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Baking cake: a mathematical model

Vivien Yeung

Supervised by Mark Nelson and Xiaoping Lu

University of Wollongong

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Abstract

Baking is an energy intensive simultaneous heat and mass transfer process ubiquitous in food industry, but few studies have focused on the transport phenomena inside cake. The development of baking models is important to reduce costs whilst maintaining product quality. The lumped reaction engineering approach (LREA) is a semi-empirical drying model that has previously been used to model the transport phenomena inside a thin-slice of white cake with good matches to experimental data, but parameter values and estimation methods were not provided. To address this, we explicitly characterise parameter estimation methods and use estimated parameters to generate moisture content and temperature profiles for oven temperature 100°C. Estimation of model parameters were found to require significant chemical engineering knowledge that is not intuitive to mathematicians. The LREA is found to reasonably fit experimental data but slightly overestimates moisture content towards the end of baking and yields a less smooth temperature profile than that obtained previously with the same model. These results demonstrate that insufficient information significantly increases difficulty in modeling and decreases accuracy of model predictions to data.

1 Introduction

Baking is an energy intensive process with relatively complex transport mechanisms. Baking involves application of heat perpendicular to the surface of the cake to induce migration of liquid water from the wet core of the cake batter to the surface through pressure-driven diffusion where it then evaporates at the surface. This can be thought of as drying. Therefore, as a first step towards an energy efficient process favoring product quality, drying models are appropriate as a predictive model for the baking process. A relatively simple model is the lumped reaction engineering approach (LREA)¹, a semi-empirical drying model that was applied to the experimental data from (Sakin et al., 2007) for modeling a thin-slice of white cake (Putranto et al., 2011) with good matches to experimental data. In general, the LREA, developed by chemical engineers (C. N. Chen X.D., 1997), is advantageous over existing empirical and mechanistic approaches as it captures the major physics of drying yet is simple in mathematical formulation. However, parameter values and methods of estimation were not provided, so duplication of modeling for further study of baking under similar conditions is not easy to conduct. To address this, we explicitly characterise methods for estimating model parameters for the LREA applied to a thin-slice of cake and use estimated parameters to generate the corresponding temperature and moisture content profiles.

¹The LREA has been used to model the drying of various food products and was extended to model baking of cake without alteration, with good matches to experimental data (X. D. Chen & Putranto, 2013)



2 Statement of authorship

Nelson conceived the main conceptual ideas and project outline. Nelson and Yeung devised the project. Nelson and Lu supervised the project. Putranto and Chen designed the model and originally performed the analytical methods using experiments carried out by Sakin (et al.). Yeung derived parameter estimation methods with support from Nelson, Lu and Putranto. Yeung analysed and verified analytical methods, performed numerical simulations and interpreted results with support from Nelson and Lu. Yeung wrote the manuscript supervised by Nelson. AMSI funded the project.

3 Experimental details

Modeling the baking of a thin layer of white cake using the LREA was conducted by (Putranto et al., 2011) using experimental data from (Sakin et al., 2007). To better understand this modeling, experimental details are reviewed below.

Cake batter ingredients are: 49.4% (of total weight) Dr. Oetkers ready dry cake mix (contains wheat flour, sugar, corn starch and baking powder), 24.7% pasteurized whole liquid egg, 16.2% vegetable margarine and 9.7% water. Batter was prepared with a three-stage mixing method using a hand mixer. The mixture was spread on a baking tray with diameter of 220 mm with initial thickness of 3 mm. The initial moisture content of the samples was 0.53 kg water/kg dry solid (53%-wt dry basis) (Sakin et al., 2007). The initial temperature of the samples is assumed to be room temperature of $T_0 = 293\text{ K}$. The baking experiments were conducted in an electrical baking oven with dimensions 0.39 x 0.44 x 0.35 m (Teba High-01 Inox) at five different oven temperatures (50, 80, 100, 140 and 160 °C) under forced convection conditions. Fresh air entered the oven cavity through a hole up in the oven to prevent moisture accumulation. The air was circulated by a fan on the back side of the oven at a constant speed of 0.56 m s^{-1} (measured by an Airflow anemometer, LCA 6000) to provide negligible external mass transfer resistance. Baking was interrupted at definite times (every 5 mins for 160°C, every 10mins for all other oven temperatures) to obtain measurements until equilibrium moisture content was reached. Once the batter was out of the oven it was not put into the oven again and was discarded after analysis.

Weight of the batter was recorded but measuring instrument used was not specified. Product temperature was measured by a thermocouple (J-type, wire size, ϕ : 1 mm) inserted inside the samples. The thickness was measured by a digital caliper so that volume change could be calculated (since the presence of a cake tin fixes the radius of the cake).



4 Mathematical model

The lumped reaction engineering approach (LREA) was developed by (C. N. Chen X.D., 1997; X. D. Chen & Putranto, 2013) based on chemical reactor principles to model drying kinetics.

In general, the drying rate of a material (for mass balance) is:

$$m_s \frac{dX}{dt} = -h_m A (\rho_{v,s} - \rho_{v,b}), \quad (1)$$

where m_s is the dried mass of the sample (kg), X is the average moisture content on dry basis (kg water/kg dry solid), $\rho_{v,s}$ is the vapor concentration at the material-air interface (ie. at the surface of the material being dried) ($kg \cdot m^{-3}$), $\rho_{v,b}$ is the vapor concentration in the drying medium ($kg \cdot m^{-3}$), h_m is the mass transfer coefficient ($m \cdot s^{-1}$) and A is the surface area of the material being dried (m^2).

The surface vapor concentration ($\rho_{v,s}$) can be scaled against saturated vapor concentration as determined by (C. N. Chen X.D., 1997; X. D. Chen & Putranto, 2013):

$$\rho_{v,s} = \exp\left(\frac{\Delta E_v}{RT}\right) \rho_{v,sat}, \quad (2)$$

where ΔE_v is an activation energy representing the additional difficulty to remove moisture from the material beyond the free water effect ($Jmol^{-1}$), R is the ideal gas constant ($Jmol^{-1}K^{-1}$), T is the temperature of the material being dried (K) and $\rho_{v,sat}$ is the saturated vapor concentration (kgm^{-3}).

