A discrete population balance to simulate the particle size distribution in a bolus of chewed rice

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ABSTRACT

In this work, a discrete element method (DEM) model is developed to simulate the particle size distribution in a rice bolus as a function of chew number. Comparisons are made to the results from a single human subject study. The model uses the selection function developed by van der Glas et al. [7] based on two-way competition between particles for breakage sites in the occlusal zone. The breakage function is based on a cleavage-pasting mechanism proposed in this work. The model simulation produces distributions similar to the experimental data. The rice bolus produces a bi-modal distribution of particles which can be fitted by a mixed Weibull distribution. In the early stages of chewing most of the bolus volume is comprised of large particles with a $d_{50}$ of approximately 2000 μm, the distribution of smaller particles has a median size approximately 300 μm. The minimum point between the two distributions remains relatively unchanged throughout mastication. As mastication progresses there is a near constant volume flux between the two distributions, this result indicates that the desire to continue chewing maybe dictated by the proportion of particles above this minimum size between the distributions. This rice system example demonstrates the flexibility of the DEM model approach, which can be extended to include other particle properties such as solubility and moisture content to account for dissolution and moisture absorption.

Keywords: mastication; simulation; distribution; rice

INTRODUCTION

The literature contains a number of models that predict with some success the change in particle size distribution (PSD) in the food bolus during mastication. These models are adapted from those used to tackle industrial comminution processes [1 - 4]. These researchers simulated the PSD of a volume basis, the number of individual particles was not considered. In this study, a discrete element method (DEM) model is proposed, where particles and their associated properties are tracked individually. This approach is particularly suited to mastication because the number of particles involved is a small finite number compared to many industrial processes.

Particle size has long been considered an important factor in the formation of a swallowable bolus [5 & 6]; size reduction through mastication is a significant part of preparing the ready-to-swallow bolus. The ability to predict the PSD as mastication occurs has a twofold benefit; firstly, a model can help formalise an understanding of the mastication process; and secondly, a model can reduce the amount of time-intensive laboratory work needed to test hypotheses.

Comminution models typically have two separate functions; a selection function and a breakage function [1 - 4]. The selection function gives the probability a particle has of being fragmented by the teeth and the breakage function describes the distribution of particles that result when a particle is fragmented by the teeth.
This study aims to simulate the PSD using a mechanistic selection function and size dependent breakage function for the mastication of rice.

**MATERIALS & METHODS**

A single subject was selected to participate in this study on the basis of dental condition, age, and rice consumption which was assessed using a questionnaire. The project was reviewed and approved by the Massey University Human Ethics Committee (Southern A) prior to beginning the experiment. The subject gave their informed consent to take part in the study. Whole kernels of brown rice (*Oryza sativa*) were cooked using an electronic rice cooker with water-to-rice ratio of 3:1 (v/v). After cooking, cooked rice samples (50-80g) were placed in plastic container, kept warm at 60±2°C in food oven warmer, and served to the subject after cooling down to approximately 40°C, which is the temperature that cooked rice is normally consumed.

The subject was trained in order to familiarize them with every step of rice chewing prior to the trials. They were instructed to take rice using a tablespoon with a normal portion size as they do at home. The subject was also instructed to use a timer clock to signal that the chewing was beginning and finishing. The serving mass was measured. The subject was asked to; (i), chew rice normally and then expectorate the chewed sample (bolus) when instructed into a small plastic container kept on ice; (ii), rinse their mouth before and after chewing the rice; (iii) to chew and expectorate the bolus after 8, 16, 24, 32 or 40 chews or when they felt the natural need to swallow. Three replicates of each chew number were performed and the trials conducted in a random order. The bolus properties including bolus mass, moisture content, and solid loss were analyzed within a day of collection.

The particle size measurement was achieved by laser light diffraction using a Mastersizer S (Malvern Instruments Ltd, Malvern, UK) equipped with a 1000-mm lens, allowing for analysis of particles between 5 and 3500 µm. The whole food bolus of rice was dispersed in distilled water at ambient temperature (20 ± 2 °C) until an obscuration of 20-25% was obtained. The sample was mixed in a dispersion chamber for 2-3 min to ensure particles were independently dispersed before measurements began. Thereafter stirring was continued throughout the measurement. This method delivers the volume weight size distribution.

