

MODELLING THE COOKING PROCESS OF A SINGLE CEREAL GRAIN

Four models are developed to assist with the uniform and accurate cooking of whole grains for Uncle Tobys breakfast cereals.

1. Heat satisfies a linear conduction equation and is found to rapidly penetrate the grain.
2. Moisture satisfies a non-linear diffusion equation, and is found to penetrate the grain more slowly than heat. The more sophisticated moisture diffusion model is solved by numerical and analytic techniques for spherical and ellipsoidal grains.

A vital role is played in the moisture diffusion model by the concept of the mean action time for wetting a grain.

These first two models are used to determine sensitivity to key cooking parameters, and to calculate the degree of over-cook in the existing batch steam process. Recommendations are made for improving and speeding up the cooking process.

The last two models are modifications of the nonlinear moisture penetration model 2. above. The results of these improved models have the potential to provide finer adjustments to estimates of wetting times.

3. A cereal grain swells significantly during wetting. A model that takes this into account is developed and solved approximately.
4. Another wetting model describes the effect of the gelatinisation reaction, slowing moisture penetration, and leading to a sharp front entering the grain. The effect of gelatinisation on the speed of moisture penetration is expected to be more important for the present high-temperature cooking process, than when soaking a grain at a lower temperature. This model is also developed and solved approximately.

1. The problem

Whole cereal grains of corn, wheat, oats and rice are cooked at Uncle Tobys Wahgunyah Plant in a rotating steam pressure-cooker, in one tonne batches.

Cooking depends on two concurrent processes, heating the grain to a high enough temperature, and hydrating the grain to a high enough moisture content. After cooking, the grains are dried, flaked, toasted and coated before packaging as a finished breakfast cereal product.

The breakfast cereal manufacturing line currently installed at Uncle Tobys Wahgunyah Plant is now running near full capacity, and the rotary cooking operation is known to be the bottle-neck in the line capacity.

An idea proposed by Uncle Tobys is to separate the wetting and heating processes, installing additional equipment to wet the grains, and using the existing rotary batch pressure cookers to heat them. If the time required in the cookers could be reduced, throughput could be increased.

Besides speeding up the cooking process, Uncle Tobys also mentioned the importance of being able to ensure a uniformly cooked product. Under-cooking of part of the grain produces a raw taste and poor binding; and over-cooking produces a sticky dough that is difficult to process, and a product that goes soggy too quickly in milk.

Uncle Tobys has asked specifically for two mathematical models:

1. one predicting the moisture content of a single cereal grain as a function of some grain property, grain size, process temperature, process pressure and time, and
2. one predicting the internal temperature of a single cereal grain as a function of some grain property, grain size, process temperature, process pressure and time.

Ideally, the models could be extended to cover the present process where both mechanisms occur together.

2. Background

Cooking involves gelatinising the starches present. It is desirable to retain the longer-chain starches, which give a product that retains its crispness when put into milk. This is one reason that whole grains are cooked — if grains are physically broken up first, too much of the starch is broken down to shorter chains, giving the over-cooking problems mentioned above.

Gelatinisation is the process whereby water and heat cause starch granules to swell, and eventually burst at the gelatinisation temperature T_{gel} . The swelling

is reversible up to a temperature somewhat below the bursting temperature, T_{gel} , and irreversible beyond it. Water is taken up by the grain, which swells by a volume equal to that of the water taken up. The water bonds with the starch, although there is evidence that there is still freedom for bonded water to interact with neighbouring dry starch.

Gelatinisation occurs over a temperature range of about 10°C , at a temperature that depends on the moisture level. The relationship is illustrated in Figure 1. If moisture content is too low, it is thought that gelatinisation cannot occur at all. The higher the moisture content, the lower the temperature at which gelatinisation occurs. Moisture content is here the dry ratio, the ratio of the mass of water to the mass of dry grain. Another measure of moisture content commonly used is the wet ratio, the ratio of the mass of water to the mass of water plus grain.

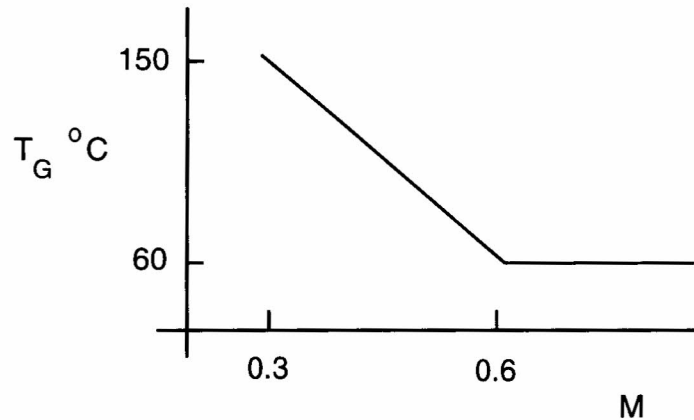


Figure 1: A sketch indicating gelatinisation temperature versus moisture content (dry ratio).

A thermodynamic treatment of the gelatinisation process is consistent with the observed inter-dependence of T_{gel} and moisture levels. In this, the starch is treated as a melting crystalline polymer, with water the diluent. The latent heats of melting obtained experimentally are tabulated in Table 1.

	cal/gm dry starch	J/gm dry starch
Corn	4.1-4.9	17.2-20.5
Wheat	2.5-3.3	10.5-13.8
Rice	3.4-3.9	14.2-16.3

Table 1: Latent heats of melting.

Grain structure and properties are summarised in Figure 2 and Table 2. Two major parts of the grain are identified in a simplified view of the actual grain, the outer cellulose skin or pericarp, and the inner region filled with starch granules.

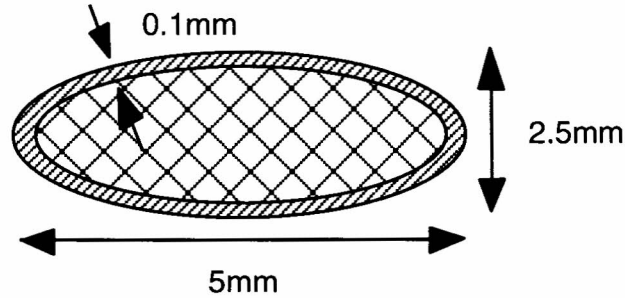


Figure 2: Sketch of a simplified rice grain.

Properties	Cellulose	Corn Starch	units
specific heat C_p	2500	2160	J/(kg °K)
density ρ	950	1400	kg/m ³
thermal conductivity λ	0.15	0.26	W/(m °K)
thermal diffusivity α_0	6.3×10^{-8}	8.6×10^{-8}	m ² /s
moisture diffusivity D at 40°C (Syarief <i>et al.</i> (1987))	$6 \times 10^{-12} e^{8.6M}$	$1.5 \times 10^{-11} e^{8.6M}$	m ² /s
lengthscale	0.1 – 0.15	1.25	mm

Table 2: Some properties of whole grains.

