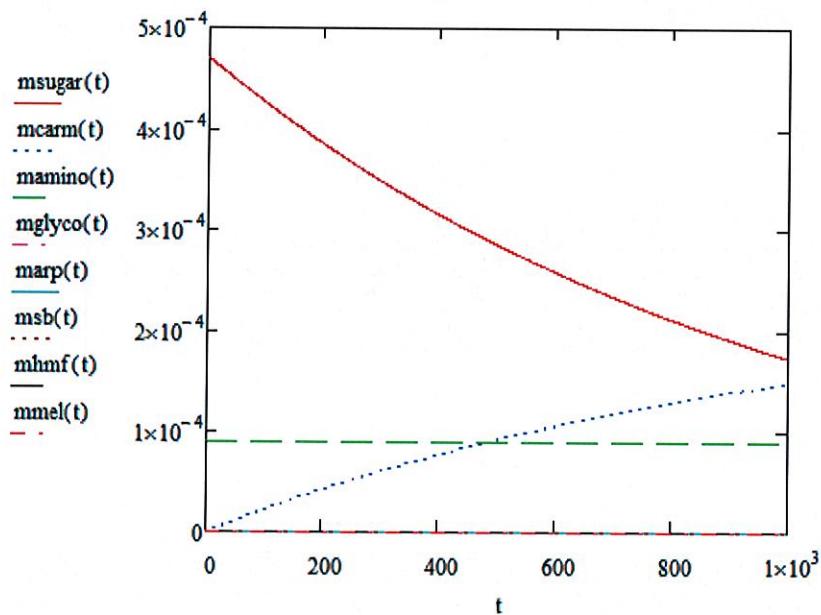
$$\frac{d}{dt} M(t) = km6 \cdot HMF(t) \cdot A(t)$$

$$M(0) = 0$$

```

  msugar
  mwater4
  mcarm
  mamino
  mglyco := Odesolve
  marp
  msb
  mhmaf
  mmel
  
```

S
W
C
A
G , t, 1000, 1000
ARP
SB
HMF
M



ITERATION 7

Iteration 7 Assumptions

All assumptions from Iteration 6 apply, except the ones given below:

- The pectin hydrolyzation reaction is no longer considered separately from the Maillard and caramelization reaction network.
 - Pectin hydrolyzation begins before caramelization and Maillard, since Tph is less than Tcarm.
 - Once caramelization and Maillard begin, all three are considered in one network.
 - This is more realistic since all three reactions have water as a reactant and/or product.

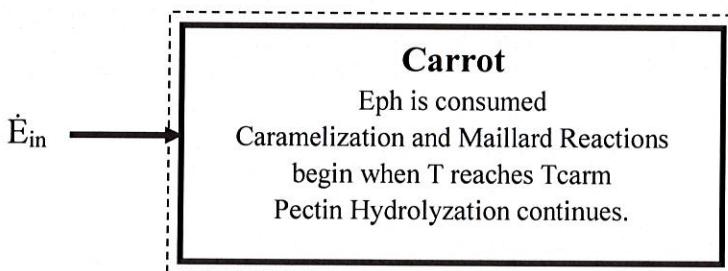
Iteration 7 Model Output: 36.2 minutes

Iteration 7 System Diagrams

Only Phase 4 changes. Refer to Iteration 1 for the other phases.

Phase 4: Temperature increases from Tph to Tcarm.

- There are no mass flows.
- There is an energy flow from the hot oven air to the carrot.
- Energy is being consumed by the pectin hydrolyzation reaction, which began at the end of the last phase.
- Caramelization begins at the end of this phase, once the temperature reaches Tcarm. This would result in a consumption of energy as the temperature continues to increase.