**Model development**

The mechanistic model developed by van der Glas et al. [7] is used here for the selection function. It is a two way competition model in which small particles compete with larger particles for breakage sites between the antagonistic teeth. The overall selection function is given by:

\[
S_i(X_i) = \frac{n_{s_i}(X_i)}{n_{i}} \cdot \left[ \frac{n_{X_i} \cdot \ln \left( 1 - O_i(X_i, 1) \right)}{\sum_{j=1}^{k} \left( n_{X_j} \cdot \ln \left( 1 - O_i(X_j, 1) \right) \right)} \right] \cdot \left[ 1 - \prod_{j=1}^{k} \left( 1 - O_i(X_j, 1) \right)^{n_{s_j}} \right] (1)
\]

where \(n_i\) is the number of selected particles of size \(X_i\) in a particle mixture, \(n_h\) is the number of breakage sites on the teeth for each respective particle size if only that size were present and it represents the maximum number of particles of a particular size that can be selected in a single chew. \(k\) is the number of particle size classes with the number of particles in each class being \(n_{X1}, \ldots, n_{Xk}\), and the total number of particles in the mixture is \(n_T\). Clearly for any one size \(n_i \leq n_{i}\) and so the selection chance for any given size particle is

\[
O_i(X_i, 1) = \frac{S_i(X_i)}{n_{s_i} \cdot n_{X_i}}
\]

and is dependent on the ability of the tongue and cheeks to capture and position particles on the antagonistic teeth. \(O_i(X_i, 1)\) is considered to be a measure of particle affinity of the oral system for size \(X\) [7]. This selection model assumes all the breakage sites are initially available for any particle size \(X_i\), but when these particles occupy a fraction of its available breakage sites \(n_{s_i}(X_i)\) it also occupies a fraction of the breakage sites \(n_{s_i}(X_i)\) available to another particle size \(X_j\). Values for the number of breakage sites (\(n_b\)) and particle
affinity $Q_i(X, 1)$ for each size class need to be specified. The complete derivation of this model is shown by van der Glas et al. [7].

In mastication, it is not unreasonable to consider a size threshold, below which particles are no longer fragmented as the result of a breakage event. Van de Bilt et al. [2] note that when predominantly large particles are present, small particles have a negligible chance of being fragmented. Selection thresholds of 1.8 and 1.0 mm have been suggested for brittle foods [7]. Such a threshold will need to be determined from the particle size data. Rice particles are not spherical but are assumed to be so here because it makes comparisons with the Mastersizer data more relevant as the Mastersizer assumes spherical particles. In this work we postulate that a rice particle is fragmented in a cleavage and pasting mechanism, where a selected particle produces a pasted fraction and the remainder of the particle forms either one or two large daughter particles. The pasted fraction consists of particles smaller than some threshold size and because they are below the size threshold they are no longer individually tracked in the system. The number and size of daughter particles is randomly determined. The random nature of the breakage mechanism reflects the way in which a particle is fragmented by the teeth (figure 1). When a particle is on the occlusal surface of the teeth, the cusps of the antagonistic teeth cut the particle at one or more contact points during jaw closure producing large fragments and a pasted fraction. The exact number of fragments produced is unknown, but within the cleavage concept, it is not unreasonable to assume that only a small number of daughter particles are formed. If a particle is positioned with a portion protruding from the teeth then a single large particle may be formed, as shown in 1 (a). The cusps may cleave a particle at a more central location on the particle which could result in a number of small particles at the cleavage point where the opposing teeth surfaces make contact and cleave off two larger particles as shown in 1 (b).

Figure 1. A schematic representation of the possible particles produced in a breakage event, the thatched volume is the pasted fraction comprised of a number of particles smaller than the threshold size.

The portion of a particle that is pasted to below the threshold size is given by:

$$P_i = \left(\frac{V_i}{V_t}\right)^{\alpha} \quad (2)$$

Where $P_i$ is the pasted fraction of a particle with volume $V_i$, $V_t$ is the threshold particle size below which all particles will be pasted, and $\alpha$ is the pasted fraction variable. If $\alpha$ equals one then the pasted volume is constant and equal to the threshold size which could relate to the contact area of opposing cusps during a chewing stroke. The volume fraction of pasted particles was not individually tracked as particles below the threshold size are regarded as unimportant in this model because they do not offer a size-related sensory reason to continue to masticate the food. However, the pasted volume of particles can still prevent the selection of larger particles, thus the volume was assigned a size in order to calculate the selection chance of the larger particles. The ratio of daughter particles produced and the value of $\alpha$ will be varied in an attempt to fit the distribution.