3. Heating

The linear diffusion equation for temperature $T(\mathbf{x}, t)$ at time t and at location \mathbf{x} in the grain is

$$\frac{\partial T}{\partial t} = \alpha_0 \nabla^2 T \quad (1)$$

with initial temperature $T(\mathbf{x}, 0) = T_0$, and $T = T_1$ at the grain surface for $t > 0$. This has solutions that depend on the grain shape.

Two different measures of time to heat or wet are used here, t^* the time for the temperature at the centre of the grain to move to 90% of its final value, and a mean action time t^{**} (McNabb, 1975, and McNabb and Wake, 1991), which is particularly useful for the nonlinear wetting problem. These time measures are illustrated in Figure 3.

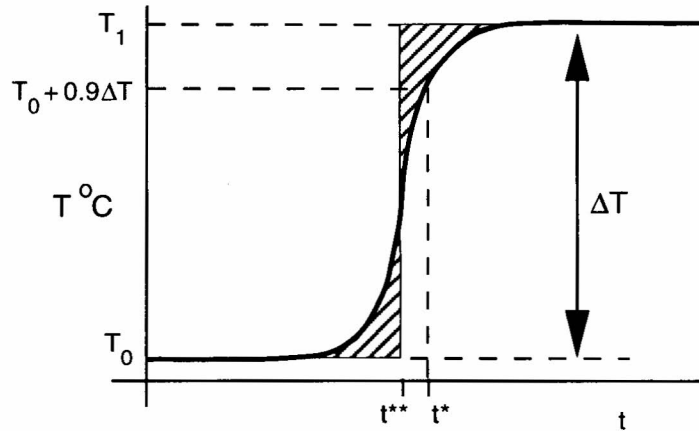


Figure 3: Sketch showing the locations of the time t^* to reach 90% of the final temperature, and of the mean action time t^{**} at a point.

3.1 Mean action time

A solid theoretical basis for heating time is given by McNabb (1975) and McNabb and Wake (1991), and is outlined briefly here. A mean action time t^{**} is defined at each point in the grain by

$$t^{**}(\mathbf{x}) = \frac{\int_0^\infty t \frac{\partial T}{\partial t}(\mathbf{x}, t) dt}{\int_0^\infty \frac{\partial T}{\partial t}(\mathbf{x}, t) dt} = \int_0^\infty \frac{T_1 - T(\mathbf{x}, t)}{T_1 - T_0} dt. \quad (2)$$

We define $\Phi(\mathbf{x})$ by setting $t^{**}(\mathbf{x}) \equiv \Phi(\mathbf{x})/\alpha_0$. Then substitution into the diffusion equation gives the result that Φ satisfies a Poisson equation,

$$\nabla^2 \Phi = -1 \quad (3)$$

inside the grain, with $\Phi = 0$ on the grain surface. The largest value of Φ , Φ_G , gives the mean action time for heat to penetrate to the centre of the grain. A graphical interpretation is given in Figure 3. The areas shaded on either side of the mean action time are equal, showing how it corresponds to locating a front in shock theory. With a sharp front, as occurs in nonlinear diffusion problems like the wetting problem introduced later in this report, there is very little difference between t^* and t^{**} . With a more diffuse front, like the present linear problem, t^* can be up to twice as large as t^{**} .

3.2 Sphere

For a sphere of radius R , reference to the solution plotted in Figure 4 shows that

$$t^* = 0.3R^2/\alpha_0. \quad (4)$$

The leftmost curve is the relevant one when temperature is fixed at the surface of the grain, which is the boundary condition used in this report. For the mean action time, the Poisson equation has solution

$$\Phi = (R^2 - r^2)/6, \quad (5)$$

$$t^{**} = R^2/(6\alpha_0). \quad (6)$$

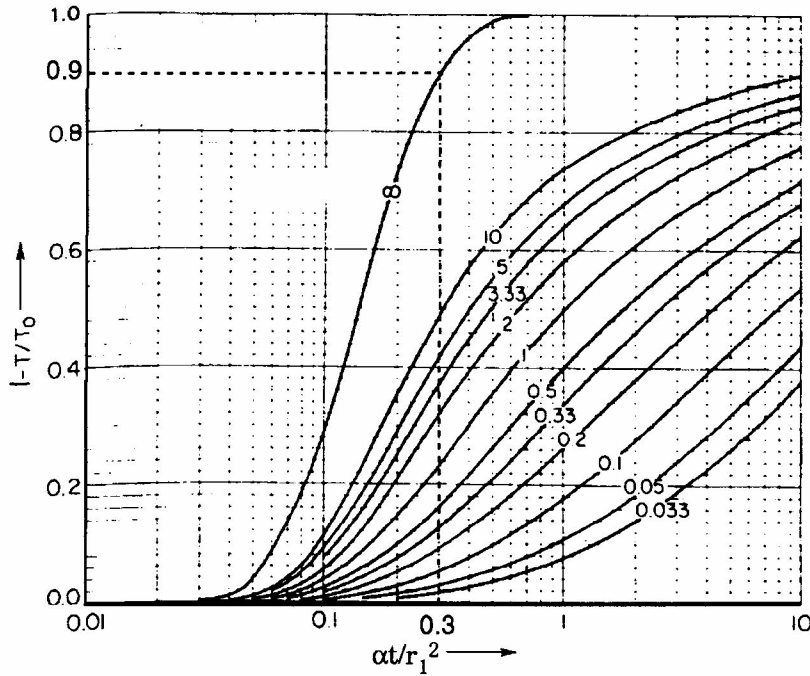


Figure 4: Solutions to the linear diffusion problem in temperature for a sphere.

3.3 Ellipsoid

For an ellipsoid

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} = 1 \quad (7)$$

the solution to the Poisson equation is

$$\Phi = \left[1 - \left(\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} \right) \right] / A \quad (8)$$

where

$$A = 2 \left(\frac{1}{a^2} + \frac{1}{b^2} + \frac{1}{c^2} \right). \quad (9)$$

The penetration of heat then follows ellipsoids, successively smaller and smaller as time progresses, like onion skins. The mean action time for heat to penetrate to the center of an ellipsoidal grain is

$$t^{**} = \frac{1}{2\alpha_0 \left(\frac{1}{a^2} + \frac{1}{b^2} + \frac{1}{c^2} \right)} \quad (10)$$

and t^* is approximately twice this.

The pericarp, which has a slightly different thermal diffusivity to the inner part of the grain, is so thin that it is of no consequence.

4. Time scales for wetting and heating — linear models

The times t^* to heat and wet in Table 3 are calculated assuming linear diffusion occurs. This is a good assumption for heating, and a poor assumption for wetting. It gives a first approximation to the times involved. It is immediately clear that a grain heats right through in a much shorter time than it takes to wet.

Times t^*	Cellulose	Corn Starch	units
timescale – linear heating	0.05	5.4	seconds
timescale – linear wetting (M=0.15)	2	145	minutes
timescale – linear wetting (M=0.5)	0.1	7	minutes

Table 3: Some timescales for heating and wetting whole grains.

This puts an entirely new picture in place for the existing batch steam pressure cooking process. Uncle Tobys had originally modelled the thermal front as following the wetting front, linking them by an Arrhenius law. Now it is clear that the present process is moisture-limited, and most of the hour or more of cooking time is spent waiting for moisture to penetrate the hot grain. It also means, given that the temperature is well above T_{gel} , that much of the grain is over-cooked.