Iteration 7 Computational Model

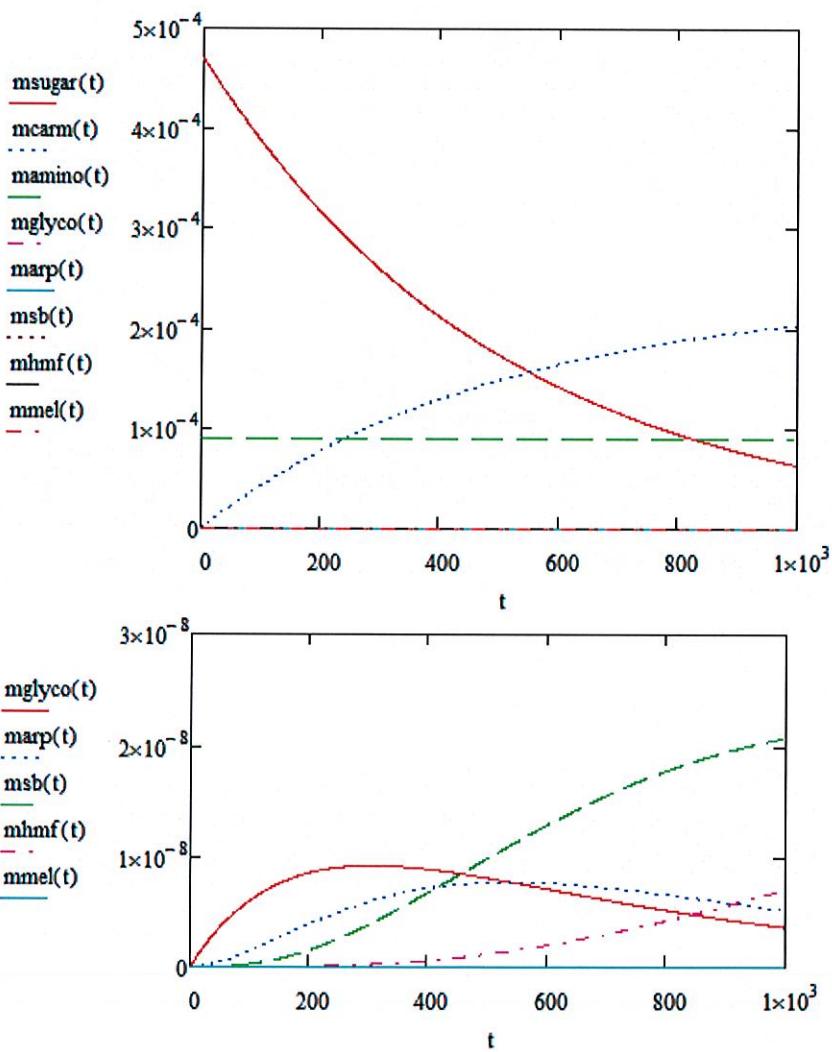
Only the sections that are different from Iteration 6 are displayed.

Given

$$\frac{d}{dt} S(t) = -k_{carm} \cdot S(t) - km1 \cdot S(t) \cdot A(t) + km2 \cdot G(t) \cdot W(t)$$

$$S(0) = msugari$$

$$\frac{d}{dt} W(t) = 2 \cdot k_{carm} \cdot S(t) + km1 \cdot S(t) \cdot A(t) - km2 \cdot G(t) \cdot W(t) + 3 \cdot km4 \cdot ARP(t) - km5 \cdot SB(t) \cdot W(t)$$

$$\left. \begin{array}{l} \text{msugar} \\ \text{mwater4} \\ \text{mcarm} \\ \text{mamino} \\ \text{mglyco} \\ \text{marp} \\ \text{msb} \\ \text{mhmf} \\ \text{mmel} \\ \text{mpectin4} \\ \text{mgacid4} \end{array} \right\} := \text{Odesolve} \left[\begin{array}{l} \text{S} \\ \text{W} \\ \text{C} \\ \text{A} \\ \text{G} \\ \text{ARP} \\ \text{SB} \\ \text{HMF} \\ \text{M} \\ \text{P} \\ \text{GA} \end{array} \right], t, 1000, 1000$$


ITERATION 8

Iteration 8 Assumptions

All assumptions from Iteration 7 apply, except the ones given below:

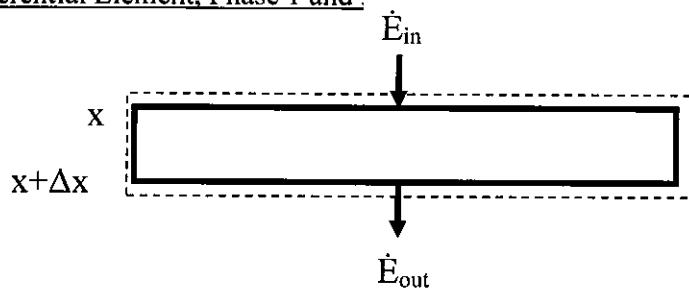
- Distributed system
 - The temperature profile is found as a function of position and time.
 - One dimensional heat transfer
 - Because of convection, the temperature at the surface of the carrot is not equal to the temperature of the oven. To determine the surface temperature boundary condition, we examine a very small thickness at the surface (5% of the total surface) and treat it as a lumped parameter system. This assumption is valid because the section is so small.
 - The surface boundary condition is the same for the top and bottom of the carrot.
 - Since we have assumed an even distribution of water, sugar, and pectin in the system, the entire carrot needs to reach each given temperature. The center of the carrot ($x=0.5*L$) takes the longest to heat, so we will determine time by finding the time it takes for the center of the carrot to reach a given temperature.
- Heat capacity and thermal conductivity are assumed to be constant. Both values are calculated using the Choi-Okos Equations (Choi & Okos, 1986).