Saturated vapor concentration ($\rho_{v,sat}$) is a property of water estimated by (Putranto et al., 2011):

$$\rho_{v,sat} = b_1 \times 10^{-9}(T-273) - b_2 \times 10^{-7}(T-273)^3 + b_3 \times 10^{-5}(T-273)^2 - b_4 \times 10^{-5}(T-273) + b_5 \times 10^{-3}, \quad (3)$$

where $b_1 = 4.844$, $b_2 = 1.4807$, $b_3 = 2.6572$, $b_4 = 4.8613$ and $b_5 = 8.342$.

Substituting equations 2 and 3 into equation 1 we obtain:

Mass balance equation:

$$m_s \frac{dX}{dt} = -h_m A \left[\exp\left(\frac{\Delta E_v}{RT}\right) \rho_{v,sat} - \rho_{v,b} \right], \quad (4)$$

Rearrange equation 4 to obtain the activation energy (ΔE_v) as the subject:

$$\Delta E_v = -RT \ln \left[\frac{-m_s \frac{dX}{dt} \frac{1}{h_m A} + \rho_{v,b}}{\rho_{v,sat}} \right] \quad (5)$$

where dX/dt is experimentally determined and all other parameters on the RHS are known.

Relative activation energy ($\Delta E_v / \Delta E_{v,b}$) is obtained by normalising activation energy ΔE_v with the equilibrium activation energy ($\Delta E_{v,b}$), which for a thin slice of cake was determined by (Putranto



et al., 2011) to be:

$$\frac{\Delta E_v}{\Delta E_{v,b}} = [1 - 1.612(X - X_b)^{1.151}] \cdot \exp[-1.28 \times 10^6(X - X_b)^{14.19}], \quad (6)$$

where X_b is the equilibrium moisture content on dry basis (kg water/kg dry solid).

Equilibrium activation energy ($\Delta E_{v,b}$) is the maximum ΔE_v under relative humidity and temperature of the drying air (RH_b) (ie. highest possible difficulty to dry material at time t):

$$\Delta E_{v,b} = -R \cdot T_b \ln(RH_b), \quad (7)$$

where R is the ideal gas constant ($J \cdot \text{mol}^{-1} \cdot K^{-1}$), T_b is oven temperature (K) and RH_b is the relative humidity of drying air.

Heat balance equation for thin sample of cake as determined by (Putranto et al., 2011) is:

$$\frac{d[m_s(1 + X)C_p T]}{dt} \approx hA(T_b - T) + m_s \frac{dX}{dt} \Delta H_v \quad (8)$$

where C_p is specific heat of the sample ($J \cdot \text{kg}^{-1} \cdot K^{-1}$), h is the heat transfer coefficient ($W \cdot m^{-2} \cdot K^{-1}$), ΔH_v is vaporisation heat of water ($J \cdot \text{kg}^{-1}$), T_b is baking oven temperature (K), T is temperature of sample (K).

Physically, $m_s(1 + X)C_p$ is the thermal mass of the sample, $hA(T_b - T)$ is Newton's law of cooling and $m_s \frac{dX}{dt} \Delta H_v$ is the heat energy required for phase change (from liquid water to water vapor during evaporation) (ΔH_v) based on the mass balance of the system ($m_s \frac{dX}{dt}$).

Mass balance and heat balance equations 4 and 8 form a coupled system of non-linear autonomous ODEs that can be solved with ode23 in MATLAB to yield moisture content and temperature profiles for the material being dried.

The physics of drying are modeled using the relative activation energy ($\Delta E_v / \Delta E_{v,b}$). Relative activation energy describes the internal behaviour of the material being dried during drying. The parameters for the LREA (except equilibrium isotherm for X_b) can be generated with one accurate drying experiment for similar drying conditions and initial moisture content, with generated parameters expressed in the relative activation energy, equation 6. The relative activation energy generated can then be implemented to the same material with different drying conditions and similar initial moisture content since relative activation energy would collapse to a similar profile.

The reaction engineering approach (LREA), 'offers advantages of accuracy, simplicity, suitability for implementation in plant and minimum experiments to generate the parameters' (Putranto et al., 2011). However, parameter values nor estimation methods were not provided in the papers. Hence one of the aims of this report is to estimate model parameters for the LREA applied to baking a thin sample of cake (see section 6).



5 Assumptions of model

5.1 General model assumptions

For better understanding of the scope of modeling we assume:

Model transport phenomena only. We only model heat and mass transfer inside the cake, not the effect of changes in recipe or oven conditions on energy requirements and product quality.

Batter temperature. Maximum batter temperature at any time is its oven temperature.

Oven temperature. In industry, oven temperatures usually range 150 to 220°C. The experimental oven temperatures (50, 80, 100, 140 and 160°C) are far lower than expected as they represent the possible batter temperatures through the complete baking process, not necessarily cake baking oven temperatures.

Cake batter composition. The experimental cake batter is simplistic and unrealistic for industry application due to the use of cake mix rather than (bleached) cake flour, homogenisation of the egg, inferior ingredient substitutions (margarine for butter, water for milk) and the omission of additives (vanilla or almond extract for flavour).

Volume change. The cake is a cylinder with radius 110 mm and initial thickness 3 mm. However, volume only changes in the thickness dimension as mass transfer cannot occur radially (radius is fixed by cake tin). Volume change of the cake during baking is ignored as equations for change of thickness determined by (Putranto et al., 2011) predict negative thickness at high values of time, which is invalid. Future work would be formulating our own empirical equations for change of thickness for incorporation into the model.

5.2 Model assumptions for parameter estimation

The following model assumptions are needed for parameter estimation in section 6.

Thin samples. Since the radius of the cake (110 mm) is much larger than its thickness (initially 3mm), we ignore temperature gradient and spatial distribution of moisture content inside the sample.

Geometry and flow of concern. As we have thin samples and air flowing over the material, the geometry and flow of concern is forced convection in a flat plate and laminar flow of air.

Dry air in oven. Air is either dry or moist depending on the amount of water vapor in the air. Since moisture in the air is removed from the oven in the experiments (Sakin et al., 2007), we have dry air in the oven. Dry air is an ideal gas. By assuming ideal gas, formulas for properties of dry air are far simpler than those for moist air. This greatly simplifies parameter estimation as many model



parameters are temperature-dependent properties of air.

6 Parameter estimation

To obtain moisture content and temperature profiles, the mass balance and heat balance equations (4 and 8) must be solved simultaneously. To do this, accurate estimation of model parameters is required. However, parameter values and methods of calculation were not provided in the papers by (Putranto et al., 2011) and (Sakin et al., 2007). In this section, we explicitly characterise parameter estimation methods for the LREA as applied to cake. For the mass balance parameters, see section 6.1. For heat balance parameters, see section 6.2.