Already this indicates that separating the processes is a good idea, particularly that it is a good idea to wet the grains before heating.

Mathematically, we can separate the heating and wetting processes because the timescales are so different, irrespective of whether the processes are separated in practice.

5. Wetting the grains — a nonlinear model

A variety of models was investigated. Convection models considered the possibility of modelling moisture penetration as flow in a porous medium, driven by capillarity or swelling. These were rejected as they do not fit with what is known about the grains. There is no air in the grain before hydration, and hence no surface tension to drive a capillary pressure. Water enters the grain by sorption processes, driven by a chemical potential called water affinity. The amount of grain swell is equal to the volume of water absorbed.

Such a process leads naturally to a nonlinear diffusion equation for moisture content. The paper by Syarief *et al.* (1987) is the best reference we found to the way grains take and lose water, below T_{gel} . Syarief *et al.* present the results of careful experiments on the uptake and loss of moisture from various parts of a corn kernel, and they fit the experimental results with a fully nonlinear numerical finite element model. They find that the following nonlinear diffusion equation accurately describes the uptake of moisture at 40°C:

$$\frac{\partial M}{\partial t'} = \nabla \cdot (D \nabla M) \quad (11)$$

where M is the ratio of the mass of water to the mass of dry starch, and the nonlinearity comes from the dependence of D on M ,

$$D \equiv D_0 \exp(\delta M),$$

where D_0 and δ are positive real constants. For corn starch, the values they find for D_0 and δ are tabulated above in Table 2. The initial value M_0 of M is typically about 0.15, and the desired final moisture content, M_1 , is usually about 0.6.

We non-dimensionalise and re-scale equation (11) by choosing

$$m = \frac{M - M_1}{M_1 - M_0} \quad (12)$$

$$t = \frac{D_0 e^{\delta M_1}}{R^2} t' \quad (13)$$

where R is a lengthscale in the problem, so that the diffusion equation becomes

$$\frac{\partial m}{\partial t} = \nabla \cdot (e^{\beta m} \nabla m) \quad (14)$$

where $\beta = \delta(M_1 - M_0)$, with initial condition $m = -1$ everywhere in the grain, and boundary condition at the grain surface $m = 0$ for $t > 0$.

Some typical values for parameters are $\delta = 8.6$, $\beta = 3.9$.

This nonlinear diffusion equation (14) has been solved numerically and analytically, as described in Sections 5.1 and 5.2 respectively. Swelling effects, and gelatinisation at the wetting front, are modelled later, in Sections 8 and 9.

5.1 Numerical solutions

The finite element package called *FastFlo*TM was used to solve equation (11) accurately with ellipsoidal geometry. *FastFlo*TM was developed by CSIRO Division of Mathematics and Statistics; it is finite-element based and has the capability to deal with a range of element types on structured and unstructured meshes. Due to symmetry, only one quarter of the ellipsoid is shown. Figure 5 shows snapshots of the contours of constant moisture content, at times 2, 10 and 20 minutes after beginning to soak the grain. Contours are evenly spaced in moisture content, with some values indicated directly on the plots. The contours at 10 minutes illustrate the sharpness of the wetting front, in the clustering near 38% moisture. After 20 minutes most of the grain is close to 37% moisture content.

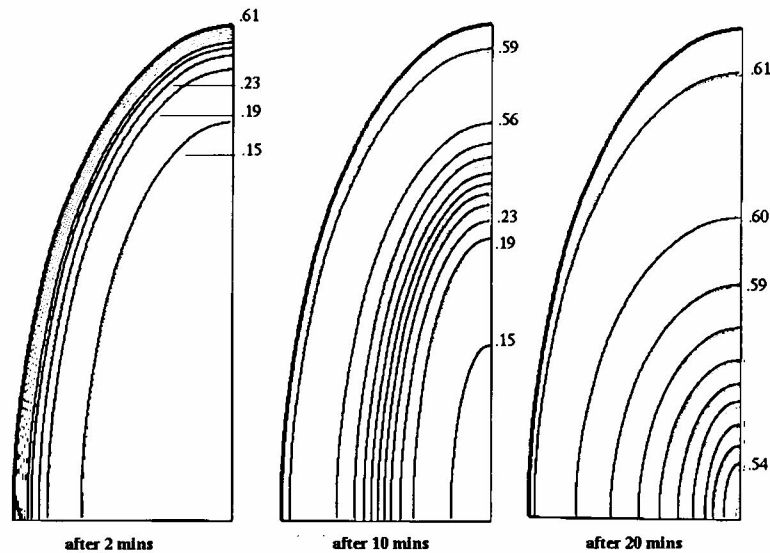


Figure 5: Numerical solutions to the nonlinear wetting problem for an ellipsoid, using *FastFlo*TM.

Another numerical approach used was to program a finite difference solution using the NAG package, for a spherical grain. The sphere radius was taken to be 1.6 mm, and the diffusivity was taken as $1.5 \times 10^{-11} \exp(8.6M)$. Moisture content profiles are shown in Figure 6 at 3 minute intervals, showing the grain

to be very close to equilibrium moisture levels after 21 minutes. These profiles are in good agreement with the *FastFlo*TM results.

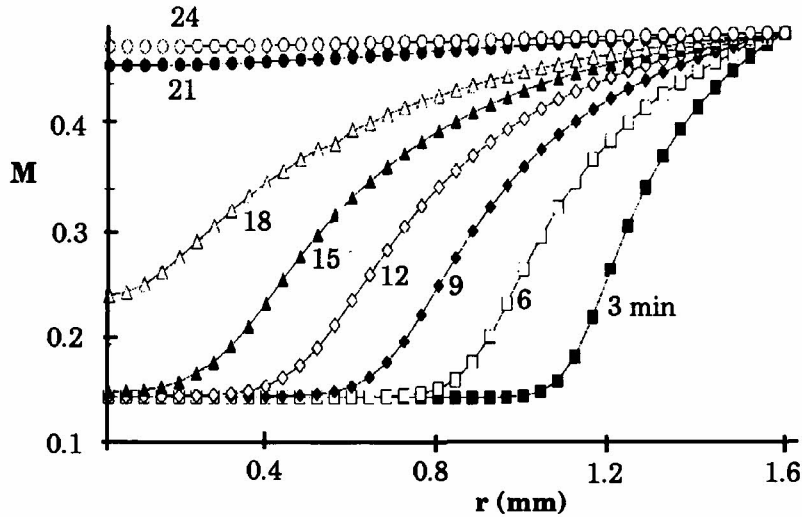


Figure 6: Numerical solutions to the nonlinear diffusion equation, for a sphere, using NAG.