Iteration 8 Model Output: 32.2 minutes

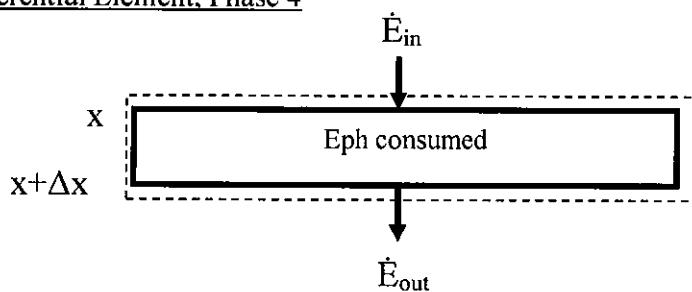
Iteration 8 System Diagrams

Refer to Iteration 1 and 7 for full system diagrams. The differential elements for the distributed system are shown.

Differential Element, Phase 1 and 3



Differential Element, Phase 4



Take limit as Δx goes to 0

$$\frac{dT}{dt} = \frac{k}{\rho_{carrot} \cdot c_p} \cdot \frac{d^2}{dx^2} T$$

$$\frac{dT(x,t)}{dt} = \alpha \cdot \frac{d^2}{dx^2} T(x,t)$$

Initial Condition:

$$\text{at } t=0, T(x,0) = T_{carrot}$$

Boundary Conditions:

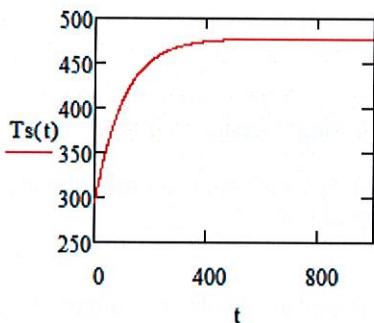
$$\text{for } t>0, T(0,t) = T_s(t)$$

$$\text{for } t>0, T(L,t) = T_s(t)$$

$$m_{surface} := 0.05 \cdot m_{total} = 5 \times 10^{-4} \quad \text{kilograms}$$

$$T_s(t) := T_{oven} + (T_{carrot} - T_{oven}) \cdot \exp\left(\frac{-h \cdot A \cdot t}{m_{surface} \cdot c_p}\right)$$

Boundary condition for the temperature at the surface



Given

$$T_t(x,t) = \alpha \cdot T_{xx}(x,t)$$

$$T(x,0) = T_{carrot}$$

$$T(L,t) = T_s(t)$$

$$T(0,t) = T_s(t)$$

$$T_1 := \text{Pdesolve}\left[T, x, \begin{pmatrix} 0 \\ L \end{pmatrix}, t, \begin{pmatrix} 0 \\ 1000 \end{pmatrix}, 100, 1000\right]$$

Temperature profile in phase 1 of cooking

$$\frac{dT(x,t)}{dt} = \alpha \cdot \frac{d^2}{dx^2} T(x,t)$$

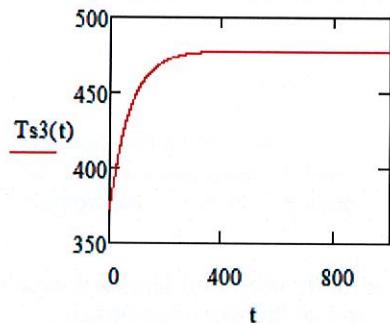
Initial Condition:
at $t=0$, $T(x,0) = T_{boil}$

Boundary Conditions:
for $t>0$, $T(0,t) = Ts3(t)$
for $t>0$, $T(L,t) = Ts3(t)$

$$msurfacenew := 0.05 \cdot mtotalnew = 3.599 \times 10^{-4} \text{ kilograms}$$

Mass of small surface
section has changed
due to water
vaporization

$$Ts3(t) := T_{oven} + (T_{boil} - T_{oven}) \cdot \exp\left(\frac{-h \cdot A \cdot t}{msurfacenew \cdot cpnew}\right)$$