6.1 Mass balance equation parameters

The mass balance equation is equation 4.

6.1.1 Dried mass of sample

Dried mass of sample m_s refers to the mass of the cake after baking is complete and is adapted from (Putranto et al., 2011):

$$m_s = \rho_s XSA L_f \quad (9)$$

where ρ_s is dry density of flour (kg m^{-3}), XSA is cross-sectional area of sample (m^2) and L_f is final thickness of the sample (m).

Dry density of flour (ρ_s) ($\text{kg} \cdot \text{m}^{-3}$) is $\rho_s = 593$.

Cross-sectional area of drying material (XSA) refers to area of the top of the cake: (m^2):

$$XSA = \pi r^2 \approx 0.038$$

where $r = 0.11$ is radius of the cake (m).

Final thickness of the cake (L_f) (m) is taken to be initial thickness:

$$L_f = 0.003. \quad (10)$$

6.1.2 Surface area of sample A

The surface area of the material exposed to the drying air A (m^2) is the top and sides of the cake since heat flows through the top of the cake by convection and through the sides by conduction:

$$A = \pi r^2 + 2\pi r L \quad (11)$$



where $r = 0.11$ is radius of the sample (m) and L is thickness of the sample (m). L is taken to be initial thickness for all time t :

$$L = 0.003, \quad (12)$$

6.1.3 Mass transfer coefficient h_m

Mass transfer coefficient h_m is determined by (Incropera et al., 2002):

$$\overline{h}_m = \frac{\overline{Sh} \cdot D_{12}}{L_c} \quad (13)$$

where D_{12} is the binary mass diffusivity of fluid ($m^2 s^{-1}$), L_c is the characteristic length of the drying material and \overline{Sh} is the Sherwood number for the geometry and flow of concern.

Calculation of the mass transfer coefficient h_m is more challenging as h_m involves generically defined engineering terms that are functions of other temperature-dependent parameters. Therefore explicit calculation of h_m is shown in Appendix C.

6.1.4 Activation energy ΔE_v

Activation energy ΔE_v represents the, 'additional difficulty to remove moisture from the material beyond the free water effect' (Putranto et al., 2011), obtained by rearranging equation 6:

$$\Delta E_v = \Delta E_{v,b} \cdot [1 - 1.612(X - X_b)^{1.151}] \cdot \exp[-1.28 \times 10^6 (X - X_b)^{14.19}], \quad (14)$$

We judge the suitability of this formula form modeling by checking the condition of $\Delta E_v = \Delta E_{v,b}$ at $t = t_f$. At $t = t_f$, $X = X_b$. Substitution into equation 14 gives $\Delta E_v = \Delta E_{v,b}$. Hence this empirical formula is suitable for modeling.

6.1.5 Equilibrium moisture content X_b

Equilibrium moisture content X_b is found by fitting an empirical line through two endpoints for X_b as a function of T_b in log-log space (see figure 1). This is appropriate as X_b and T_b have an inverse non-linear relationship and moisture sorption isotherm equations such as the Guggenheim-Anderson-de Boer (GAB) equation are unusable.

For the two endpoints, X_b was experimentally determined by (Sakin et al., 2007) to range from 0.0165 to 0.0710 kg water/kg dry solid over the oven temperatures T_b tested. Since X_b and T_b have an inverse relationship, our two points are ($T_b = 50^\circ\text{C}$, $X_b = 0.0710$ kg/kg) and ($T_b = 160^\circ\text{C}$, $X_b = 0.0165$ kg/kg). Table 1 gives values of X_b for each oven temperature T_b .



T_b (C)	X_b (kg/kg)
50	0.0710
80	0.0457
100	0.034
140	0.0209
160	0.0165

Table 1: Oven temperature and corresponding equilibrium moisture content

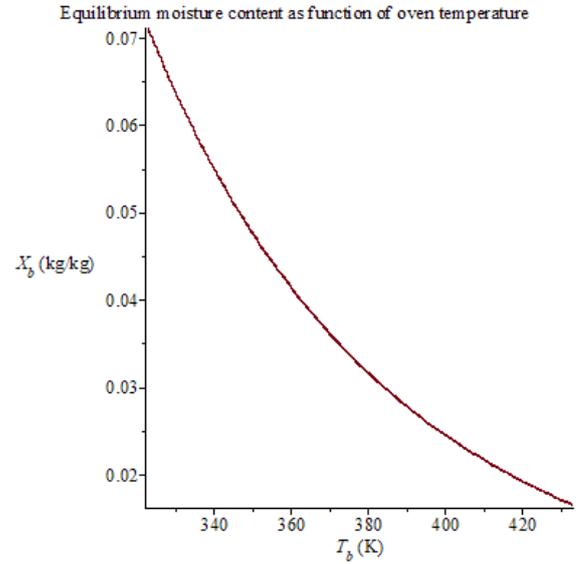


Figure 1: Equilibrium moisture content as a function of oven temperature in log-log space

6.1.6 Equilibrium activation energy $\Delta E_{v,b}$

Equilibrium activation energy ($\Delta E_{v,b}$) is defined by equation 7. It involves drying air temperature T_b and relative humidity of drying air RH_b .

At oven temperature $T_b = 100^\circ\text{C}$ or $RH_b = 0.0015$ (see section 6.1.7 for calculation) and $\Delta E_{v,b} \approx 20000 \text{ J mol}^{-1}$. This is a reasonable value as activation energy for drying tomato slices is $22.28 \text{ kJ mol}^{-1}$ (Abano et al., 2011). Hence equation 7 obtained for $\Delta E_{v,b}$ by (Putranto et al., 2011) is reasonable.

6.1.7 Relative humidity of drying air RH_b

Relative humidity of drying air RH_b refers to the the ratio between amount of water vapor present in air and amount of water vapor needed for saturation (or maximum amount it could be before condensation occurs) at the same temperature, expressed as a percentage.

Relative humidity is calculated using the mass balance equation and the condition of $\frac{dX}{dt} = 0$, $T = T_b$ and $\Delta E_v = \Delta E_{v,b}$ at the end of baking as we are unable to use psychrometric charts for



relative humidity³. The only way to obtain $\frac{dX}{dt} = 0$ ⁴ is if:

$$\exp\left(\frac{\Delta E_{v,b}}{R \cdot T_b}\right) \rho_{v,sat}(T_b) = \rho_{v,b} \quad (15)$$

where the exponential term on the LHS is just equation 7 rearranged to obtain RH_b as the subject:

$$RH_b = \frac{\rho_{v,b}}{\rho_{v,sat}(T_b)} \quad (16)$$

where $\rho_{v,b}$ is vapour concentration in drying medium and $\rho_{v,sat}(T_b)$ is saturated vapour concentration evaluated at drying air temperature T_b . See section 6.1.9 and equation 3 for respective calculations.

