Computer Simulation of Flavor Release from Solid Foods in the Mouth

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A computer simulation describing flavor release from solid foods in the mouth is presented. The rate-limiting step for flavor release is assumed to be the transport of flavor volatiles across the food−saliva interface, which can be described by the stagnant-layer theory of mass transfer. Saliva flow, mastication, and swallowing are incorporated into the model. The mastication process is simulated by introducing selection and breakage functions to generate particle size distributions after each chew. The results predict that the initial rate of flavor release primarily depends on the mass transfer coefficient and the fracture mechanics of the food, which, in turn, depend on the food's structure and composition. In contrast, an individual's mastication and swallowing pattern greatly influences the rates of flavor release at longer times.

Keywords: *Interfacial mass transfer; swallowing; saliva; partitioning; mastication*

INTRODUCTION

The past few years have seen rapid progress in the development of mechanistic models of flavor release from foods in the mouth (de Roos and Wolswinkel, 1994; Hills and Harrison, 1995; Harrison and Hills, 1996; Harrison et al., 1997). The ultimate goal of these efforts is to be able to mathematically predict the effect of varying food composition, food structure, and mastication behavior on the perceived time−intensity flavor release profile. If successful, it would then be possible to use computer simulations to formulate foods for a desired flavor profile, taking into account individual or group differences in mastication behavior.

The first step in achieving this goal is understanding the physical mechanism of aroma release from the food into the saliva and mouth headspace. Formulating these release mechanisms for solid or semisolid foods is somewhat more difficult than for liquids due to the added complication of a matrix, which first has to be broken down so that the flavors can be released into the saliva. Despite these difficulties, models have been developed to predict flavor release from foods that dissolve (Hills and Harrison, 1995) and melt (Harrison and Hills, 1996) in the mouth. These models were developed for the ideal case of spherically shaped foods, which retain their initial form as they disintegrate and reduce in size.

Although these models have been developed for simple bulk foods, they have revealed two important points: first, that the rate-limiting step for flavor release for solid and semisolid foods is mass transfer of the volatiles across the solid−liquid (de Roos and Wolswinkel, 1994; Hills and Harrison, 1995) and liquid−gas interfaces (Harrison et al., 1997; Bakker et al., 1998), respectively; second, that the rate of release across the interfaces is proportional to the mass transfer coefficient and the interfacial surface area (Hills and Harrison, 1995).

Modeling the effects of in-the-mouth mastication is a much more challenging task and is one of the primary objectives of this paper. We need to incorporate the effect of saliva flow into the oral cavity (Harrison, 1998), increase in surface area during mastication (Hills and Harrison, 1995), swallowing (Prinz and Lucas, 1995), and transport of flavor volatiles to the olfactory epithelium (Harrison and Hills, 1997a).

The theoretical headspace concentration profiles can be tested experimentally with both instrumental and sensory methods. Until recently, most instrumental analysis has been confined to measuring the aroma concentrations in the headspace above the food. Although these techniques have revealed a great deal of information on flavor release, they do not investigate the physical changes occurring during eating. It is well-known that the eating process changes the amounts and nature of chemicals in foods. For example, when cellular foods are eaten, certain flavors undergo an enzymatic change once the cells have been ruptured (Linforth et al., 1994). Recent developments, however, now permit monitoring of aroma compounds at extremely low concentrations passing out of the nose breath-by-breath during eating (Taylor and Linforth, 1994).

Predicting and measuring the concentration−time profiles of aroma compounds in the mouth headspace is, of course, only part of the complex physiological and psychological process conveniently labeled "flavor perception". The perception of a volatile compound depends on the concentration of the compound, threshold levels of the individual, and duration of exposure. An individual's perception of a particular food product will therefore primarily depend on the amounts and rates of volatile release from the food matrix; however, the overall perception will also depend on cognitive factors, such as pattern recognition and mood.

Sensory panels are often employed and trained to perceive certain characteristics of a food during eating. Subjects are usually asked to record their perception of a particular flavor attribute with time by moving a

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pointer between the extremes of zero and maximum flavor perceived. In general though, due to large variations among subjects, it is often difficult to analyze the data produced. It is easier, and more informative, to compare the differences between similar food products for one particular individual. More recently, EMG mastication and swallowing patterns have been used in conjunction with sensory techniques (Wilson and Brown, 1997). This approach has revealed that the perceived flavor of a food depends greatly on how an individual interacts with the food as well as the initial flavor composition.

Such individual differences are important and, at least in principle, can be explored theoretically. As a first step all that is required is a mathematical relationship between the "perceived" response and the concentration of aroma in the headspace. Stevens' law (Overbosch et al., 1991) is one example of this type of relationship that could be used to calculate perceived time−intensity profiles from theoretical concentration−time profiles.