Given

$$T_t(x,t) = \alpha \cdot T_{xx}(x,t)$$

$$T(x,0) = T1(x,t_{boil})$$

$$T(L,t) = Ts3(t)$$

$$T(0,t) = Ts3(t)$$

$$T3 := \text{Pdesolve}\left[T, x, \begin{pmatrix} 0 \\ L \end{pmatrix}, t, \begin{pmatrix} 0 \\ 1000 \end{pmatrix}, 100, 1000\right] \text{ Temperature profile in phase 3 of cooking}$$

$$\frac{dE_{\text{total}}}{dt} := -m_{\text{total}} \cdot c_p \cdot \frac{dT}{dt}$$

$$\frac{dE_{\text{total}}}{dt} := -A \cdot \Delta x \cdot \rho_{\text{carrot}} \cdot c_p \cdot \frac{dT}{dt}$$

$$E_{\text{in}} := kA \cdot \left(\frac{d}{dx} T \right)_x$$

$$E_{\text{out}} := kA \cdot \left(\frac{d}{dx} T \right)_{x+\Delta x}$$

$$E_{\text{rxn}} := A \cdot \Delta x \cdot E_{\text{ph}}$$

$$\frac{dT}{dt} := \frac{-k \cdot \left(\frac{d}{dx} T \right)_x + k \cdot \left(\frac{d}{dx} T \right)_{x+\Delta x} - E_{\text{ph}}}{\Delta x \cdot \rho_{\text{carrot}} \cdot c_p}$$

Take limit as Δx goes to 0

$$\frac{dT}{dt} := \frac{k}{\rho_{\text{carrot}} \cdot c_p} \cdot \frac{d^2}{dx^2} T - \frac{E_{\text{ph}}}{\rho_{\text{carrot}} \cdot c_p}$$

$$\frac{dT(x,t)}{dt} := \alpha \cdot \frac{d^2}{dx^2} T(x,t) - \frac{E_{\text{ph}}}{\rho_{\text{carrot}} \cdot c_p}$$

Initial Condition:

$$\text{at } t=0, T(x,0) = T_{\text{ph}}$$

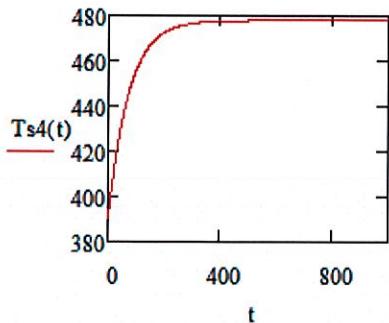
Boundary Conditions:

$$\text{for } t>0, T(0,t) = T_{\text{s4}}(t)$$

$$\text{for } t>0, T(L,t) = T_{\text{s4}}(t)$$

$$T_{\text{s4}}(t) := T_{\text{oven}} + (T_{\text{ph}} - T_{\text{oven}}) \cdot \exp\left(\frac{-h \cdot A \cdot t}{m_{\text{surface}} \cdot c_p}\right)$$

Boundary condition for the temperature at the surface, phase 4



ITERATION 9

Iteration 9 Assumptions

All assumptions from Iteration 8 apply, except the ones given below:

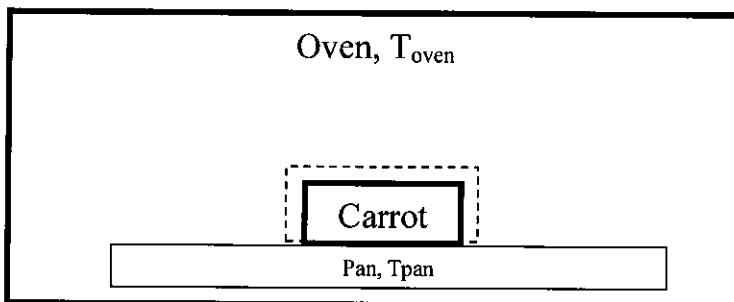
- The carrot is on a pan. The bottom surface has a new boundary condition.
 - The pan has a very high thermal conductivity, so it immediately reaches a temperature very close to the temperature of the oven.
 - The temperature of the pan is constant.
 - The top surface boundary condition is still found in the same way as Iteration 8.
 - The center is no longer the cold point of the carrot. The new cold point location is calculated iteratively.

Iteration 9 Model Output: 30.8 minutes

Iteration 9 System Diagrams

Refer to Iteration 8 for the differential element diagrams.

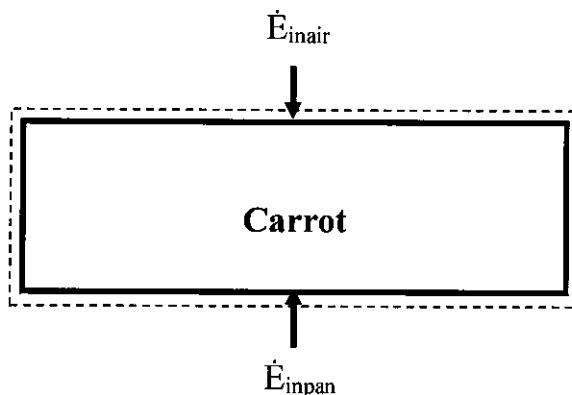
System Definition: Carrot Piece. System boundary is shown with a dotted line. Note that the pan is in contact with the carrot, but it is not inside the system boundary.