6.1.8 Saturated vapour concentration $\rho_{v,sat}$

Saturated vapor concentration $\rho_{v,sat}$ is the maximum concentration of the vapour of a liquid or solid that can exist in air at a particular temperature. It is a property of water that depends on temperature. There are two methods of calculation.

6.1.8.1 Method 1: Given for LREA

$\rho_{v,sat}$ for water can be estimated with equation 3. Since this formula has been used for all other applications of the LREA (X. D. Chen & Lin, 2005; Putranto & Chen, 2012; X. D. Chen & Putranto, 2013), we judge that this formula is correct and hence suitable for our modeling.

6.1.8.2 Method 2: Vapor pressures

We can relate saturated vapor concentration ($\rho_{v,sat}$) to saturated water vapor pressure ($P_{v,sat}$) (saturated water vapor pressure) by using the ideal gas assumption:

$$\rho_{v,sat} = \frac{P_{v,sat}M}{R \cdot T} \quad (17)$$

where $M = 18.01534$ is molar mass of water ($kgmol^{-1}$) (Singh & Heldman, 2014) and $P_{v,sat}$ (Pa) is saturated vapor pressure.

Saturated vapor pressure ($P_{v,sat}$) is a property of water that can be calculated using the Antoine equation as we are assuming ideal gas and dry air in the oven. Antoine equation is a function that

³Relating absolute humidity (kg water/kg drying air) and drying air (dry-bulb) temperature T_b to each other intersected far below the lowest relative humidity curve of 10%, and were unable to interpolate between relative humidity curves for the same reason.

⁴Since mass transfer coefficient h_m and surface area of drying material A are positive and never 0.



will relate the vapor pressure of some species to a temperature and is widely published in engineering textbooks (such as (Smith et al., 2004b)):

$$\ln(P_{sat}[kPa]) = A_1 - \frac{B_1}{T[^\circ C] + C_1} \quad (18)$$

where P_{sat} is the saturated vapor pressure (and is a property of water), T is the drying air temperature (as P_{sat} is pressure exerted by *drying air*) and A_1 , B_1 and C_1 are constants that depend on the substance of concern as well as the units of pressure P_{sat} and temperature T . Table 2 provides these constants for water as obtained from Appendix B in (Smith et al., 2004b):

Substance	A_1 (kPa)	B_1 ($kg \cdot m^{-1} \cdot s^{-1} \cdot ^\circ C$)	C_1 ($^\circ C$)	Temp. Range ($^\circ C$)
Water	16.3872	3885.70	230.170	0 - 200

Table 2: Antoine Equation parameters (P_{sat} in kPa, Temp. Range in $^\circ C$)

For baking cake, we need to convert units for P_{sat} to Pa and T to K for use in further parameter estimation and modeling.

Substitution into equation 17 generates similar results to those from equation 17. This validates use of both formulas for calculating $\rho_{v,sat}$.

6.1.9 Vapor concentration in drying material

$\rho_{v,b}$ refers to the concentration of water vapour in the drying material (kg water vapour/ m^3). It is experimentally determined. It is humidity with different units, obtained by multiplying two properties of the medium used to dry it (air in the oven):

$$\rho_{v,b} = H_b \cdot \rho_{air} \quad (19)$$

where H_b is the humidity of the drying air (kg water vapor/kg drying air) and ρ_{air} is the density of dry air (kg dry air/ m^3).

Since $\rho_{v,b}$ is dependent on drying air properties, it is different for each oven temperature T_b but remains constant through the baking process.

6.1.9.1 Humidity of drying air

Humidity of drying air is $H_b \approx 0.001$ kg water/kg dry solid provided by Putranto¹¹ (2018).

¹¹Value of H_b was provided by email



We had initially attempted to calculate H_b from (Treybal, 1981):

$$RH_b = \frac{P_{vap}}{P_{vap,sat}}, \quad (20)$$

$$H_b = \frac{P_{vap}}{P_{total} - P_{vap}} \times \frac{18}{29} \quad (21)$$

where P_{vap} is partial water vapor pressure (Pa), $P_{vap,sat}$ is saturated water vapor pressure, P_{total} is total pressure of system and $18/29$ is a conversion factor where 18 is molar mass water and 29 is molar mass air.

Although $P_{vap,sat}$ was calculated using Antoine equation 18 and P_{total} was assumed to be standard atmospheric pressure of $101\,325\ Pa$, we were unable to calculate partial water vapor pressure (P_{vap}), as equations for P_{vap} required knowledge of mass of water vapor in air (which is unknown) and using equation 20 requires assumption of RH_b to calculate P_{vap} then using that value of P_{vap} to calculate H_b , which is counter-intuitive.

Fortunately we were provided the value of $H_b \approx 0.001\ \text{kg water/kg dry solid}$ by Putranto¹¹ (2018), which we have used for our calculations.

6.1.9.2 Density of dry air

Density of dry air ρ_{air} is calculated using the formula for density of ideal gas and is evaluated at oven temperature T_b : (ie. $\rho_{air} = f(T_b)$):

$$\rho_{air} = \frac{p}{R \cdot T} \quad (22)$$

where p is total pressure of the system (Pa) (assume standard atmospheric pressure $p = 101\,325\ Pa$), R is the ideal gas constant for dry air ($\text{J mol}^{-1}\ \text{K}^{-1}$) and $T = T_b$ (oven temperature) (K).

6.2 Heat balance equation parameters

In this section, we estimate model parameters for the heat balance equation 8).

6.2.1 Specific heat of sample C_p

Specific heat of cake batter C_p ($\text{J kg}^{-1}\ \text{K}^{-1}$) is assumed to be constant within the range of experimental oven temperatures. It is determined experimentally using empirical models. Neither were provided by (Sakin et al., 2007). Therefore we used the average of the endpoints of the range $2516 - 2658\ \text{J kg}^{-1}\ \text{K}^{-1}$, which was obtained by (Baik et al., 1999) for baking cupcake:

$$C_p = 0.5(2516 + 2658) = 2587 \quad (23)$$

¹¹Value of H_b was provided by email



Future work would be using an empirical model for specific heat of the sample based on mass fractions of each component since predictions using empirical models are fairly accurate (Berk, 2013).