5.2 Analytic solutions — mean action time

Following McNabb and Wake (1991) (see also McNabb, 1975), we define a mean action time at each point x in the grain for equation (14) as follows:

$$t^{**}(x) \equiv \frac{\int_0^\infty t \left[\frac{\partial}{\partial t} \int_{-1}^m e^{\beta s} ds \right] dt}{\int_0^\infty \left[\frac{\partial}{\partial t} \int_{-1}^m e^{\beta s} ds \right] dt}. \quad (15)$$

The integrals can be simplified to give

$$t^{**}(x) = \frac{\int_0^\infty (1 - e^{\beta m}) dt}{1 - e^{-\beta}}. \quad (16)$$

Note that as $\beta \rightarrow 0$ the definition in equation (16) is the same as that in the linear definition equation (2).

If we define

$$\Phi \equiv \frac{1}{\beta} \int_0^\infty (1 - e^{\beta m}) dt, \quad (17)$$

so that

$$t^{**} = \frac{\beta \Phi}{1 - e^{-\beta}}, \quad (18)$$

then substitution into the nonlinear diffusion equation reveals that Φ satisfies a (linear) Poisson equation inside the grain:

$$\nabla^2 \Phi = -1, \quad (19)$$

with boundary condition $\Phi = 0$ on the surface of the grain. This Poisson equation can be solved for an ellipsoidal shaped grain,

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} \leq 1. \quad (20)$$

Here, (x, y, z) and (a, b, c) are the non-dimensional variables and semiaxes of the ellipsoid. The same equation for the ellipsoid applies, when (x, y, z) and (a, b, c) have dimensions. The analytic solution Φ is given in equations (8) and (9).

The largest value of Φ is at the centre of the grain. This gives the maximum mean action time, so that

$$\Phi_G = \frac{1}{2 \left(\frac{1}{a^2} + \frac{1}{b^2} + \frac{1}{c^2} \right)}, \quad (21)$$

$$t_G^{**} = \frac{\beta}{1 - e^{-\beta}} \Phi_G. \quad (22)$$

The term Φ_G can be seen to be a shape factor, dependent on grain shape, in the expression for the maximum mean action time t_G^{**} . The expression for maximum mean action time in seconds is then

$$t'_G(s) = \frac{R^2 e^{-\delta M_1} \beta \Phi_G}{D_0(1 - e^{-\beta})}. \quad (23)$$

Using the properties tabulated for corn starch in Table 2, and the grain shape illustrated in Figure 2, leads to a wetting time $t'_G = 18$ minutes. Note that while this falls between the extreme values of 7 minutes and 145 minutes calculated using linear theory in Table 3, it is closer to the value of 7 minutes calculated using $M = 0.5$. Note also the excellent agreement with numerical results for spherical and ellipsoidal shapes.

5.3 Log mean diffusivity

A significant way to rewrite the maximum mean action time is as

$$t'_G(s) = \frac{R^2 \Phi_G}{D_{\text{equiv}}}, \quad (24)$$

where the equivalent diffusivity is the log mean of the extreme values taken by the nonlinear diffusivity,

$$D_{\text{equiv}} \equiv \frac{D_{\text{wet}} - D_{\text{dry}}}{\ln(D_{\text{wet}}/D_{\text{dry}})}, \quad (25)$$

where

$$D_{\text{wet}} \equiv D_0 e^{\delta M_1}, \quad D_{\text{dry}} \equiv D_0 e^{\delta M_0}. \quad (26)$$

Even though the moisture penetration problem is a nonlinear diffusion one, the definition used for mean action time justifies the treatment of the diffusion of moisture as an equivalent linear diffusion problem, at least in terms of the times taken to wet grains. That is, the form of equation (24) is the same as the time scaling obtained with a linear diffusion equation with a diffusion equal to D_{equiv} .

5.4 Degree of over-cook for the present process

The present cooking process at Uncle Tobys involves high temperature steam pressure-cooking. The grains quickly establish a constant temperature, and gelatinisation depends on the penetration of the moisture front. In this section we give a formula for calculating how the degree of over-cook varies with time and temperature for a single grain, for this process. The first step is to calculate the volume of grain that has been cooked.

The volume that has been gelatinised can be calculated using the mean action time to locate the wetting front as it enters an ellipsoidal grain. First we calculate the volume that is not yet cooked. After t' seconds, assuming the mean action time gives the front location, the moisture front has penetrated to x, y, z values satisfying

$$t' = \frac{R^2 e^{-\delta M_1} \beta \Phi(x, y, z)}{D_0 (1 - e^{-\beta})} = \frac{t'_G \Phi(x, y, z)}{\Phi_G}. \quad (27)$$

Substituting for Φ_G and Φ from equations (21) and (8) gives

$$\frac{\Phi_G}{\Phi} = 1 - \frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2}. \quad (28)$$

Hence, after t' seconds, all points inside the ellipsoid

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} = 1 - \frac{t'(s)}{t'_G(s)} \quad (29)$$

are not yet cooked. This ellipsoid has semiaxes (Ba, Bb, Bc), where

$$B^2 = 1 - \frac{t'}{t'_G}. \quad (30)$$

The volume uncooked is the volume inside this ellipsoid,

$$\frac{4}{3} \pi abc \left(1 - \frac{t'}{t'_G}\right)^{3/2}. \quad (31)$$

Hence the volume overcooked is

$$V_{oc} = \frac{4}{3}\pi abc \left[1 - \left(1 - \frac{t'}{t'_G} \right)^{3/2} \right]. \quad (32)$$

This volume is sketched in Figure 7. It has been normalised on the total grain volume, and the time variable has been divided by the mean action time,

$$\tilde{t} = t'/t'_G.$$

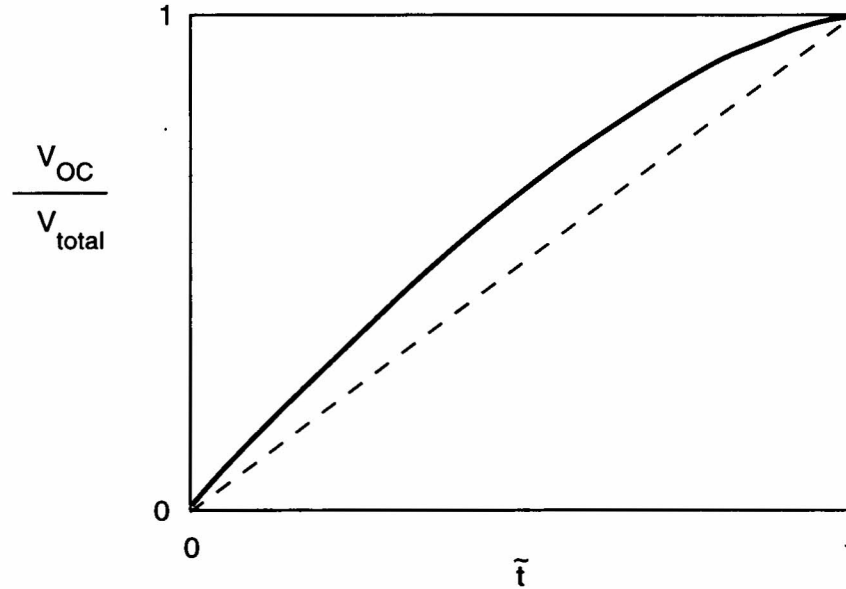


Figure 7: A sketch of the calculated volume (over)cooked, for an ellipsoidal grain. The dashed line is a straight line of slope 1, for comparison.