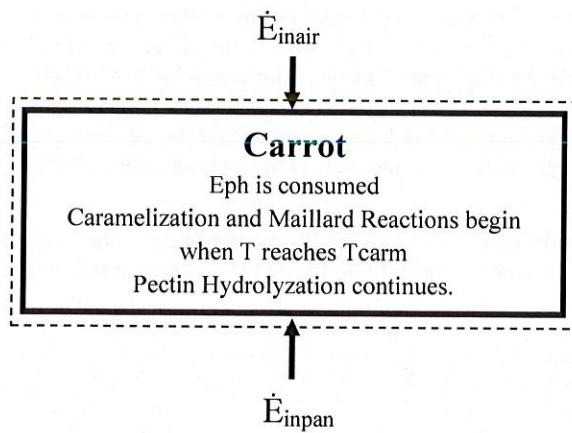


All of the following diagrams show only the carrot piece.

Phase 1: Temperature increases from $T_{carroti}$ to T_{boil} .

- There are no mass flows.
- The only energy flow is from the hot oven air to the carrot.





Iteration 9 Computational Model

Only the sections that are different from Iteration 8 are displayed.

Given

$$T_t(x, t) = \alpha \cdot T_{xx}(x, t)$$

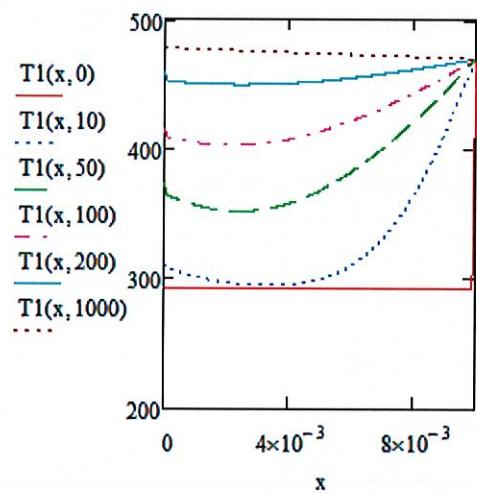
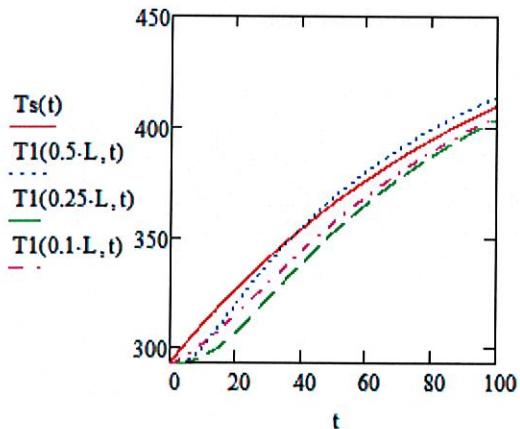
$$T(x, 0) = T_{carroti}$$

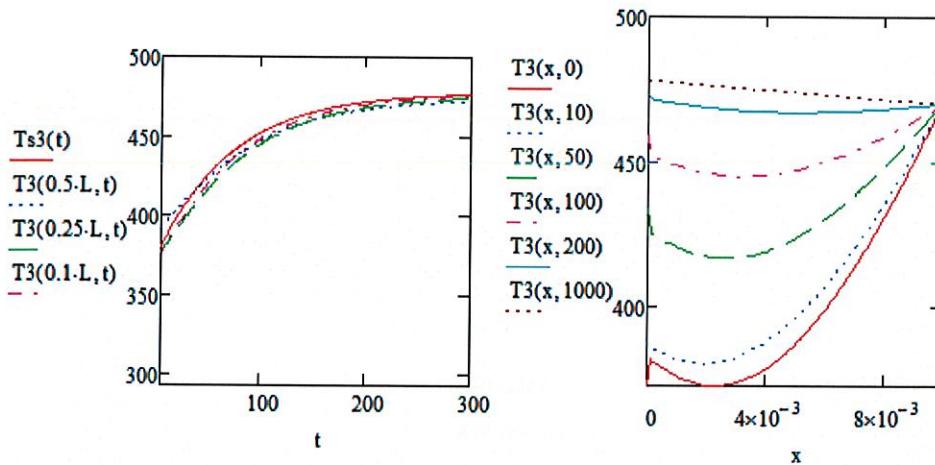
$$T(L, t) = T_{pan}$$

$$T(0, t) = T_s(t)$$

$$T1 := \text{Pdesolve}\left[T, x, \begin{pmatrix} 0 \\ L \end{pmatrix}, t, \begin{pmatrix} 0 \\ 1000 \end{pmatrix}, 100, 1000\right]$$