6.2.2 Heat of vaporisation of water ΔH_v

Heat of vaporisation of water ΔH_v ($J \cdot mol^{-1}$) is the amount of heat energy required for phase change of water from liquid to vapor. ΔH_v is temperature-dependent and is determined using Watson's equation, which is available in engineering textbooks such as (Smith et al., 2004a; Singh & Heldman, 2014):

$$\frac{\Delta H_v}{\Delta H_{v1}} = \left(\frac{1 - \frac{T}{T_c}}{1 - \frac{T_1}{T_c}} \right)^{0.38} \quad (24)$$

where:

- ΔH_v is heat of vaporisation of water at cake batter temperature T , in $J \cdot mol^{-1}$
- ΔH_{v1} is heat of vaporisation of water at reference temperature T_1 , in $J \cdot mol^{-1}$
- T is temperature of cake batter, in K
- $T_1 = 373$ is reference temperature, in K
- $T_c = 647.1$ is critical temperature of water, in K

6.2.3 Heat transfer coefficient h

Heat transfer coefficient h is determined by (Incropera et al., 2002):

$$\bar{h} = \frac{\overline{Nu} \cdot k_f}{L_c} \quad (25)$$

where k_f is thermal conductivity of fluid ($W \cdot m^{-1} \cdot K^{-1}$), L_c is the characteristic length of the drying material (m) and Nu is the Nusselt number as determined by (Putranto et al., 2011) for the geometry and flow of concern:

$$\overline{Nu} = 0.664 Re^{0.5} Pr^{0.37} \quad (26)$$

where Re is the Reynolds number for fluid and Pr is the Prandtl number for fluid.

Calculation of the heat transfer coefficient h is similarly complex to that of the mass transfer coefficient h_m and is thus shown in Appendix B.



7 Moisture content and temperature profiles

The mass balance 4 and heat balance 8 equations were solved simultaneously in MATLAB (using ode23) and MAPLE to yield moisture content and temperature profiles in figures 2 and 3 for 100°C. Due to difficulties parameter estimation, we have only plotted results for one oven temperature. However, similar problems to those detailed in this section would be expected to arise when plotting predictive profiles for the other oven temperatures.

The behaviour of moisture content profiles are highly sensitive to errors the order of the mass transfer coefficient h_m whereas temperature profiles remain similar regardless of model parameter errors (see Appendix D). The lack of change in temperature profile even when moisture content profile significantly changes is also true when LREA is applied to model roasting of coffee (Nikolic, 2018). Figures 2 and 3 were obtained using the mass transfer coefficient $h_m = f(T_{film})$ obtained in Appendix C, which is order 10^{-2} .

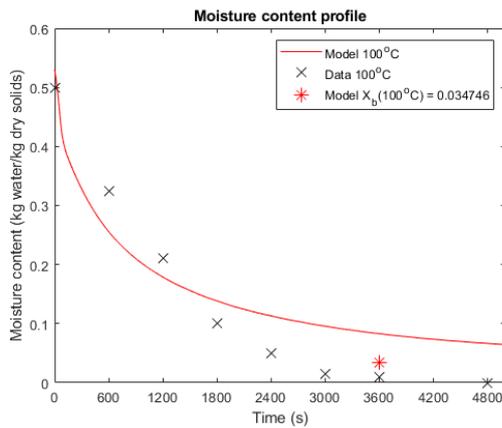


Figure 2: Moisture content profile at baking temperature of 100°C, $h_m = f(T_{film})$

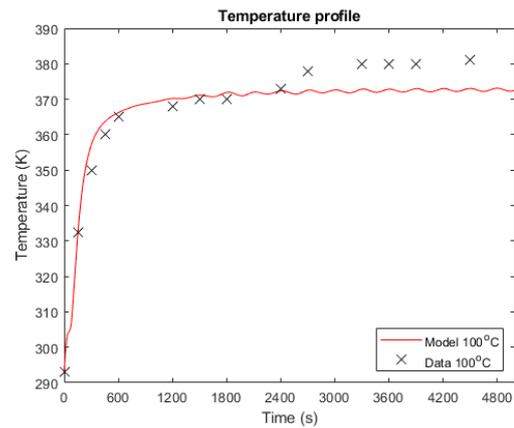


Figure 3: Temperature profile at baking temperature of 100°C, $h_m = f(T_{film})$

Predicted moisture content profile overestimate moisture content values and do not appear to closely match experimental data as mass transfer coefficient h_m is of order 10^{-2} rather than order 10^{-1} as desired (see Appendix D). However, we had to estimate the experimental data points as the raw experimental data points were not provided. Data points were estimated by hand using graphs with poor resolution obtained by (Putranto et al., 2011) and (Sakin et al., 2007). This crude method for estimation mean that estimated data points are not a reliable benchmark for modeling and the true accuracy of predicted results cannot be obtained.

Furthermore, the raw data point for equilibrium moisture content is $X_b = 0.01$ kg water/kg dry



solid, which is below the lower bound of the range X_b 0.0165 to 0.0710 kg/kg given by (Sakin et al., 2007) and below the theoretically estimated value of $X_b = 0.034746$ kg/kg (calculated in section 6.1.5). On the other hand, predicted equilibrium moisture content using LREA with $h_m = f(T_{film})$ is $X_b = 0.08312$ kg/kg, which is above both the upper bound of the given range and the theoretical value. Since the raw data point, theoretical (our benchmark) and predicted values of X_b have all been estimated, it is difficult to tell which value is correct. Fortunately, all X_b are order 10^{-2} so estimated values are somewhat reasonable.

Predicted temperature profiles reasonably match experimental data. However, inaccuracies in h_m carry over to the temperature profile as the LREA is a coupled system of ODEs. Experimental data points were estimated in the same crude way as those for the moisture content profile. The fluctuations in the temperature profile at later times match the behaviour shown in the temperature history profile (Sakin et al., 2007). However, (Putranto et al., 2011) predicted smoother behaviour using the LREA and plateau at temperature slightly above T_b . This suggests that our assumption of maximum batter temperature being the oven temperature T_b is incorrect. Future work would be to remove this assumption.