RESULTS & DISCUSSION

The rice bolus exhibits a bimodal distribution (figure 1); a mixed Weibull distribution is fitted to the data, where the change in fitting parameters can help explain how the PSD changes with chew number,

$$Q = \pi \times \left(1 - \exp \left(-1 \times \left(\frac{X}{d_{50(1)}}\right)^b\right)\right) + \left(1 - \pi\right) \times \left(1 - \exp \left(-1 \times \left(\frac{X}{d_{50(2)}}\right)^b\right)\right)$$

where $Q$ is the volume fraction of particles with a size smaller than $X$, $\pi$ is the volume fraction in the smaller size distribution, $X$ is the particle size, $d_{50}$ is the aperture of a theoretical sieve through which 50% of the volume can pass and $b$ is variable that determines the width of the distribution. The fitting parameters at each chew number are listed in table 1. There is a small accumulation of particles which appear to make up a third
distribution centred on 10 µm; these particles are starch granules [8] which comprise a very small portion of the volume and are well below the size of interest in this study.

The bimodal distribution provides evidence for a cleavage and pasting mechanism as proposed previously, where a portion of a selected particle is pasted below a threshold size and the remainder is cleaved to produce 1 or 2 daughter particles. The narrow distribution of larger particles supports the cleavage mechanism as demonstrated by higher $b$ values. The distribution of pasted particles is much broader.

The minimum size between the two distributions (650 µm) does not change significantly as the number of chews increases and there is an almost constant volume flux of particles across this size minimum. The larger particle distribution is of particular interest here as the quantity of particles in this size range may be important in determining the swallow point. In this work the natural swallow point for the subject was 32 chewing strokes. At this chew number the fraction of particles above the threshold was ≈ 20%.

Table 1. Parameters for the double Weibull fit to the experimental data after various number of chews.

<table>
<thead>
<tr>
<th>No. Chews</th>
<th>8</th>
<th>16</th>
<th>24</th>
<th>32</th>
<th>40</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\bar{x}$</td>
<td>0.053</td>
<td>0.30</td>
<td>0.51</td>
<td>0.67</td>
<td>0.89</td>
</tr>
<tr>
<td>$b_1$</td>
<td>1.89</td>
<td>1.25</td>
<td>1.19</td>
<td>1.34</td>
<td>1.49</td>
</tr>
<tr>
<td>$d_{501}$</td>
<td>300</td>
<td>249</td>
<td>262</td>
<td>217</td>
<td>194</td>
</tr>
<tr>
<td>$b_2$</td>
<td>4.30</td>
<td>3.14</td>
<td>1.93</td>
<td>1.93</td>
<td>0.25</td>
</tr>
<tr>
<td>$d_{502}$</td>
<td>2708</td>
<td>2048</td>
<td>1677</td>
<td>801</td>
<td>799</td>
</tr>
<tr>
<td>$R^2$</td>
<td>0.99</td>
<td>0.99</td>
<td>0.99</td>
<td>0.99</td>
<td>0.96</td>
</tr>
</tbody>
</table>

The experimental data indicates that beyond 32 chews the threshold particle size between pasting and cleavage changes and particles as small as 320 µm are comminuted. However, as the natural swallow point for the subject is at 32 chews, the model is less interested in following behaviour beyond this point. Because only particles greater than 650 µm are individually tracked in the simulation it is assumed that all particles above this size are able to be fragmented. It is worth noting that some size reduction could be a result of attrition as the bolus is moved around in the mouth. Leaching of starch from the surface of the particles could lead to size reduction, indeed the emergence of starch granules may result from leaching rather than fragmentation of larger particles.

**Model Simulation**

The model was programmed in MathWORKS MATLAB.

1. A normal distribution of $n$ rice particles is generated to represent the initial mouthful, the initial mean of the distribution is the average initial particle volume $v_i$. The initial number of rice particles was chosen such that the initial volume was similar to the volume of the subject’s initial mouthful.
2. From this distribution the theoretical selection chance for each particle is determined using the selection model. A random number is generated for each particle, if the selection chance is less than the corresponding random number that particle is selected to undergo breakage.
3. A selected particle produces a pasted volume according to equation (2), and either one or two larger daughter particles, the average ratio of daughter particles can be manipulated.
4. Daughter particles are added to the particles that were not selected to update the distribution after chew stroke.
5. The selection and breakage process continues with the new distribution in a loop for the specified number of chewing strokes.

Figure 3 A & B. A comparison between the PSD simulation and the Mastersizer data for particles in the large size range, as a volume distribution on the left and as a cumulative distribution of total bolus volume on the right (8, 16 and 32 chews are plotted).