Temperature profile in phase 1 of cooking





$$T_{phapprox}(t) := T3(0.5 \cdot L, t) - T_{ph}$$

$$x := 100$$

$$t_{phapprox} := \text{root}(T_{phapprox}(x), x) = 3.011$$

Approximate time for the system
to reach pectin hydrolyzation
temperature (s)

$$T_{phcoldpt}(x) := T3(x, t_{phapprox})$$

$$z := 0.003$$

$$coldpt := \text{Minimize}(T_{phcoldpt}, z) = 1.515 \times 10^{-3}$$

Location of cold point (m)

$$T_{phapprox2}(t) := T3(coldpt, t) - T_{ph}$$

$$x := 100$$

$$t_{phapprox2} := \text{root}(T_{phapprox2}(x), x) = 18.822$$

Approximate time for the system
to reach pectin hydrolyzation
temperature (s)

$$T_{phcoldpt2}(x) := T3(x, t_{phapprox2})$$

$$z := 0.003$$

$$coldpt2 := \text{Minimize}(T_{phcoldpt2}, z) = 2.121 \times 10^{-3}$$

Location of cold point (m)

$$T_{ph1}(t) := T3(coldpt2, t) - T_{ph}$$

$$x := 100$$

$$t_{ph1} := \text{root}(T_{ph1}(x), x) = 19.412$$

Additional time for the system to
reach hydrolyzation temperature
once the water has vaporized (s)

Given

$$T_t(x, t) = \alpha \cdot T_{xx}(x, t) - \frac{E_{ph}}{\rho_{carrot} \cdot c_{pi}}$$

$$T(x, 0) = T3(x, t_{ph1})$$

$$T(L, t) = T_{pan}$$

$$T(0, t) = T_{s4}(t)$$

ITERATION 10

Iteration 10 Assumptions

All assumptions from Iteration 9 apply, except the ones given below:

- The chemical formulas and molecular weights are considered for the reactants and products of all chemical reactions.
- Stoichiometry is considered.
- Conversion from kmol to kg is performed, and graphs are presented in terms of mass.

Iteration 10 Model Output: 37.4 minutes

Iteration 10 System Diagrams

Refer to Iteration 8 and 9.

Iteration 10 Computational Model

Only the sections that are different from Iteration 9 are displayed.

Molecular Weights of Hydrolyzation, Caramelization, and Maillard Products and Reactants

$\text{mwP} := 12 \cdot 12 + 18 \cdot 1 + 13 \cdot 16 = 370$	kg/kmol Pectin
$\text{mwW} := 2 \cdot 1 + 16 = 18$	kg/kmol Water
$\text{mwGA} := 6 \cdot 12 + 10 \cdot 1 + 7 \cdot 16 = 194$	kg/kmol Glucuronic Acid
$\text{mwS} := 12 \cdot 12 + 22 \cdot 1 + 11 \cdot 16 = 342$	kg/kmol Sucrose
$\text{mwC} := 24 \cdot 12 + 36 \cdot 1 + 18 \cdot 16 = 612$	kg/kmol Caramelin
$\text{mwGL} := 6 \cdot 12 + 12 \cdot 1 + 6 \cdot 16 = 180$	kg/kmol Glucose
$\text{mwA} := 12 \cdot 1 + 14 + 2 \cdot 1 = 28$	kg/kmol Amino Groups
$\text{mwG} := 7 \cdot 12 + 12 \cdot 1 + 1 \cdot 14 + 5 \cdot 16 = 190$	kg/kmol Glycosylamine
$\text{mwARP} := 7 \cdot 12 + 12 \cdot 1 + 1 \cdot 14 + 5 \cdot 16 = 190$	kg/kmol Amadori rearrangement product
$\text{mwSB} := 7 \cdot 12 + 6 \cdot 1 + 14 + 2 \cdot 16 = 136$	kg/kmol Schiff's Base
$\text{mwHMF} := 6 \cdot 12 + 6 \cdot 1 + 3 \cdot 16 = 126$	kg/kmol Hydroxymethylfurfural
$\text{mwM} := 7 \cdot 12 + 8 \cdot 1 + 14 + 3 \cdot 16 = 154$	kg/kmol Melanoidin

Pectin Hydrolyzation



P= Pectin ($\text{C}_{12}\text{H}_{18}\text{O}_{13}$)
W= Water (H_2O)
GA=Glucuronic Acid ($\text{C}_6\text{H}_{10}\text{O}_7$)