8 Discussion

Methods for estimating model parameters were clearly explained to account for insufficient information in papers. It was found that significant chemical engineering knowledge is required for parameter estimation as many model parameters are functions of temperature-dependent parameters and the properties each parameter belonged to were not specified. The parameter estimation methods derived in this report could be used in other applications of the LREA such as drying of other thin samples ((X. D. Chen & Lin, 2005; Putranto & Chen, 2012, 2012)) where varying information on parameter values are available. They may be applicable to modeling similar food engineering problems such as frying and freezing.

The mass and heat balance equations were solved simultaneously to yield moisture content and temperature profiles for oven temperature 100°C . Moisture content profiles are more sensitive to errors in parameter estimation compared to temperature profiles. Physically this may explain differing product outcomes even when cakes appear to be baked in the same oven conditions. Raw experimental data points are desired for accurately judging how well predicted values from the LREA match experimental data.



9 Conclusion

In this report, the baking of a thin sample of white cake was modeled using the LREA. Parameter estimation methods were explicitly characterised due to insufficient information in experimental papers. Results of modeling indicate that the model slightly overestimates the moisture content profile for baking temperature 100°C , which may have affected the corresponding temperature profile. However, results are inconclusive as all values used as benchmarks have been crudely estimated. Future work would involve obtaining moisture content and temperature profiles for oven temperatures $50, 80, 140$ and 160°C , incorporating volume change into the model, removing the assumption of maximum batter temperature being equal to the oven temperature and incorporating a mathematical formulation of the specific heat of cake into the model.

10 Acknowledgements

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A Appendix: Estimating heat and mass transfer coefficients

A.1 Properties for heat and mass transfer coefficients

The heat and mass transfer coefficients h and h_m (sections B and C) involve characteristic length of material L_c and (functions of) thermophysical properties of fluid. However, neither characteristic length nor fluid are explicitly defined in the experimental papers. We will define these terms in sections A.1.1 and A.1.2 below.

A.1.1 Characteristic length of material L_c

The characteristic length of the material L_c refers to the main dimension across which heat and mass transfer occur. It is defined as:

$$L_c = \frac{V_{body}}{A} \quad (27)$$

where L_c is the characteristic length of the material (m), V_{body} is the volume of the material (m^3) and A is the surface area of the material (m^2).

Volume of the material V_{body} (m^3) refers to the volume of a cylindrical cake:

$$V_{body} = \pi r^2 L \quad (28)$$

Surface area of the material A is calculated using equation 11:

$$A = \pi r^2 + 2\pi r L \quad (29)$$

Substitution into equation 27 yields characteristic length of the cake to be its half-thickness:

$$L_c = 0.5 \cdot L \quad (30)$$

where L is thickness of the cake (m).

Therefore, characteristic length L_c is half-thickness of the cake. Physically, this makes sense as heat and vapor flux occur perpendicular to the surface (thickness) and symmetry is present inside the cake (half).

A.1.2 Fluid of concern

Heat and mass transfer coefficients are functions of parameters that are properties of fluid. Fluid refers to the medium flowing over an object and can be either liquid or gas depending on the situation modeled. Therefore, fluid of concern for baking is air (gas) as it is the medium used to dry the liquid cake batter.



B Heat transfer coefficient h

Heat transfer coefficient (h) is a property of dry air and is a function of thermophysical properties that depends on film temperature (justified in section B.2) and is determined by (Incropera et al., 2002):

$$\bar{h} = \frac{\overline{Nu} \cdot k_f}{L_c} \quad (31)$$

where k_f is thermal conductivity of fluid ($Wm^{-1}K^{-1}$), L_c is the characteristic length of material (m) and Nu is the Nusselt number.

Nu is determined by (Putranto et al., 2011) for the geometry and flow of concern (laminar flow of air, forced convection in flat plate):

$$\overline{Nu} = 0.664Re^{0.5}Pr^{0.37} \quad (32)$$

where Re is the Reynolds number for fluid and Pr is the Prandtl number for fluid:

$$Re = \frac{\rho u L_c}{\mu} \quad (33)$$

where ρ is density of the fluid (kgm^{-3}), u is velocity of the fluid with respect to the object (ms^{-1}), μ is the dynamic viscosity of the fluid ($kg s^{-1}m^{-1}$).

$$Pr = \frac{c_p \mu}{k_f}, \quad (34)$$

where c_p is specific heat of the fluid at constant pressure ($Jkg^{-1}K^{-1}$) and k_f is thermal conductivity of the fluid ($Wm^{-1}K^{-1}$).

Therefore we can rewrite the heat transfer coefficient h purely as a film-temperature-dependent function of thermophysical properties and characteristic length of the material:

$$h(T_{film}) = 0.664 \left(\frac{\rho u L_c}{\mu} \right)^{0.5} \left(\frac{c_p \mu}{k_f} \right)^{0.37} \left(\frac{k_f}{L_c} \right), \quad (35)$$

where T_{film} is film temperature (see section B.2).

Substitution into equation 35 yield $h \approx 72$. This is reasonable as convective heat transfer coefficient for forced convection of air is between 10 and 120 (Singh & Heldman, 2014).

B.1 Characteristic length L_c

From section A.1.1, characteristic length of the cake L_c is its half thickness (equation 30).



B.2 Thermophysical properties k_f , ρ , u , μ and c_p

Heat transfer coefficient h is a function of engineering parameters such as the Nusselt number Nu , Reynolds number Re , Prandtl number Pr , which are functions of thermophysical properties. Thermophysical properties belong to fluid (drying air, not materials A.1.2) and are evaluated at film temperature, which is the average of material temperature T and drying air temperature T_b :

$$T_{film} = \frac{T + T_b}{2} \quad (36)$$

Film temperature is appropriate as batter temperature and oven temperature differ greatly, particularly at the start of drying, and the temperature in different parts of the system would be somewhere in between.

Equations for thermophysical properties of dry air for the heat transfer coefficient are summarised in table 3 and calculated in sections B.2.1 to B.2.5.

Thermophysical property	Definition	Value or Calculation
ρ (kg m^{-3})	Density of dry air	$\rho_{dryair} = \frac{p}{R \cdot T}$
μ ($\text{kg} \cdot \text{m}^{-1} \cdot \text{s}^{-1}$)	Dynamic viscosity of dry air	Sutherland's law with 3 coefficients
k_f ($\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$)	Thermal conductivity of dry air	Sutherland's law with 3 coefficients
c_p ($\text{Jkg}^{-1}\text{K}^{-1}$)	Specific heat of dry air	1012 to 1030 from 50 to 160°C
u (ms^{-1})	Velocity of dry air	0.56 (Putranto et al., 2011)

Table 3: Thermophysical properties of dry air

B.2.1 Density of dry air ρ_{dryair}

Density of dry air is calculated using the ideal gas law expressed in terms of pressure and temperature, evaluated at film temperature T_{film} :

$$\rho_{dryair} = \frac{p}{R \cdot T_{film}} \quad (37)$$

where $p = 101\,325$ (Pa) is total pressure of the system.