The degree of over-cook might usefully be defined to be

$$D_{oc} \equiv e^{T_{excess}} \int_0^{V_{oc}(t')} t' dv, \quad (33)$$

where T_{excess} is the excess temperature above the gelatinisation temperature for the equilibrium moisture content of the grain. Transforming the integral so that everything is in terms of the time variable t' , and dropping the primes for the remainder of this section, gives

$$D_{oc} = e^{T_{excess}} \frac{2\pi abc}{t_G} \int_0^t t \left(1 - \frac{t}{t_G} \right)^{1/2} dt, \quad (34)$$

for $t \leq t_G$, and

$$\mathcal{D}_{oc} = e^{T_{excess}} \frac{2\pi abc}{t_G} \int_0^{t_G} t \left(1 - \frac{t}{t_G}\right)^{1/2} dt + \frac{4}{3}\pi abc(t - t_G) \quad (35)$$

for $t \geq t_G$, when all of the grain is cooked, and it continues to over-cook at a rate proportional to time. These integrals are evaluated by elementary methods to give in explicit form

$$\mathcal{D}_{oc} = e^{T_{excess}} \begin{cases} 4\pi abct_G \left[\frac{2}{15} + \frac{1}{5} \left(1 - \frac{t}{t_G}\right)^{5/2} - \frac{1}{3} \left(1 - \frac{t}{t_G}\right)^{3/2} \right], & t \leq t_G, \\ \frac{8\pi abct_G}{15} + \frac{4}{3}\pi abc(t - t_G), & t \geq t_G. \end{cases} \quad (36)$$

The way that the degree of over-cook depends on time is illustrated in Figure 8. The value plotted on the y axis is a normalised degree of over-cook,

$$D'_{oc} = \frac{\mathcal{D}_{oc}}{\frac{4}{3}\pi abct_G e^{T_{excess}}},$$

and the variable along the \tilde{t} -axis is a normalised time,

$$\tilde{t} = \frac{t}{t_G}.$$

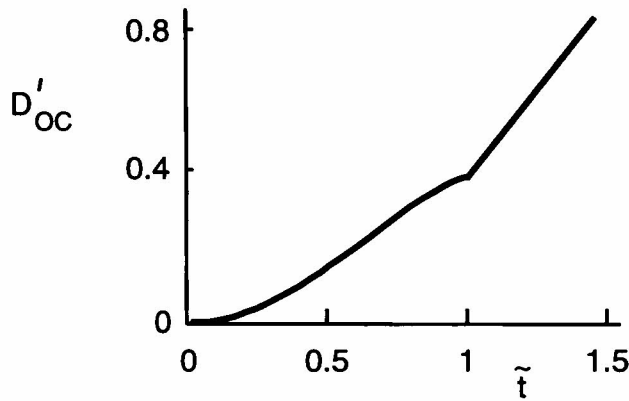


Figure 8: A sketch of the normalised degree of over-cook against a normalised time, for an ellipsoidal grain.

6. Temperature dependence of wetting times

This is adequately incorporated into the model by taking the well-known Arrhenius dependence of D_0 on temperature T ,

$$D_0 = K e^{E_a/(RT)}, \quad (37)$$

where K and E_a are constants, R is the gas constant, and by allowing for the dependence of M_1 on temperature. Uncle Tobys is already well aware of these dependencies, obtained through experiments. M_1 , the final stabilised value of moisture content, increases with temperature. However, D_0 decreases rapidly with increasing temperature, slowing the time to wet. So the optimum temperature at which to wet the grains fastest is that which is just hot enough to raise M_1 to the desired moisture level before cooking.

7. Sensitivity analysis

The previous analytical studies lead to Table 4 identifying the sensitivity of the wetting time to parameters such as variations in grain size, diffusivity, and final moisture content.

Sensitivity of t^{**} to:	Linear Model	Nonlinear Model
R	R^2	R^2
$\beta = \delta(M_1 - M_0)$	none	$\beta/(1 - e^{-\beta}) \sim \beta, \beta \rightarrow \infty$
D_0	$1/D_0$	$1/D_0$
M_1	none	$e^{-\delta M_1}$

Table 4: Sensitivity of wetting times to model parameters.

8. Swelling of the grain due to moisture absorption

In the previous Section 5, a model has been examined which considers the motion of the water into the grain interior due to gradients in water affinity but excludes the effects of swelling of the grain. In this section we shall consider how the swelling may be incorporated into the model and outline the solution structure in the case where the water diffusion in the original grain is much less than the diffusion at the surface during hydration.

8.1 A grain swelling model

Swelling of materials as fluids are absorbed has been considered in several situations such as soil wetting and absorption of solvents in polymers. We shall give an outline derivation of the underlying equations indicating the approximations made.

The basis of the model will be that at any point in the grain we can consider the water to occupy a volume fraction ϕ and that the remaining volume fraction, $1 - \phi$, is completely taken up by the solids of the grain. As water moves through the grain it is assumed to displace the solids on an equal volume basis. Taking \mathbf{u}_s to be the actual velocity ($m^3/(m^2s)$) of the solid at any point, \mathbf{u}_w as the actual velocity of the water and assuming each material has constant density we can consider the conservation of solid and of water at each point in the grain to give

$$\frac{\partial(1 - \phi)}{\partial t} + \nabla \cdot (\mathbf{u}_s(1 - \phi)) = 0 \quad (38)$$

$$\frac{\partial\phi}{\partial t} + \nabla \cdot (\mathbf{u}_w\phi) = 0. \quad (39)$$

For the purposes of analysis it is easier to work with these in a slightly different form, representing total conservation and a relative change. We add and subtract them to give

$$\nabla \cdot ((\mathbf{u}_w - \mathbf{u}_s)\phi + \mathbf{u}_s) = 0 \quad (40)$$

$$2\frac{\partial\phi}{\partial t} + \nabla \cdot ((\mathbf{u}_w + \mathbf{u}_s)\phi - \mathbf{u}_s) = 0. \quad (41)$$

We take the velocity of the water to be driven, as before, by gradients in the water affinity. Equation (11), for the case when the solid is stationary and no swelling is accounted for, is

$$\frac{\partial M}{\partial t} = \nabla \cdot (D_0 e^{\delta M} \nabla M) \quad (42)$$

where M is the mass fraction of water on a dry basis, δ is a constant with a value around 8.6 and D_0 is also constant. This definition corresponds to

$$M = \frac{\rho_w \phi}{\rho_s(1 - \phi)} \quad (43)$$

where ρ_w and ρ_s are the densities of water and solid.