In this paper we therefore present a computer simulation of aroma release from foods in the mouth, which incorporates saliva flow, mastication, and swallowing behavior. For simplicity we focus on solid and semisolid foods that, on fragmentation, retain their shape and do not further disintegrate and mix with saliva. Other categories of food matrix will be analyzed in subsequent papers. For initial simplicity we leave the simulation output in the form of an aroma concentration−time profile in the oral cavity. Subsequent processes, such as aroma transport to the olfactory epithelium and the relationship to the "perceived" sensory response, are left for later developments.

GENERAL FLAVOR RELEASE MODEL

Transport of flavor volatiles from the food product to the gaseous phase is essentially a three-phase problem involving the food, saliva, and air phases. The rate-limiting step for flavor release into the headspace is assumed to be mass transfer across the macroscopic solid−liquid interface. During eating the surface area of the food increases dramatically, therefore allowing a greater proportion of the flavor to be released from the matrix into the surrounding saliva. For foods possessing a well-defined surface, transfer of flavor volatiles across the interface can be described by the stagnant-layer theory of interfacial mass transfer (Hills and Harrison, 1995). Once in the aqueous phase the concentration of volatiles will be diluted by saliva flow into the oral cavity. At the same time, volatiles partition from the saliva into the gas phase that then transports them to the olfactory epithelium. In addition to removing sufficiently comminuted food, swallowing aids the transport of volatiles to the olfactory epithelium by coating the airways with flavor-enriched saliva.

In this section we therefore discuss the ideas behind our computer simulation and present mathematical descriptions of the effects of saliva flow, mastication, and swallowing.

Saliva Flow. It is well-known that the sight of food can stimulate the salivary glands to increase the rate of saliva flow into the oral cavity from an average of 0.5 mL/min to ≈3−4 mL/min when stimulated, thereafter decreasing exponentially to the base value of 0.5 mL/min (Dawes and MacPherson, 1992). However, in our simulation we assume, for simplicity, that the saliva flow rate, Q, is constant and in the range 1−4 mL/min. Saliva, once released into the oral cavity, performs a number of important functions that assist flavor release. First, it provides lubrication by forming a thin aqueous layer around the food and mouth; second, it aids in the breakdown of the food microstructure through a variety of mechanisms both enzymatically and physically, for example, hydration. Finally, it provides an intermediate medium for flavors to pass through as they are transported from the food to the gaseous phase.

Mastication. The primary purpose of mastication is to transform the ingested food into a form that is easily swallowed and later digested. The breakdown can be considered the composite result of two physical processes, selection and breakage (Lucas and Luke, 1983; Voon et al., 1986).

Selection. Selection is defined as the chance that a food particle is placed between the teeth and is either completely or partially damaged during the chewing cycle. Selection of a particular particle depends on a number of factors. These include movements of the jaw, tongue, and cheeks to load particles onto the working surfaces of the teeth; the occlusal area of the postcanine teeth; the number of teeth in relation to the distribution of particle sizes in the mouth; and the ability of the tongue and cheeks to prevent food particles from falling into inaccessible areas of the oral cavity (Thexton, 1992).

The chance of selecting a particle of a particular size, x, can be described mathematically by a power law relationship

$$S(x) = k_1(x/x_0)^{\beta} \tag{1}$$

where k_1 is a constant and x_0 is the initial size of the food. Increasing the exponent β means a greater chance of selecting large particles rather than small ones.

Breakage. Once selected, a particle may or may not break into smaller fragments. Breakage of the food matrix is clearly a characteristic of the product material. However, fragmentation of the matrix also depends on the shape of the particle distribution in relation to the occluding surfaces and probably also on the rate and extent at which the load is applied. The fragmentation of a parent particle can again be described mathematically by a power law relationship

$$B(y,x) = k_2(y/x)^{\alpha} \tag{2}$$

where k_2 is a constant and y/x is the ratio of the fragment size relative to the parent particle size. The exponent α determines the degree to which the particles fragment: a small value of α denotes a greater degree of fragmentation on breakage.

Particle Size Distributions. The repeated selection and breakage processes that occur during mastication produce a distribution of particle sizes. If the percentage of the total volume of size x to $x + dx$ before the nth chew is $P_{n-1}(x)\,dx$, then the percentage of particles below size y after the nth chew is given by (Voon et al., 1986)

$$Q_n(y) = \int_y^{\infty} P_{n-1}(x)B(y,x)S(x)\,dx + \int_0^y P_{n-1}(x)\,dx \tag{3}$$

where the second term on the right-hand side represents the percent of particles that exist below size y in the ingested foodstuff before the nth chew. The percentage of particles of size x to $x + dx$ before the $(n + 1)$th chew,