B.2.2 Dynamic viscosity of dry air μ

Dynamic viscosity of dry air is calculated using Sutherland's equation with constant coefficients:

$$\mu = \mu_{ref} \left(\frac{T_b}{T_{ref}} \right)^{3/2} \frac{T_{ref} + S}{T_b + S} \quad (38)$$

where:



- μ is dynamic viscosity ($kg\ m^{-1}s^{-1}$)
- μ_{ref} is reference dynamic viscosity ($kg\ m^{-1}s^{-1}$)
- T_{ref} is reference temperature (K)
- S is an effective temperature (Sutherland's constant) (K)

For air at moderate temperatures and pressures, $\mu_{ref} = 1.716 \times 10^{-5}$ ($kg\ m^{-1}s^{-1}$), $T_{ref} = 273.11\ K$, and $S = 110.56\ K$.

Calculations of μ using equation 38 were benchmarked against tabulated values for viscosity of dry air by (Singh & Heldman, 2014). Values were found to closely match. Hence the assumption of moderate temperatures and pressures is appropriate.

B.2.3 Thermal conductivity of dry air k_f

Thermal conductivity of dry air was calculated using Sutherland's equation with three coefficients (so the same way as for dynamic viscosity of dry air (equation 38)) except using reference thermal conductivity ($k_f = 0.0237$ at $T_{ref} = 273.11\ K$) instead of reference viscosity.

B.2.4 Specific heat of dry air c_p

Tabulated values of specific heat of dry air c_p ($Jkg^{-1}K^{-1}$) at film temperature T_{film} obtained from (Singh & Heldman, 2014). Relevant values are shown in table 4. Lowest value of T_{film} is $35^\circ C$ at $t = 0$ for $T_b = 50^\circ C$, $T_0 = 20^\circ C$. Highest value of T_{film} is $160^\circ C$ at $t = t_f$ for $T_b = 50^\circ C$.

$T_{film}(^\circ)C$	20	35	50	80	100	140	160
c_p ($Jkg^{-1}K^{-1}$)	1012	≈ 1013.5	1016	1019	1022	1027	1030

Table 4: Film temperature and corresponding specific heat of dry air.

B.2.5 Velocity of dry air u

Velocity of dry air (ms^{-1}) is given by (Putranto et al., 2011):

$$u = 0.56 \tag{39}$$



C Mass transfer coefficient h_m

Similarly, the mass transfer coefficient (h_m) is a property of dry air and is a function of film-temperature-dependent thermophysical properties and is determined by (Incropera et al., 2002):

$$\overline{h_m} = \frac{\overline{Sh} \cdot D_{12}}{L_c} \quad (40)$$

where Sh is the Sherwood number, D_{12} is the binary diffusivity of fluid (or the diffusion coefficient or effective moisture diffusivity) and L_c is the characteristic length of the material.

Sherwood number Sh is based on geometry and flow of concern and is the mass transfer equivalent of the Nusselt number Nu . For forced convection in a flat plate, Sh is:

$$\overline{Sh} = 0.664Re^{1/2}Sc^{1/3}, \quad (41)$$

where Re is the Reynolds number (equation 33) and Sc is the Schmidt number. Schmidt number Sc is the mass transfer equivalent of the Prandtl number and is defined by:

$$Sc = \frac{\mu}{\rho D_{12}}, \quad (42)$$

where D_{12} is the binary diffusivity of fluid and μ is density of fluid.

Similarly to the heat transfer coefficient h , we can rewrite the mass transfer coefficient h_m purely as a film-temperature-dependent function of thermophysical properties, characteristic length and binary diffusivity:

$$h_m = 0.664 \left(\frac{\rho u L_c}{\mu} \right)^{1/2} \left(\frac{\mu}{\rho D_{12}} \right)^{1/3} \left(\frac{D_{12}}{L_c} \right) \quad (43)$$

where μ , ρ , u and L_c have already been obtained (see sections B.2 and A.1.1).

Therefore for calculation of h_m , we only need to find binary diffusivity D_{12} (see section C.1).

Substitution into equation 43 yield h_m of order 10^{-2} .

C.1 Binary diffusivity D_{12}

The effective moisture diffusivity D_{12} (or binary diffusivity) for mass transfer coefficient is a property of drying air (gas).

The Slattery-Bird equation (Bird et al., 2007) is an empirical correlation that can be used to estimate binary gas diffusivity D_{12} (m^2s^{-1}) at low pressures (such as standard atmospheric pressure of $p = 1$ atm):

$$D_{12} = 10^{-4} \cdot \frac{1}{p} \cdot (p_{c,1}p_{c,2})^{1/3} (T_{c,1}T_{c,2})^{5/12} \left(\frac{1}{M_1} + \frac{1}{M_2} \right)^{1/2} \cdot a \left(\frac{T}{\sqrt{(T_{c,1}T_{c,2})}} \right)^b \quad (44)$$



where 10^{-4} is a conversion factor for D_{12} from (cm^2/s) to (m^2/s) and 1 (water) and 2 (air) index the two types of molecules present in the gaseous mixture and:

- $p = 1$ is total pressure (assume standard atmospheric pressure) (atm)
- $p_{c,1} = 217.616$ is critical pressure of species A (water) (atm)
- $p_{c,2} = 37.36294$ is critical pressure of species B (air) (atm)
- $T_{c,1} = 647.1$ is critical temperature of species A (water) (K)
- $T_{c,2} = 132.48$ is critical temperature of species A (air) (K)
- $M_1 = 18.01534$ is molar mass of species A (water)
- $M_2 = 28.9645$ is molar mass of species B (air)
- $a =$ and $b =$ (water with non-polar gas (air))

Using equation 44, D_{12} is order 10^{-5} , as expected for gases.

The Chapman-Enskog equation (Chapman & Cowling, 1970) is better than the Slattery-Bird equation as it is the standard theoretical model for gas diffusivity D_{12} . However, we cannot use it as it involves average collision diameter (tabulated) and temperature-dependent collision integral (tabulated) which could not be found for both water and air in (Bird et al., 2007).