From equation (42) we conclude that the flux of M at any point is

$$-D_0 e^{\delta M} \nabla M$$

and, since the flux is the concentration times the velocity, that the actual velocity of the water through a stationary solid is

$$-D_0 e^{\delta M} \frac{\nabla M}{M}. \quad (44)$$

We can now use this expression to give the following expression for the velocity of the water in the case where the solid is moving

$$\mathbf{u}_w = \mathbf{u}_s - D_0 e^{\delta M} \frac{\nabla M}{M}. \quad (45)$$

Putting this definition of water velocity into the conservation equations gives

$$\nabla \cdot \left(-D_0 e^{\delta M} \frac{\nabla M}{M} \phi + \mathbf{u}_s \right) = 0, \quad (46)$$

$$2 \frac{\partial \phi}{\partial t} + \nabla \cdot \left(-D_0 e^{\delta M} \frac{\nabla M}{M} \phi + (2\phi - 1) \mathbf{u}_s \right) = 0. \quad (47)$$

The model is complete except for the fact that we have stated nothing about the forces acting on the solid that may result due to its motion. Models may either take the solid as a visco-elastic material or some other behaviour based on the properties of the grain. Such models have been considered by several authors, for instance King (1989). We do not anticipate that the resulting forces will be sufficient to influence the water transport except to change the position of the outer surface of the grain.

We integrate the first equation from the center of the grain, and choose a frame of reference such that the net flux of grain and water mass is zero there, to give

$$D_0 e^{\delta M} \frac{\phi}{M} \nabla M = \mathbf{u}_s. \quad (48)$$

Note that this corresponds to a particular choice of velocity of frame of reference, moving with the grain itself, and the results are independent of this choice.

This completes the model of the behaviour, and the equation of motion for the water in the swelling grain is

$$\frac{\partial \phi}{\partial t} = \nabla \cdot \left((1 - \phi) D_0 e^{\delta M} \frac{\nabla M}{M} \phi \right). \quad (49)$$

Using the relationship between M and ϕ in equation (43), we can express these equations in terms of either M or ϕ . Hence either

$$\frac{\partial}{\partial t} \left(\frac{M}{1 + (\rho_s/\rho_w)M} \right) = \nabla \cdot \left(\frac{D_0 e^{\delta M} \nabla M}{[1 + (\rho_s/\rho_w)M]^2} \right) \quad (50)$$

or

$$\frac{\partial \phi}{\partial t} = \nabla \cdot \left(D_0 e^{\delta \rho_w \phi / (\rho_s (1-\phi))} \nabla \phi \right). \quad (51)$$

When considering a particular problem to solve we take the grain to have an initial moisture content M_0 and we assume that the outer surface is kept at the moisture level M_1 . The equation must be solved inside the grain with this initial condition and boundary condition. The boundary condition, however, must be imposed on the outer surface which will move at a velocity given by

$$D_0 e^{\delta M} \frac{\phi}{M} \nabla M \cdot \mathbf{n}$$

where \mathbf{n} is the outward facing normal to the surface. The problem is therefore a moving boundary problem for a nonlinear diffusion equation.

8.2 Approximate solutions

In order to gain some insight into the behaviour of the water movement when there is swelling, we derive an approximate solution in a region of parameter space of physical interest. It appears that one of the main situations of interest to Uncle Tobys is when the moisture content is changed substantially, and in particular where the resulting water diffusivities at the initial M_0 level and at the M_1 level are significantly different, perhaps an order of magnitude different. We could formally consider this problem using matched asymptotic expansions. However, it is more instructive to outline the structure of the solution and indicate the different physical balances in the various regions. The analysis is not novel and has been done in various contexts elsewhere.

The basic structure of the solution is that the water moves into the region from the surface and because the diffusivity is such a strong function of the concentration the flux in the region immediately adjacent to the surface is nearly uniform. This uniform flux region extends until the concentration approaches the initial value where a narrow layer separates the region of constant flux from a region where there is no substantial change from the initial value. This transition layer has the form of a travelling wave and its position changes as the water moves into the grain.

To illustrate the structure consider the 1-D problem with the grain initially in the region $0 \leq x \leq L$ and the outer wetted surface at the point $x = R(t)$, with $R(0) = L$ and where $x = 0$ is a stationary point impermeable to water (to represent a line of symmetry). The problem is then

$$\frac{\partial}{\partial t} \left(\frac{M}{1 + (\rho_s / \rho_w) M} \right) = \frac{\partial}{\partial x} \left(\frac{D_0 e^{\delta M}}{[1 + (\rho_s / \rho_w) M]^2} \frac{\partial M}{\partial x} \right) \quad (52)$$

with

$$M = M_0 \text{ at } t = 0, \quad (53)$$

$$M = M_1 \text{ at } x = R(t), \quad (54)$$

$$\frac{\partial M}{\partial x} = 0 \text{ at } x = 0, \quad (55)$$

$$\frac{dR}{dt} = D_0 e^{\delta M_1} \frac{\rho_s}{\rho_s M_1 + \rho_w} \frac{\partial M}{\partial x}, \quad (56)$$

$$R(0) = L. \quad (57)$$

The relevant dimensionless groups within this problem can be identified by introducing the non-dimensional variables

$$\bar{x} = x/L, \quad \bar{R}(\bar{t}) = R(t)/L$$

$$\bar{M} = \frac{M - M_1}{M_1 - M_0}, \quad \bar{t} = \frac{D_0}{L^2} e^{\delta M_1} t.$$

Hence the problem becomes

$$\frac{\partial}{\partial \bar{t}} \left(\frac{\alpha + \bar{M}}{\gamma + \nu \bar{M}} \right) = \frac{\partial}{\partial \bar{x}} \left(\frac{e^{\beta \bar{M}}}{(\gamma + \nu \bar{M})^2} \frac{\partial \bar{M}}{\partial \bar{x}} \right) \quad (58)$$

with

$$\bar{M} = -1 \text{ at } \bar{t} = 0, \quad (59)$$

$$\bar{M} = 0 \text{ at } \bar{x} = \bar{R}(\bar{t}), \quad (60)$$

$$\frac{\partial \bar{M}}{\partial \bar{x}} = 0 \text{ at } \bar{x} = 0, \quad (61)$$

$$\frac{d\bar{R}}{d\bar{t}} = \frac{\nu}{\gamma} \frac{\partial \bar{M}}{\partial \bar{x}}, \quad (62)$$

$$\bar{R}(0) = 1. \quad (63)$$

Within these equations the non-dimensional parameters are

$$\alpha = \frac{M_1}{M_1 - M_0}, \quad \gamma = 1 + \frac{\rho_s M_1}{\rho_w}$$

$$\nu = \frac{\rho_s (M_1 - M_0)}{\rho_w} = \frac{\gamma - 1}{\alpha}, \quad \beta = \delta (M_1 - M_0)$$

and hence there are three separate non-dimensional groups to consider. For practical situations of interest the typical value of each of these parameters is between 0.5 and 3.

Because the parameter β is in the exponential it has a significant influence on the solution and the approximate solution described below can be generated by performing a large activation energy asymptotic analysis on the system in the limit $\beta \rightarrow \infty$.

The approximate solution is found by breaking the solution into two main regions. The first has $0 \leq x < \bar{s}(\bar{t})$ and is where no additional water has diffused while the second region $\bar{s}(\bar{t}) < x \leq \bar{R}(\bar{t})$ is where the flux is nearly constant. The interface between these regions is designated by $\bar{s}(\bar{t})$, which is the position of the wetting front.