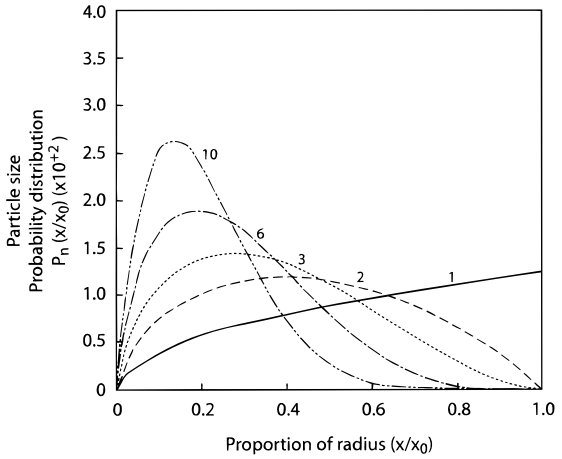

Figure 1. Probability distributions for particle size $P_n(x)$ as a function of number of chews as generated from eqs 3−9.

that is, $P_n(x)\,dx$, can be obtained from the following:

$$P_n(x) = \frac{dQ_n(x)}{dx} \tag{4}$$

The integrals in eq 3 are evaluated numerically using Simpson's rule to generate values of $Q_n(x)$. Particle size distributions, $P_n(x)$, were then obtained by numerically evaluating eq 4 with a finite difference method

$$P_n(x) = \frac{dQ_n(x)}{dx} = \frac{Q_n(x+1) - Q_n(x-1)}{2\delta x} \tag{5}$$

with the appropriate boundary conditions:

$$P_n(0) = 0 \qquad \forall\ n \tag{6}$$

and

$$P_n(x_0) = 0 \qquad \text{for } n \geq 1 \tag{7}$$

Initially, the probability, $P_0(x)$, of finding a particle of size x, before chewing begins, is defined as

$$P_0(x) = 0 \qquad \text{for } x < x_0 \tag{8}$$

and

$$P_0(x) = 1 \qquad \text{for } x = x_0 \tag{9}$$

Each time a chew occurs the integer n is incremented and a new $P_n(x)$ distribution is generated using eqs 3−5. An iterative computer simulation was written to generate the particle size distributions. Figure 1 shows a set of typical particle size distributions, $P_n(x)$, as a function of the chew number, n. As expected, with successive chews there is a definite shift in the maximum of the $P_n(x)$ distribution toward smaller particles sizes. Furthermore, Figure 1 shows that the width of particle sizes decreases with an increasing number of chews. This result indicates that, as the mastication proceeds, the teeth become less efficient at breaking down the smaller particles.

As new surfaces are created and covered with a thin film of saliva, flavor is released from the food matrix into the surrounding aqueous phase. This process can be described by the stagnant-layer theory of interfacial mass transfer (Hills and Harrison, 1995), which results in the expression

$$\frac{dM}{dt} = h_D A_{sf}\left[c_f - \frac{c_s(t)}{K_{sf}}\right] \tag{10}$$

where M is the total mass of volatile diffusing across the interface, h_D is the mass transfer coefficient, A_{sf} is the surface area of the saliva−food interface, K_{sf} is the saliva−food partition coefficient, and c_f and c_s denote the concentration of flavor in the food and saliva, respectively.

Equation 10 predicts that the rate of flavor release is proportional to the surface area of the food. If it is assumed that all fragments produced during mastication are spherical, it is possible to calculate the total surface area of the food in the mouth as

$$\text{total surface area of food in mouth, } A_{food} = (\text{av surface area, } A_{av}) \times (\text{no. of particles, } N) \tag{11}$$

where

$$A_{av} = \frac{4\pi}{3}\int_0^{x_0} x^2 P_n(x)\,dx \tag{12}$$

and

$$\text{no. of particles, } N = \frac{\text{volume of food remaining in the mouth, } V_{food}}{\text{av particle volume, } V_{av}} \tag{13}$$

with

$$V_{av} = \frac{4\pi}{3}\int_0^{x_0} x^3 P_n(x)\,dx \tag{14}$$

The volume of food remaining in the mouth, V_{food}, is calculated by the integral

$$V_{food} = V_0\frac{4\pi}{3}\int_0^{x_0} P_n(x)\,dx \tag{15}$$

where V_0 is the initial volume of food consumed. The integral in eq 15 is again evaluated numerically using Simpson's rule.

Swallowing. After a succession of chews, the distribution of particle sizes in the mouth will shift toward smaller particle sizes. Combined movements by both the tongue and teeth then select the larger particles present and retain them for further mastication, while the smaller particles are transported to the back of the oral cavity where they are swallowed. We therefore assume that particles of less than a critical size, x_c, constitute the bolus so that after a swallow the probability of finding a particle below the size x_c is 0 (Figure 2)

$$P_n(x \leq x_c) = 0 \tag{16}$$

On swallowing, a quantity of saliva will also be removed from the oral cavity. For simplicity we assume that after swallowing the volume of saliva in the mouth returns to the base level, V_0. In addition, swallowing will remove a proportion of dissolved flavor from the oral cavity, although the flavor concentration in the saliva will remain constant. The mass of flavor remaining in the oral cavity after swallowing is therefore given as