The simulation shows a close fit to the data, particularly in the earlier stages of chewing. The fitting parameters for the breakage mechanism and the input values for the selection function are given in table 2.

Table 2: The number of breakage sites ($\log_{10}$) and particle affinity ($\log_{10}$) for each size class are shown with the fitted breakage mechanism parameters.

<table>
<thead>
<tr>
<th>$X$ (µm)</th>
<th>4367</th>
<th>3749</th>
<th>3218</th>
<th>2762</th>
<th>2371</th>
<th>2035</th>
<th>1747</th>
<th>1499</th>
<th>1287</th>
<th>1104</th>
<th>948</th>
<th>814</th>
<th>698</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n_b$</td>
<td>1.53</td>
<td>1.74</td>
<td>1.94</td>
<td>2.14</td>
<td>2.35</td>
<td>2.55</td>
<td>2.76</td>
<td>2.96</td>
<td>3.17</td>
<td>3.37</td>
<td>3.57</td>
<td>3.77</td>
<td>3.98</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>1.54</td>
<td>1.76</td>
<td>1.98</td>
<td>2.20</td>
<td>2.42</td>
<td>2.65</td>
<td>2.87</td>
<td>3.09</td>
<td>3.31</td>
<td>3.53</td>
<td>3.75</td>
<td>3.97</td>
<td>4.19</td>
</tr>
</tbody>
</table>

Average number of larger daughter particles = 1.6 (all sizes)

The selection and breakage mechanism used here can sufficiently describe the changing particle size distribution as a function of chew number for particles above the threshold size. The average number of large daughter particles produced to achieve this fit was 1.6, with a value of $\alpha$ of 0.75. The cumulative plot best illustrates the reduction in the volume of particles above the threshold size. After eight chews over 90% of the bolus volume is in the large size range, the volume flux across the 650 µm boundary is a relatively constant and after 32 chews there is approximately 20% of the bolus volume is made up of large particles.

The simulation under predicts the volume in the later stages of chewing, which suggests one of two things is occurring; (i), either too many particles are being selected for breakage or (ii), the particles that are being selected in the lower half of the distribution are producing a larger pasted fraction than the particles in the bolus. If the selection chance of particles is changing this may be the result of particle and bolus properties changing. As mastication progresses the moisture content of the bolus increases as saliva is incorporated, this may make the bolus behave in a more fluid manner resulting in particles having a decreased chance of staying on the teeth and being fragmented in a chewing stroke. It was assumed that the physical properties of rice remain constant throughout mastication and the same breakage mechanism is used for all the particles.
However, the properties of the rice particles will change during the course of mastication, moisture will be absorbed from the saliva which could alter the distribution of particles produced during fragmentation [9]. It is also possible particles undergo work softening as a result of being subject to plastic deformation without fracturing. Over a number of chews this could lead to a change in the fragmentation properties of the rice.

In the model simulation the total volume was conserved. However, in the experiments solids recovery was between 85-92% of the ingested rice (table 3). This loss of solids from the bolus is due to particles being stuck in the teeth and on the oral surfaces after expectoration [5 & 6]. It is assumed the unrecovered solids have a similar distribution to the bolus.

Table3. Mass of solids lost from the expectorated bolus, values expressed are the mean ± the standard deviation.

<table>
<thead>
<tr>
<th>No. chews</th>
<th>Mass (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>7.26 ± 0.75</td>
</tr>
<tr>
<td>16</td>
<td>7.84 ± 1.27</td>
</tr>
<tr>
<td>24</td>
<td>11.73 ± 0.85</td>
</tr>
<tr>
<td>32</td>
<td>13.28 ± 1.82</td>
</tr>
<tr>
<td>40</td>
<td>14.57 ± 2.83</td>
</tr>
</tbody>
</table>

In future experiments water used to rinse the mouth after expectoration should be recovered and analysed as the mass of unrecovered solids can be significant. The loss of solids from the bolus is as much as 50% for some foods [5 & 6], a mechanism for displacement of particles should be incorporated into future comminution models. This may be achieved through a two/multi compartmental model where portions of the bolus are tracked separately as the food is manipulated around the mouth, if this could be done it would better replicate the bolus in the mouth.

**CONCLUSION**

A number based simulation using mechanistic selection and breakage functions has been shown to produce a PSD for the large particles (above 650 μm) in a rice bolus similar to the experimental data from a single subject. The model presented here could be extended to include the saliva in the mouth and incorporate mass transfer of moisture and solutes across the solid liquid interface.

**REFERENCES**