Caramelization Reaction



S = Sugar (sucrose $\text{C}_{12}\text{H}_{22}\text{O}_{11}$)
W = Water (H_2O)
C = Caramelin ($\text{C}_{24}\text{H}_{36}\text{O}_{18}$)

$$\text{ARP}(0) = 0$$

$$\frac{d}{dt} \text{SB}(t) = km4 \cdot \text{ARP}(t) - km5 \cdot \text{SB}(t) \cdot W(t)$$

$$\text{SB}(0) = 0$$

$$\frac{d}{dt} \text{HMF}(t) = km5 \cdot \text{SB}(t) \cdot W(t) - km6 \cdot \text{HMF}(t) \cdot A(t)$$

$$\text{HMF}(0) = 0$$

$$\frac{d}{dt} M(t) = km6 \cdot \text{HMF}(t) \cdot A(t)$$

$$M(0) = 0$$

$$\frac{d}{dt} P(t) = -kph \cdot P(t) \cdot W(t)$$

$$P(0) = \frac{m\text{pectin}(\text{tcam1})}{\text{mwP}}$$

$$\frac{d}{dt} GA(t) = 2 \cdot kph \cdot P(t) \cdot W(t)$$

$$GA(0) = \frac{m\text{gacid}(\text{tcam1})}{\text{mwGA}}$$

$$\left(\begin{array}{l} \text{sugar} \\ \text{water4} \\ \text{cam} \\ \text{amino} \\ \text{glyco} \\ \text{arp} \\ \text{sb} \\ \text{hmf} \\ \text{mel} \\ \text{pectin4} \\ \text{gacid4} \\ \text{glucose} \end{array} \right) := \text{Odesolve} \left[\begin{array}{l} S \\ W \\ C \\ A \\ G \\ ARP \\ SB \\ HMF \\ M \\ P \\ GA \\ GL \end{array} \right], t, 2000, 2000$$

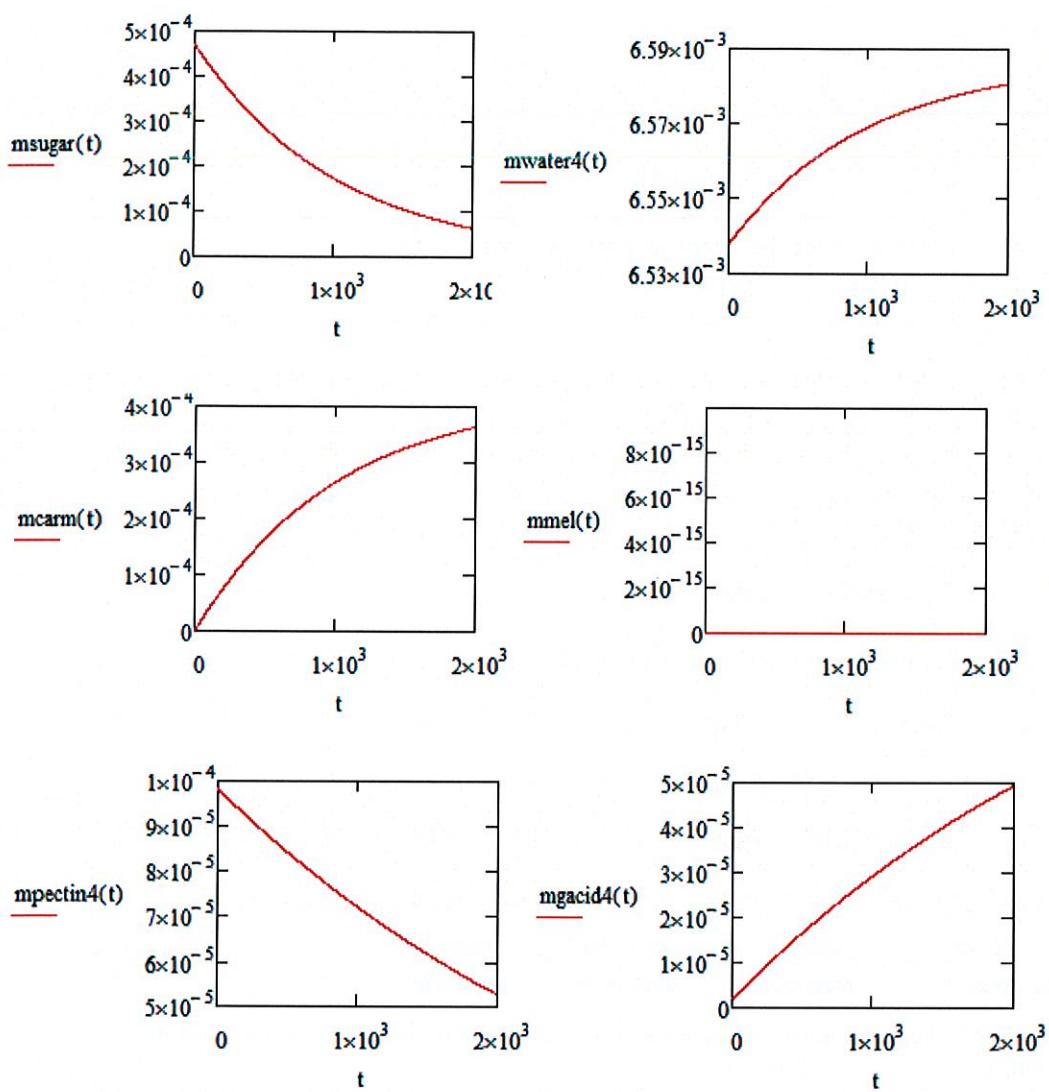
$$msugar(t) := \text{mwS} \cdot \text{sugar}(t)$$