Hence in $\bar{s}(\bar{t}) < x \leq \bar{R}(\bar{t})$ we have

$$\frac{e^{\beta \bar{M}}}{(\gamma + \nu \bar{M})^2} \frac{\partial \bar{M}}{\partial \bar{x}} \sim A(\bar{t}), \quad (64)$$

which integrates to give

$$\int \frac{e^{\beta \bar{M}}}{(\gamma + \nu \bar{M})^2} d\bar{M} \sim A(\bar{t})\bar{x} + B(\bar{t}). \quad (65)$$

The integral on the left-hand side of equation (65) is well-defined for \bar{M} in the range $[-1, 0]$, and is related to the exponential integral E_2 and to an incomplete gamma function.

This solution is required to satisfy the conditions

$$\bar{M} = 0 \text{ at } \bar{x} = \bar{R}(\bar{t}), \quad (66)$$

$$\frac{d\bar{R}}{d\bar{t}} = \frac{\nu}{\gamma} \frac{\partial \bar{M}}{\partial \bar{x}} \text{ at } \bar{x} = \bar{R}(\bar{t}), \quad (67)$$

$$\bar{R}(0) = 1, \quad (68)$$

and in addition either by a careful local analysis around $\bar{s}(\bar{t})$ or by conservation of mass at this point we also insist that it satisfy

$$\bar{M} = -1 \text{ at } \bar{x} = \bar{s}(\bar{t}), \quad (69)$$

$$\frac{d\bar{s}}{d\bar{t}} \left(\frac{\alpha}{\gamma} - \frac{\alpha - 1}{\gamma - \nu} \right) = -\frac{1}{\gamma^2} \frac{\partial \bar{M}}{\partial \bar{x}} \text{ at } \bar{x} = \bar{s}(\bar{t}), \quad (70)$$

$$\bar{s}(0) = 1. \quad (71)$$

The solution in the other region is $\bar{M} = -1$. So the problem reduces to one of solving the algebraic and ordinary differential equations for A , B , \bar{R} and \bar{s} . The full system is

$$g_2 \equiv \int_{-1}^0 \frac{e^{\beta y}}{(\gamma + \nu y)^2} dy = A(\bar{t})\bar{R}(\bar{t}) + B(\bar{t}), \quad (72)$$

$$\frac{d\bar{R}}{d\bar{t}} = \frac{\nu}{\gamma} A(\bar{t}), \quad (73)$$

$$0 = A(\bar{t})\bar{s}(\bar{t}) + B(\bar{t}), \quad (74)$$

$$\frac{d\bar{s}}{d\bar{t}} \left(\frac{\alpha}{\gamma} - \frac{\alpha - 1}{\gamma - \nu} \right) = -A(\bar{t}), \quad (75)$$

$$\bar{R}(0) = 1, \quad \bar{s}(0) = 1. \quad (76)$$

Simple manipulations result in the solution in the implicit form

$$E\bar{R} + F\bar{s} = E + F, \quad (77)$$

$$E\bar{R}^2 + F\bar{s}^2 = 2g_2\bar{t} + E + F, \quad (78)$$

where g_2 is defined above, and the constants E and F are defined to be

$$E \equiv \frac{\gamma}{\nu} = \frac{\rho_w + \rho_s M_1}{\rho_s (M_1 - M_0)} \quad (79)$$

and

$$F \equiv \frac{\alpha}{\gamma} - \frac{\alpha - 1}{\gamma - \nu}. \quad (80)$$

Equations (77) and (78) can be solved to obtain \bar{R} and \bar{s} explicitly as

$$(\bar{R} - 1)^2 = \frac{2Fg_2}{E(E + F)} \bar{t}, \quad (81)$$

and

$$(1 - \bar{s})^2 = \frac{2Eg_2}{F(E + F)} \bar{t}. \quad (82)$$

The dimensionless time for moisture to fully penetrate a one-dimensional swelling grain is the time when \bar{s} reaches zero, that is

$$\bar{t}^* = \frac{F(E + F)}{2Eg_2}. \quad (83)$$

The penetration time in seconds is given by

$$t_{\text{swelling}}^* = \frac{L^2}{D_0} e^{-\delta M_1} \frac{F(E + F)}{2Eg_2}. \quad (84)$$

Note that the form of this wetting time is the same as without swelling, relating time to the square of the length. The new feature is the dependence on E , F and g_2 , which in turn depend in a moderately complicated way on ρ_w , ρ_s , M_0 and M_1 .

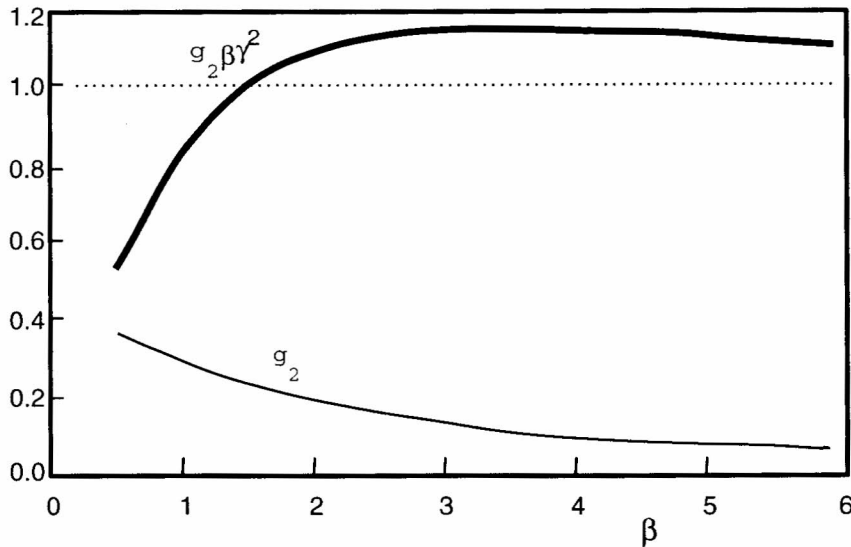


Figure 9: Sketch showing dependence of g_2 on β .

Note also that for large β , Laplace's method gives the leading behaviour $g_2 \sim 1/(\beta\gamma^2)$, $\beta \rightarrow \infty$. This approximation can be quite good even when β is only 3, as illustrated in Figure 9. The thin line shows g_2 when $\gamma = 1.7$ and $\nu = 0.5$, while the thick line shows $g_2\beta\gamma^2$, which is close to one when the leading behaviour is a good approximation.

When $M_1 = 0.5$, values for the parameters based on the corn starch properties listed in Table 2 are $\gamma = 1.7$, $\alpha = 1.4$, $\nu = 0.5$, $\beta = 3$, $E = 3.4$, $F = 0.5$ and $g_2 = 0.13$. Hence the time to penetrate a swelling grain of length L is $t_{\text{swelling}}^* = 50$ minutes. This is significantly longer than the time of 18 minutes from the nonlinear moisture diffusion model of Section 5, which makes no allowance for the effect of swelling.