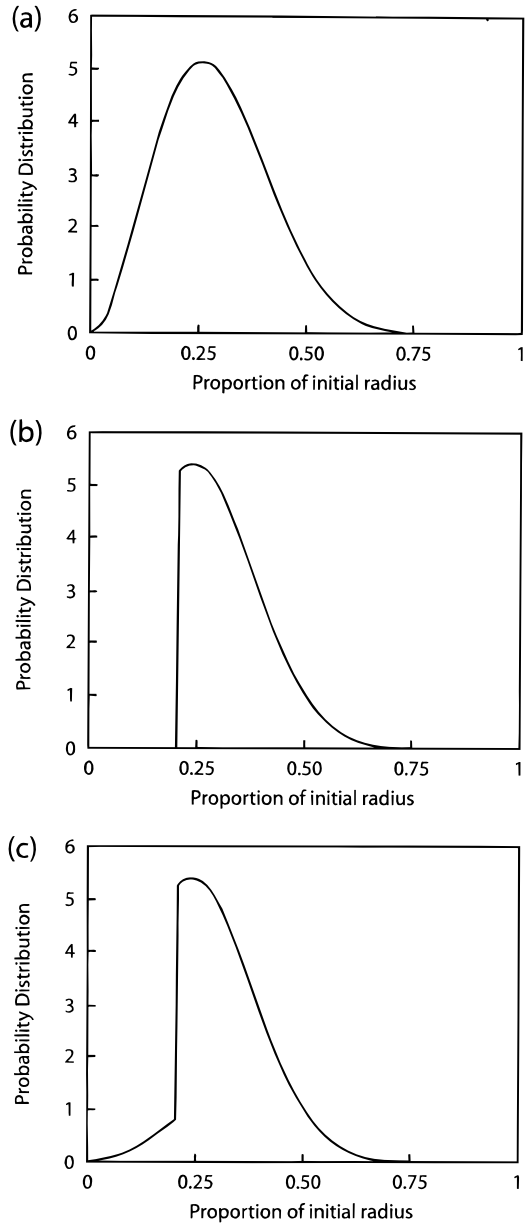

Figure 2. Schematic diagram to represent swallowing of particle sizes, x, smaller than the threshold, x_c. After a succession of chews, the particle size probability distribution shifts toward the smaller sizes (a). Prior to swallowing, the smaller particles are transported to the back of the oral cavity and swallowed (b). During the proceding chew the remaining large particles that were not swallowed are fragmented (c).

$$\text{mass of flavor in saliva after a swallow} = \frac{\text{vol of saliva after a swallow}}{\text{vol of saliva before a swallow}} \times (\text{mass of flavor in saliva before a swallow}) \quad (17)$$

SIMULATION ALGORITHM

Having mathematically described the effects of saliva production, mastication, and swallowing we can now incorporate them into a computer simulation of the time course of flavor concentration in the gaseous phase, $c_g(t)$, released from a solid food. It should be noted that at this stage the simulation is a physicochemical model and ignores the psychological and physiological steps of flavor perception. However, it should be straightforward to incorporate certain aspects of perception, such as threshold concentrations and pattern recognition into future versions.

Table 1. Parameters and Corresponding Values Used in the Simulation

parameter	description	value
V_s	initial saliva volume	1 mL
Q	saliva flow rate	3 mL/min
h_D	mass transfer coefficient	5×10^{-8} m/s
K_{sf}	saliva−food partition coefficient	1×10^{-3}
K_{gs}	gas−saliva partition coefficient	6.4×10^{-3}
α	breakage function exponent	1.5
β	selection function exponent	1.5
x_0	initial radius of ingested food	10 mm
x_c	threshold radius for swallowing	2 mm
Δt	incremental time step	0.05 s

Initialization. First, the data files containing the chewing and swallowing times for each individual are input into the simulation and stored in arrays. Other parameters, such as mass transfer and partition coefficients, are input from separate data files and stored as constants. All of the parameters used in this simulation are listed in Table 1 and unless otherwise stated will take on the values tabulated. It is assumed that at zero time the food is placed into the mouth and immediately coated with saliva. Furthermore, it is assumed that the concentration of flavor in both the aqueous and gaseous phases is zero. The simulation commences by incrementing the time, t, by Δt.

Main Simulation Loop. After each time step, the time, t, is incremented and then compared to the chew and swallow times stored in the input arrays. There are three possible outcomes: First, if t corresponds to a chew time, then a new particle probability distribution is evaluated using eqs 3−5 and the total surface area of the food is recalculated using Simpson's rule. Second, if t corresponds to a swallow time, then all particles of sizes smaller than the threshold, x_c, and a proportion of the flavor-enriched saliva are removed from the oral cavity. Again the total surface area of the food has to be recalculated, unless of course the food is completely removed from the mouth. Finally, if t corresponds to neither a chew nor a swallow time, then the volume of saliva is simply incremented by $Q\Delta t$ and the total surface area of food remains constant.

