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Effect of flake shape on packing characteristics of popped popcorn

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Abstract

The purpose of this study was to determine the role of flake shape on the packing characteristics of popped popcorn. Unilateral, bilateral, and multilateral popcorn flakes, named for the direction of expansion of the popcorn flake, were digitized and packed into a virtual conical frustum-shaped container using a digital packing algorithm to simulate particle packing. Corresponding laboratory experiments were also conducted. Number of flakes required to fill the container agreed between simulated and laboratory experiments ($r=0.996$; $p<0.0001$) and ranged from about 340 for 50% bilateral+50% multilateral to >600 for 100% unilateral. Statistical modeling revealed 36.9% bilateral+63.1% multilateral would minimize the number of flakes required to fill the container. Packing fraction varied from $\rho=0.14$ for 10% unilateral+75% bilateral+15% multilateral to $\rho=0.28$ for 100% unilateral shape. These results offer insights into the packing characteristics of irregularly-shaped materials.

Keywords: irregular; packing fraction; flakes; modeling; simulation

1. Introduction

Particle packing is a pervasive topic of interest in the engineering and physical sciences with applications in soil sedimentation, pharmaceutical powders, and food systems (Clusel et al., 2009). Understanding such phenomena is often described using geometric shapes of the same or discrete sizes (Donev et al. 2004; Torquato and Jiao 2009). However, in reality granular materials in nature tend to be irregularly shaped, which has a strong effect on packing characteristics (Yu and Zoh, 1996).

Popcorn is an irregularly-shaped particle for which particle packing is extremely important. For popcorn, low bulk density, described in commercials as “lighter and fluffier”, is desirable to consumers (Lyerly, 1942; Levy, 1988) and increases profits for commercial venues like movie theatres where popcorn is purchased by weight and sold by volume (Song et al., 1991; Hosney et al., 1983).

Previous studies have shown that variations in bulk density of popped popcorn is influenced by many factors including flake size (Dofing et al., 1990), flake density (Sweley et al., 2012a), and the void spaces between kernels (Tian et al., 2001). Although modeling experiments with other particles have shown that shape influences bulk density (Zou and Yu, 1996; Jia et al., 2007), the role that popcorn flake shape plays in bulk density has not been comprehensively reported.

We have described a method for modeling packing of irregular materials into any space by digitization of particle shapes and the packing space, rather than using mathematical equations (Jia and Williams, 2001; Jia et al., 2002, 2007). In this approach, particles are digitized by x-ray computed tomography (CT) scanning and packed into a container that is also digitized in an identical manner (Moreno-Atanasio et al. 2010; Caulkin et al. 2009). Particles are added at

a defined rate either from one point (causing heaping) or from random points above the container. Each particle moves one grid cell at a time in a randomly selected direction, out of 26 possible directions, with upward moves restricted (by a rebounding probability) to encourage settling. The simulation can model loose packing or dense packing by simulating shaking.

Popcorn is an attractive candidate for modeling irregularly-shaped particle packing because popcorn flakes have been shown to assume discrete, irregular shapes when popped (Sweley et al., 2011), and the relatively large size of popcorn flakes makes it possible to perform controlled experiments. Thus, the purpose of this study was to determine the role of flake shape on the packing characteristics of popped popcorn using both laboratory experiments and modeling approaches.

2. Materials and methods

2.1. Popcorn popping and sorting

A composite sample of commercial, butterfly-type popcorn hybrid (YP-213) produced in Nebraska, Iowa, and Ohio in 2010 was obtained from ConAgra Foods (Omaha, NE). Kernels were tempered to 14% moisture by storing at 21.5 °C and 73% relative humidity for about 30 d. Kernels (60 g) were then added to microwave popcorn bags ($15 \times 30 \text{ cm}^2$) containing an inlaid aluminum-polyester susceptor ($14 \times 17 \text{ cm}^2$) positioned on the bottom center of the bag. The kernels were then heated in a 1200 W microwave oven (Model PEB2060, General Electric) until the interval between pops was 2-3 s. The contents of the bag were then poured into a sieve with 7.94 mm diameter round-hole openings (Seedburo, USA Model 007) to remove unpopped kernels. A total of 56 bags of popcorn were popped.