This analysis can be extended to the case when the region is either cylindrical or spherical and this merely requires more algebra. In these cases we again do not need to consider the law governing the motion of the material. For more realistic shapes, including those with cusped initial shapes such as occur in real grains, more work is required accounting for the forces acting on the solid as well as approximating the solution to the model for the case $\beta \rightarrow \infty$. Such cases are of theoretical as well as practical interest since analysis around such cusps may indicate if such cusps remain or are smoothed out by the process.

9. A gelatinisation model

This model is directed at the present cooking process, with a temperature of about 140°C rapidly establishing throughout the grain, and moisture penetrating more slowly. At these high temperatures, gelatinisation is taking place at the wetting front. This is a chemical reaction, and focusing on this aspect leads to a different treatment of the advancing cooking front. The approach in this section is an approximate analytic technique.

The idea of the technique is to use steady state moisture content profiles on either side of the front, and is similar to that used in Carslaw and Jaeger (1959), p. 286. It depends on the gelatinisation process *holding up* the movement of the moisture front into the grain. The method used in this section is also quite similar to that of the previous section on grain swelling.

The grain is taken to be at a constant temperature. The nonlinear diffusion equation (11) describes the movement of moisture in regions excluding the gelatinisation front. This front is also the moisture front, and is assumed to be sharp. At this front, virgin starch is (irreversibly) gelatinised by the water arriving from the outside of the grain. Inside the front, there is not enough water to cause gelatinisation. Outside the front, there is no more virgin starch — it is all gelatinised. This sets the problem up with the usual Stephan conditions, with the one difference that the critical water content at which irreversible gelatinisation takes place is temperature dependent.

The reaction front is at the variable location $a(t)$. At the front,

$$M(a(t), t) = M_G(T), \quad (85)$$

a known value. Furthermore, the flux of water supplied by diffusion through the already gelatinised region has to be sufficient to gelatinise the virgin starch there, so that

$$f \frac{da}{dt} = -D \nabla M / M. \quad (86)$$

The left-hand side is the amount of water required to change virgin starch to gelatinised starch, f is a Stochis number (non-dimensional), and the right-hand side is as in expression (44), the velocity of water arriving at the front ($m^3/(m^2s)$). These two equations, together with

$$\frac{\partial M}{\partial t} = \nabla \cdot (D_0 e^{\delta M} \nabla M), \quad (87)$$

in $r > a$, and

$$M(b, t) = M_1, \quad t > 0, \quad (88)$$

$$M(r, 0) = M_0, \quad (89)$$

form the complete model, where b is the outer boundary of the grain.

9.1 Approximate solution, one-dimensional case

We use the steady state profile as a shape function to solve the problem approximately, in the case where the grain is one-dimensional. That is, we integrate

$$\frac{\partial}{\partial x} \left(D_0 e^{\delta M} \frac{\partial M}{\partial x} \right) = 0, \quad (90)$$

from the outer boundary at distance R to a distance x (and a moisture content M) to get

$$D_0 \left(e^{\delta M} - e^{\delta M_1} \right) = \delta A(x - R), \quad (91)$$

where A is a constant of integration. This satisfies the boundary condition (88) at $x = R$. Now A is chosen so that the boundary condition (85) at $x = a$ is satisfied,

$$A = \frac{D_0 \left(e^{\delta M_G} - e^{\delta M_1} \right)}{\delta(a - R)}, \quad (92)$$

so that the moisture profile is given by

$$\frac{e^{\delta M} - e^{\delta M_1}}{e^{\delta M_G} - e^{\delta M_1}} = \frac{x - R}{a - R}, \quad (93)$$

where $a(t)$ is determined by solving the remaining flux condition (86), which can be written

$$f M_G \frac{da}{dt} = -A. \quad (94)$$

Using the expression (92) for A , evaluated at $x = a$, then gives

$$\frac{da}{dt} = \frac{C_1}{a - R}, \quad (95)$$

where all constants have been gathered into

$$C_1 = \frac{D_0 \left(e^{\delta M_1} - e^{\delta M_G} \right)}{\delta f M_G}. \quad (96)$$

Equation (95) easily integrates to give

$$a^2 - 2Ra + R^2 - 2C_1 t = 0. \quad (97)$$

The constant of integration has been chosen to ensure $a = R$ when $t = 0$. The appropriate solution of this quadratic is

$$a = R - \sqrt{2C_1 t}. \quad (98)$$

The time to cook is when a reaches zero, that is,

$$t_G = \frac{R^2}{2C_1} = \frac{R^2 f M_G \delta}{2D_0 (e^{\delta M_1} - e^{\delta M_G})}. \quad (99)$$

We can estimate $f = 1$ from the observation that the volume of water taken up by the grain is about the same as the original grain volume. Note that this gives the same sensitivity of wetting time to the parameters R , D_0 and δ , as that obtained from equation (23) for the maximum mean action time. If the association

$$\frac{M_G}{2} \equiv (M_1 - M_0)\Phi_G$$

is made, then both expressions (99) and (23) for wetting time are the same.

The present process has a temperature of about 140°C, which corresponds to $M_G = 0.33$ according to Figure 1. The value to use for M_1 is not accurately known. It will be at least 0.6, so that value will be used here. The value for D_0 depends on temperature, as noted in Section 6, but it is not clear exactly what this dependence is. Values for an effective diffusivity have been calculated at Uncle Tobys from experiments with wetting rice grains. The way these are calculated, by fitting linear diffusivity to experimental results, suggests that they should be the same as D_{equiv} in equation (25). More work is needed to properly incorporate these experimental results into this analysis.

If the value of D_0 for a temperature of 40°C is used, the penetration time for the present process, for a typical grain, is $t_G = 16$ minutes. This is very close to the results obtained in the previous models, but more work is needed before meaningful comparisons can be made.

It is useful to refer here to other work, particularly that of Stapley (1995), comparing the models of Suzuki *et al.* (1977) and Cabrera *et al.* (1984). Stapley uses NMR imaging techniques to track moisture penetration into the grain.

10. Conclusions

Four models have been presented and solved for the movement of heat and moisture into whole cereal grains.

Heat is found to penetrate a grain in about 5 seconds, according to a simple linear diffusion model.

Moisture movement at temperatures below gelatinisation has been treated as a nonlinear diffusion problem in the second model, leading to penetration

times of about 20 minutes. The concept of mean action time allows analytic solutions, and leads to formulae for the volume of grain cooked, and for the degree of overcook of a grain, versus time.

A third model allows for the effect of grain swelling, which slows down moisture penetration by about 10%.

The fourth model, incorporating the high temperatures used in the present process, allows for the effect of gelatinisation slowing down moisture penetration along a sharp front.

The third and fourth models are still under development, and need more work.

All models identify relevant parameters, and give the sensitivity of cooking times to the parameters.

Our recommendation to Uncle Tobys is that grains be presoaked at a temperature that is just high enough for the moisture level to equilibrate at the desired level. We estimate typical soaking times to be about 20 minutes. Then the wet grains can be heated at a temperature that is set at T_{gel} . The heating time should be quite short, as an individual grain is expected to heat through in about 5 seconds. Such a process will allow a grain to be fully cooked, and will minimise the degree of overcook.

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