$$mwater4(t) := \text{mwW} \cdot \text{water4}(t)$$

$$mcam(t) := \text{mwC} \cdot \text{cam}(t)$$

$$mamino(t) := \text{mwA} \cdot \text{amino}(t)$$

$$mglyco(t) := \text{mwG} \cdot \text{glyco}(t)$$



Calculation of new value for thermal diffusivity

$$\alpha_2 := \frac{k_2}{\rho_{carrot2} \cdot cp_2} = 3.821 \times 10^{-7}$$

Equation for Thermal Conductivity based on the Choi-Okos Equation (1987)

$$kw3 := .001 [0.57109 + 1.725 \cdot 10^{-3} \cdot (Tph - 273) - 6.7306 \cdot 10^{-6} \cdot (Tph - 273)^2] = 6.808 \times 10^{-4}$$

$$kc3 := .001 [2.014 + 1.3874 \cdot 10^{-3} \cdot (Tph - 273) - 4.3312 \cdot 10^{-6} \cdot (Tph - 273)^2] = 3.044 \times 10^{-4}$$

$$kf3 := .001 [1.8331 + 1.2497 \cdot 10^{-3} \cdot (Tph - 273) - 3.1683 \cdot 10^{-6} \cdot (Tph - 273)^2] = 2.862 \times 10^{-4}$$

$$kp3 := .001 [-1.788 + 1.1958 \cdot 10^{-3} \cdot (Tph - 273) - 2.7178 \cdot 10^{-6} \cdot (Tph - 273)^2] = 2.815 \times 10^{-4}$$

$$k3 := \frac{mwated}{m_{totalnew}} \cdot kw3 + \frac{msugari}{m_{totalnew}} \cdot kc3 + \frac{mpectini}{m_{totalnew}} \cdot kf3 + \frac{mprotein}{m_{totalnew}} \cdot kp3 = 6.457 \times 10^{-4} \text{ kW/mK}$$

Note that the thermal conductivity has increased slightly due to the rise in temperature.

Equation for Heat Capacity based on the Choi-Okos Equation (1987)

$$cpw3 := .001 [4176.2 - 9.0862 \cdot 10^{-5} \cdot (Tph - 273) + 5473.1 \cdot 10^{-6} \cdot (Tph - 273)^2] = 4.251$$

$$cpc3 := .001 [1548.8 + 1962.5 \cdot 10^{-3} \cdot (Tph - 273) - 5939.9 \cdot 10^{-6} \cdot (Tph - 273)^2] = 1.697$$

$$cpf3 := .001 [1845.9 + 1930.6 \cdot 10^{-3} \cdot (Tph - 273) - 4650.9 \cdot 10^{-6} \cdot (Tph - 273)^2] = 2.008$$

$$cpp3 := .001 [2008.2 + 1208.9 \cdot 10^{-3} \cdot (Tph - 273) - 1312.9 \cdot 10^{-6} \cdot (Tph - 273)^2] = 2.132$$

$$cp3 := \frac{mwated}{m_{totalnew}} \cdot cpw3 + \frac{msugari}{m_{totalnew}} \cdot cpc3 + \frac{mpectini}{m_{totalnew}} \cdot cpf3 + \frac{mprotein}{m_{totalnew}} \cdot cpp3 = 4.027 \text{ kJ/kgK}$$

Note that the heat capacity has increased slightly due to the rise in temperature.

Calculation of new value for thermal diffusivity

$$\alpha_3 := \frac{k_3}{\rho_{carrot3} \cdot cp_3} = 3.832 \times 10^{-7}$$

References

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