Having calculated the total surface area of the food in the mouth, $A_{sf}(t)$, it is used to compute the mass of flavor, ΔM_s, released from the food into the saliva during the time interval Δt using Euler's approximation of eq 10:

$$\Delta M_s = A_{sf}(t) h_D \left[c_f - \frac{c_s(t)}{K_{sf}} \right] \Delta t \quad (18)$$

The mass of flavor in the saliva is then incremented by ΔM_s and used to recalculate the flavor concentration in the saliva, $c_s(t)$

$$\text{concn of flavor in saliva} = \frac{\text{mass of flavor in saliva}}{\text{vol of saliva}} \quad (19)$$

which then partitions into the gas phase to provide $c_g(t)$:

$$c_g(t) = K_{gs} c_s(t) \quad (20)$$

Note that this assumes instantaneous equilibrium partitioning from the saliva into the gas phase so that the rate-limiting step is release from the food into the

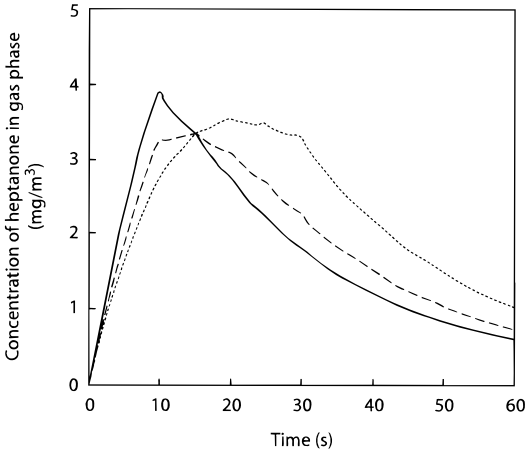

Figure 3. Time-dependent release profiles of heptanone as a function of the exponent α in the breakage function: α = 2, solid line; α = 3, dashed line; α = 4, dotted line.

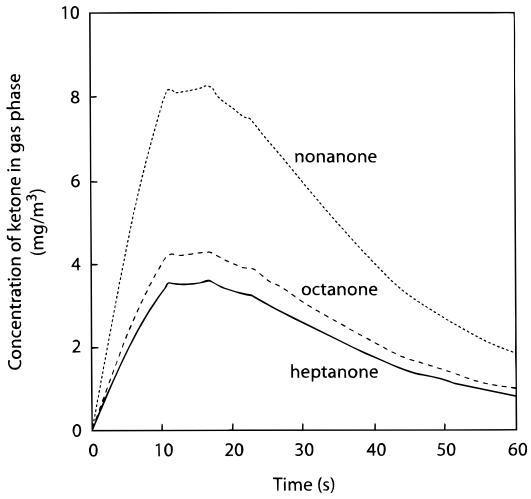

Figure 4. Time-dependent release profiles of three ketones released in the mouth.

saliva. However, this is not a necessary assumption, and more sophisticated rate expressions can be considered. Once the new $c_g(t)$ has been computed, t can be incremented by Δt repeatedly until the food has been cleared from the mouth, at which point $A_{sf}(t)$ is set to zero. In the absence of food, volatiles will still be released into the gaseous phase from the flavor-enriched saliva coating the oral cavity. Further saliva flow will dilute the remaining flavor, and subsequent swallows will remove the remaining flavors from the mouth. The simulation was developed in a Windows environment using a commercial software package (Microsoft Visual C++, v 1.0) so that multiple outputs could be viewed simultaneously. The simulation had a CPU time of approximately 60 s.

THEORETICAL ANALYSIS

There are large numbers of parameters in the model that can be varied and which result in differing flavor release profiles. These parameters can be separated into two groups: first, those that are related to the nature of the food, such as its composition, structure, and flavor content; and second, those that predict the eating behavior of individuals. In this section we will examine the effects of varying these parameters on the time-dependent flavor release profiles in the mouth.

Food Composition. The computer simulation allows us to examine the effects of varying the internal characteristics of the food, such as its structure fragmentation behavior and flavor composition, on volatile release. The fracture mechanics of the solid food will determine the rate of surface area increase during mastication. In our model the breakage function (eq 2) determines the degree of fragmentation. Increasing the value of the parameter α in eq 2 corresponds to a slower rate of surface area increase and hence reduced rates of flavor release (Figure 3). Furthermore, foods that easily fracture will break down into particles smaller than the threshold size more quickly. Such foods will reside in the mouth for shorter periods of time, and therefore the total quantity of flavor released is likely to be less than for foods that remain in the mouth for longer periods of time.

Flavors will also be released from the food into the saliva at different rates depending on their partition and mass transfer coefficients. Figure 4 predicts the time-dependent release curves of three ketones of increasing hydrophobicity (heptanone, octanone, and nonanone). As expected, the more hydrophobic compounds are released at a faster rate and to a greater extent than the less hydrophobic volatiles. In this calculation it has been assumed that the mass transfer coefficient, h_D, is constant for all volatiles. However, in reality this may not be the case, as the mass transfer coefficient is greatly dependent on the diffusion coefficients, which may vary among volatiles.