The diffusion coefficient for mass transfer coefficient h_m is a property of air. This is contrary to the equation for moisture diffusivity in (Sakin et al., 2007) as that diffusivity is a property of the cake itself used explicitly for a diffusion model rather than implicitly for the LREA in this report. This means we must carefully check whether equations for engineering parameters are for the material being dried (cake) or the medium used to dry it (air). The property that moisture diffusivity D_{12} referred to was not provided in the papers This is yet another vital aspect of modeling baking and drying processes that is not explained in any of the papers yet is not intuitive to mathematicians.

D Moisture content and temperature profiles varying orders of h_m

In our first attempt at modeling, we incorrectly used the value $h_m = 2 \times 10^{-5}$ ¹. Resultant moisture content profile 4 exhibits an entirely different relationship (linear) to the experimental data (negative exponential) while temperature profile and 5 plateaus too early.

¹This value of h_m was obtained from the experimental data used for modeling the roasting of coffee using the LREA (Fabbri et al., 2011; Putranto & Chen, 2012)

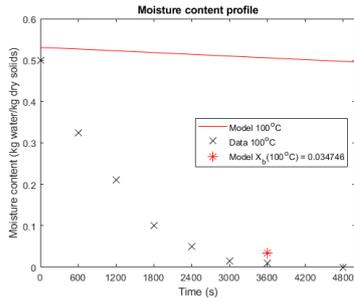


Figure 4: Moisture content profile at baking temperature of 100°C , $h_m = 2 \times 10^{-5}$.

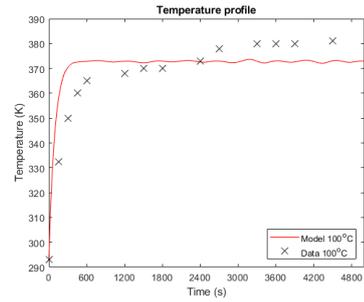


Figure 5: Temperature profile at baking temperature of 100°C , $h_m = 2 \times 10^{-5}$.

We then incorrectly assumed that the binary diffusivity D_{12} used to calculate the mass transfer coefficient h_m is a property of the cake batter (using equations obtained by (Sakin et al., 2007)). This resulted in mass transfer coefficient h_m of order 10^{-4} and a similarly poor moisture and temperature profiles:

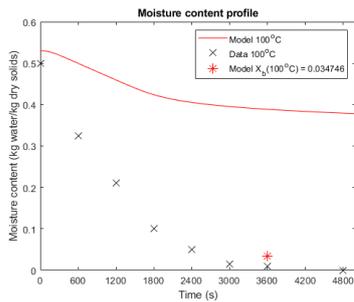


Figure 6: Moisture content profile at baking temperature of 100°C , $h_m = 2 \times 10^{-4}$.

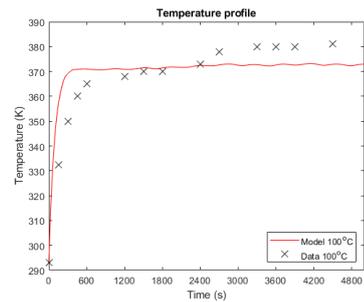


Figure 7: Temperature profile at baking temperature of 100°C , $h_m = 2 \times 10^{-4}$.

We then increased the order of the mass transfer coefficient h_m until we obtained a negative exponential moisture content profile that reasonably fit the experimental data. h_m of order 10^{-1} (figure 12 and 13) was found to generate profiles with the best fit.

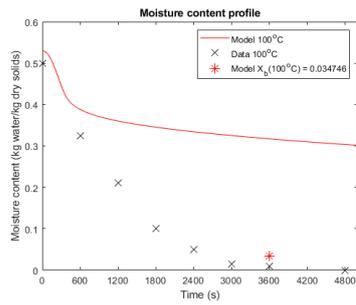


Figure 8: Moisture content profile at baking temperature of 100°C , $h_m = 2 \times 10^{-3}$.

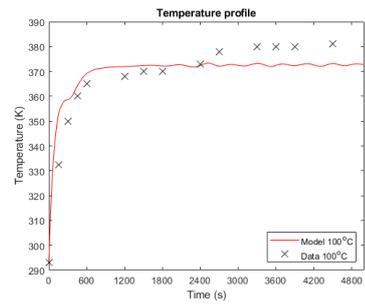


Figure 9: Temperature profile at baking temperature of 100°C , $h_m = 2 \times 10^{-3}$.

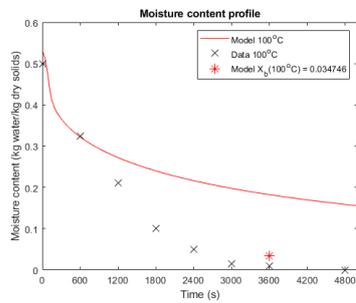


Figure 10: Moisture content profile at baking temperature of 100°C , $h_m = 2 \times 10^{-2}$.

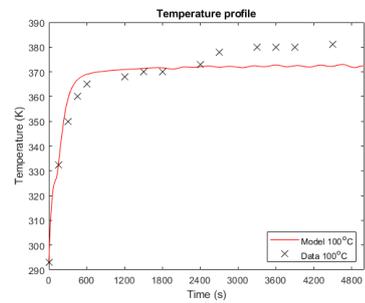


Figure 11: Temperature profile at baking temperature of 100°C , $h_m = 2 \times 10^{-2}$.

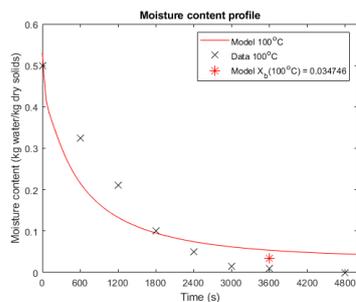


Figure 12: Moisture content profile at baking temperature of 100°C , $h_m = 2 \times 10^{-1}$.

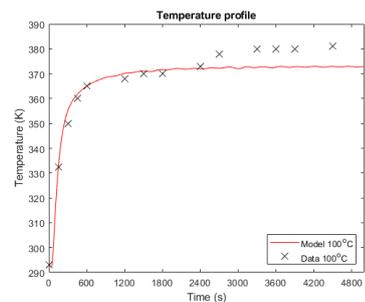


Figure 13: Temperature profile at baking temperature of 100°C , $h_m = 2 \times 10^{-1}$.



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