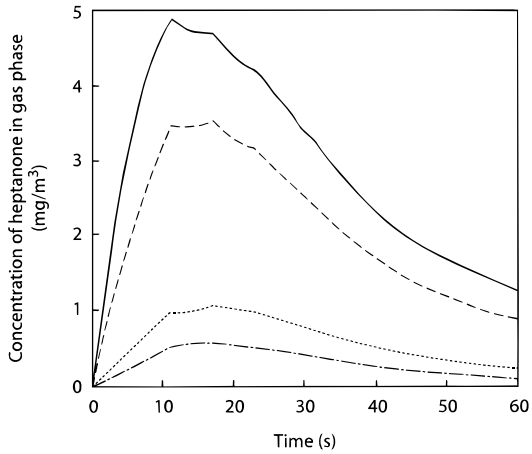

Figure 5. Time-dependent release profiles of heptanone as a function of the mass transfer coefficient: $h_D = 5 \times 10^{-8}$ m/s, solid line; $h_D = 1 \times 10^{-8}$ m/s, dashed line; $h_D = 5 \times 10^{-9}$ m/s, dotted line; $h_D = 1 \times 10^{-9}$ m/s, dotted−dashed line.

The mass transfer coefficient is also extremely sensitive to the viscosity of the liquid phase. Increasing the viscosity of the liquid phase will increase the thickness of the stagnant layer adjacent to the solid food and therefore decrease the mass transfer coefficient. Figure 5 predicts that the rate and extent of the release of flavor from the food product is extremely sensitive to the mass transfer coefficient. In this example we have assumed a constant h_D and that, once fragmented, no other constituents of the food matrix are released into the saliva. However, in reality, as the food matrix disintegrates, lipids and macromolecules are released into the saliva, thereby increasing the saliva viscosity and decreasing h_D. It should also be possible to incorporate these complications into the computer simulation. The ability to predict the effect of varying composition on flavor release profiles is obviously of great

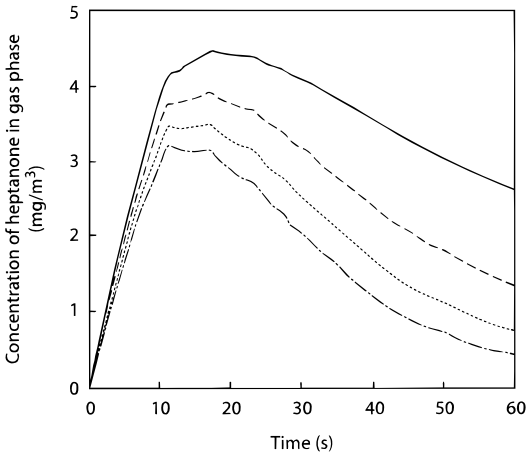

Figure 6. Time-dependent release profiles of heptanone as a function of the saliva flow rate: $Q = 1$ mL/min, solid line; $Q = 2$ mL/min, dashed line; $Q = 3$ mL/min, dotted line; $Q = 4$ mL/min, dashed−dotted line.

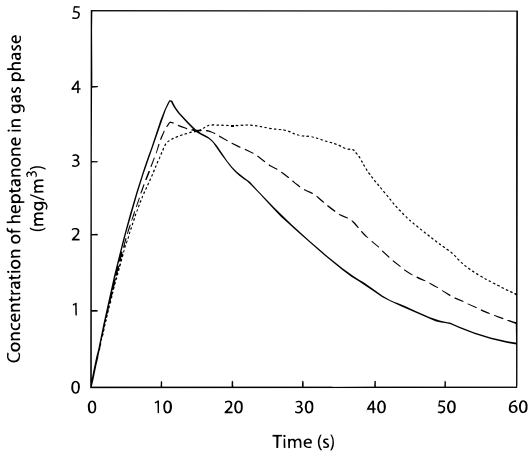

Figure 7. Time-dependent release profiles of heptanone as a function of the exponent β in the selection function: $\beta = 1.5$, solid line; $\beta = 2.5$, dashed line; $\beta = 4$, dotted line.

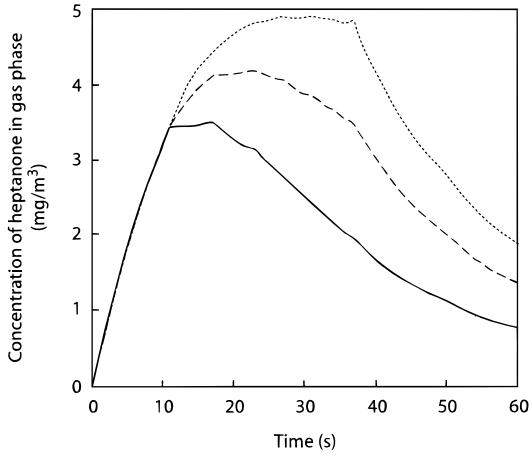

Figure 8. Time-dependent release profiles of heptanone for three swallowing threshold particle sizes: $x_c = 3$ mm, solid line; $x_c = 2$ mm, dashed line; $x_c = 1$ mm, dotted line.

importance to food companies, especially when developing new products. However, another aspect of the simulation that could be important is its ability to examine the differences in eating behavior among individuals. This is achieved by reading in chewing and swallowing times from mastication patterns (Wilson and Brown, 1997) acquired during eating.

Flavor Release from Individual Subjects. EMG studies on mastication provide a record of the exact chewing and swallowing times for an individual, and this can be read as input into the simulation. With this in vivo information, it is then possible to predict the total surface area of the food and hence the time-dependent flavor release profile for the individual. In this section we will therefore focus on differences in eating behavior among individuals and in particular the effects of different chewing and swallowing rates. First, however, we examine the differences in saliva flow rate on flavor release.

Figure 6 predicts time-dependent release curves of heptanone for a range of saliva flow rates (1−4 mL/min). At short times, the rate of heptanone release from solid foods is independent of the saliva flow rate. Similarly, it has been predicted that at short times the rate of flavor release from liquid foods is independent of the saliva flow rate (Harrison, 1998). At the time of the first swallow (10 s) there is an observable difference in the gaseous volatile concentration, and soon after a maximum concentration is observed. The maximum concentration is found to depend on the saliva flow rate: increasing Q dilutes the flavor in the saliva to a greater degree and hence decreases the maximum concentration. Thereafter, increasing Q induces more frequent swallowing, thereby flushing the flavor-enriched saliva from the oral cavity.

Mastication of a food increases the total surface area available for flavors to diffuse from the matrix into the surrounding saliva. The rate of increase of surface area for a particular food is determined by the efficiency of the individual at selecting larger particles for breakage and the rate at which they are chewed. In this model, the selection function (eq 1) describes the efficiency of the individual at selecting larger particles. Decreasing the value of the parameter β in eq 1 increases the efficiency of the selection process. Figure 7 predicts the effect of increasing β on the time-dependent flavor release profiles. For efficient particle selectivity (small β) the food is rapidly fragmented, producing a rapid rate of heptanone release followed by a sharp maximum at the first swallow. The efficient selectivity enables the food to be quickly broken down into particles smaller than the threshold size and, on swallowing, the majority of the food is removed from the oral cavity. Furthermore, the ability to swallow larger food particles greatly reduces the time that food is retained in the mouth (Figure 8). Conversely, for poor particle selectivity (large β) the food matrix is broken down more slowly, and thus the food will reside in the oral cavity for a longer period of time, allowing greater quantities of flavor to be released.

Increasing the chewing frequency also increases the rate at which new surfaces are created and, hence, the quantity of flavor released (Figure 9). Figure 9 shows that initially the rate of flavor increase is independent of the chewing frequency, but as the total surface area increases at longer times, a greater proportion of flavor is released. At longer times, however, it is extremely difficult to draw any conclusions except that, for the slower chewing frequencies, food remains in the mouth for longer periods of time. In this calculation we have assumed that all subjects swallow simultaneously at regular intervals, the last of which was after 30 s. This calculation is somewhat artificial as it is highly unlikely that under normal eating conditions individuals would swallow the same product simultaneously, except of

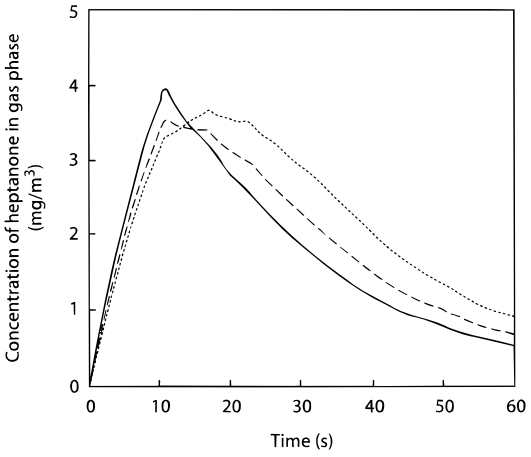

Figure 9. Time-dependent release profiles of heptanone for three chewing rates and simultaneous swallowing: two chews per second — solid line; one chew per second, dashed line; one chew every 2 seconds, dotted line.

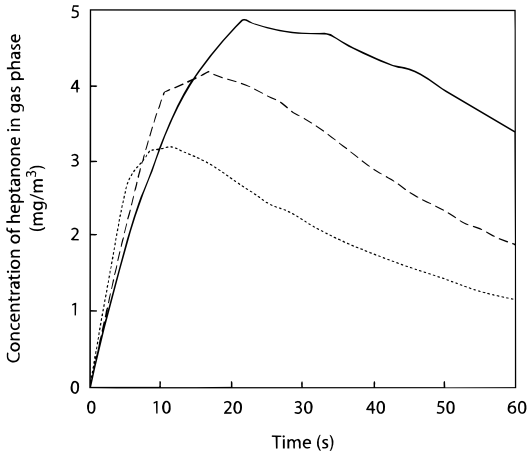

Figure 10. Time-dependent release profiles of heptanone for three chewing rates and swallowing after specified number of chews: two chews per second, solid line; one chew per second, dashed line; one chew every 2 seconds, dotted line.

Table 2. Mastication Pattern Used in Figure 10

10 chews, swallow, 5 chews, swallow, 5 chews, swallow, 3 chews, swallow, 3 chews, swallow, 2 chews, swallow, 2 chews, swallow, and thereafter swallows every 10 s

course under controlled conditions. In reality, individuals swallow when the food has been reduced to a certain consistency with an adequate amount of saliva to provide lubrication to aid swallowing.

Figure 10 shows time-dependent flavor release profiles for the same three chewing rates used in Figure 9; however, in this simulation each curve was plotted using the mastication pattern listed in Table 2. In contrast to Figure 9, the curves in Figure 10 are all very similar to one another in shape. Again at short times the chewing frequency has little influence upon the initial rate of flavor release. Both the maximum concentration and the time to reach this point increase with decreasing chew rate, indicating that the longer food resides in the mouth, the greater the quantity of flavor released into the gaseous phase.

Clearly, it will be important to test these predictions with real experimental data. On-line mass spectrometry (Taylor and Linforth, 1994) could be employed to monitor the concentrations of flavor volatiles in the mouth as they are released during eating. This coupled with EMG studies on mastication patterns (Wilson and Brown, 1997) would yield chewing and swallowing times that could be fed into the computer simulation. Combining the above techniques simultaneously with sensory time–intensity studies would assist in understanding the link between the concentrations of flavor passing the olfactory epithelium and perception. Together this collection of techniques would provide a more comprehensive understanding of flavor release in the mouth during eating.

CONCLUSIONS

In this paper we have presented a mathematical model of flavor release from solid foods in the mouth. It is assumed that transport of flavor volatiles from the food product to the gaseous phase is essentially a three-phase problem involving saliva as the intermediate medium. The rate-limiting step for release is assumed to be the transport of volatiles across the solid–liquid interface, which can be described by the stagnant-layer theory of interfacial mass transfer. This theory requires that the interfacial area between the food and saliva be known during eating. Therefore, mathematical descriptions of the physical processes occurring during eating, such as saliva flow, mastication, and swallowing, have been incorporated into the model. An estimate of the total surface area of the food can be obtained by using selection and breakage functions to generate particle size distributions after each chew. From these distributions the total surface area can be calculated. Once released into saliva, volatiles are then free to partition into the gas phase.

Our simulation can be used to examine both the effects of food composition and differences in eating behavior between individuals on flavor release from solid foods. In general, our results also predict that the initial rates of flavor release are less sensitive to the chewing frequency and saliva flow rate but extremely dependent on the fracture mechanics of the food and mass transfer coefficient. This result implies that primarily the structure and composition of the food determine the initial rate of flavor release.

At longer times the eating behavior of an individual begins to influence the flavor release rates. Increasing either the chewing frequency or the efficiency of particle selection increases the rate at which new surfaces are created and therefore the rate of flavor release into the saliva phase. The maximum flavor concentration in the gaseous phase depends on a number of factors, such as mass transfer and partition coefficients, selection efficiency, and chewing and swallowing frequencies. Sensory studies suggest that an individual's perceived maximum flavor intensity coincides approximately with the first swallow; however, our calculations predict that maximum flavor concentration in the oral cavity may occur later for some subjects. We found that the time to reach maximum flavor concentration in the mouth depends on many factors, such as saliva flow rate, chewing frequency, and swallow thresholds, in a complex way. These factors also influence the time that food remains in the mouth. Furthermore, once the food has been completely removed from the mouth, the flavor-enriched saliva will continue to release volatiles into the oral cavity.

This paper has focused on the effects of saliva flow, mastication, and swallowing on flavor release from solid foods in the mouth. This model, however, has only

considered solid food that, once fragmented by the teeth, does not disintegrate into the surrounding saliva. A more realistic simulation will need to focus on the microscopic breakdown of the food matrix. This may occur through a number of mechanisms, such as dissolution (Hills and Harrison, 1995), melting (Harrison and Hills, 1996), or hydration (Ingham et al., 1995) of the food matrix. As the food microstructure breaks down, the saliva viscosity will increase, therefore reducing the rate at which volatiles are released from the food product. Furthermore, flavor volatiles released from the food matrix will bind to macromolecules (Harrison and Hills, 1997b) and partition into lipids (Harrison et al., 1997), therefore reducing the free flavor present in the saliva and hence available for perception. These aspects of flavor release in the mouth will be the subjects of future papers.

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