Popped flakes were sorted into unilateral, bilateral, or multilateral depending on the directions of flake expansion, as described (Sweley et al., 2011; 2012a, b). Several thousand pieces of each flake type were obtained from the 56 bags of popped popcorn.

Because flake size has been shown to affect expansion volume (Dofing et al., 1990) and the objective was to determine the influence of flake shape on packing characteristics, only “medium” size flakes were selected to reduce the effect of flake size. Medium flake size was determined by randomly selecting 400 flakes of each shape type and measured along three mutually perpendicular axes using digital calipers to the nearest 0.01 mm (Mitutoya America Corp., Aurora, IL). Flake size was the geometric mean diameter, which was calculated as the cubic root of the multiplied lengths of each of the three measured axes. The flake sizes of all three shapes were normally distributed by the Shapiro-Wilk test (Shapiro and Wilk, 1965), with geometric mean diameters of 18.8 ± 3.0 mm for unilaterally-expanded flakes, 22.8 ± 2.3 mm for bilateral, and 24.0 ± 2.4 mm for multilateral. Thereafter, flakes that were within 0.5 standard deviations of the mean were deemed “medium” and selected for further study. Aspect ratio for each popcorn shape was determined by dividing the length of the longest axis by the average of the other two orthogonal axes. To maintain consistency, the same researcher conducted the sorting and measuring of individual popcorn flakes.

2.2. Popcorn packing

2.2.1. Laboratory measurements

A conical frustum-shaped tub having interior cavity height of 15.4 cm, bottom rim diameter 14.0 cm, and upper rim diameter of 17.0 cm was obtained from the Solo Cup Company (Spec No. VP130-00061, Lake Forest, IL). Medium-size popcorn flakes (as defined in section 2.1) were manually added to the packaging tub by dropping the flakes from a height

approximately 10 cm above the rim of the container at 1 flake/s. Individual flakes were dropped from different positions above the tub, since adding particles from a single, fixed point above the container would result in undesirable heaping (Jia et al., 2007). Treatment combinations included each of the three flake shapes alone, all three binary mixtures (one flake shape excluded and the other two present at 50%), the ternary mixture of equal amounts of each shape, as well as an unbalanced ternary mixture of 75% bilateral, 15% multilateral, and 10% unilateral shapes (percentage given as number of flakes), which was previously reported in a typical bag of popcorn (Sweley et al., 2011). Flakes were added until the tub was filled to the interior tub height, as determined using qualitative observation at eye-level of the rim. The number and weight of added popcorn flakes were then recorded. All runs were performed in triplicate.

2.2.2. Digital simulation

To model popcorn packing, the DigiPac algorithm was used, which treats 3D solid objects as coherent collections of voxels (as in 3D digital images) instead of mathematically-described geometries (Jia and Williams, 2001). For each popcorn shape, nine or ten medium-sized pieces of popcorn (as defined in section 2.1) were randomly selected and CT scanned using a Nanotom NF160 (GE Measurement & Control, Wunstorf, Germany). CT scan settings were: 40 kV, 800 μ A, no filter, 500 ms exposure time per image, with a resolution 50 μ m/pixel (Fig. 1). For the simulations, the digitized pieces were scaled down to an effective resolution of 240 μ m/pixel, to save memory and computing time while keeping sufficient details of their shapes. Each digitized piece of popcorn was replicated 100 times, yielding a feed stock of 900 or 1000 particles of each shape for simulation. The tub used in empirical measurements was also digitized and mapped onto a grid at the same (240 μ m/pixel) resolution using the dimensions

given above (section 2.1). The tub itself was not scanned because of its regular shape and also because it was physically too large to fit in the sample holder.

Since both the popped popcorn and package container were digitized, particle movements were also digitized. The model was built on two simple rules: all particles undergo biased random walks and they do not overlap. At each step and for each particle, a random move to a neighboring site was tried and accepted if it resulted in no overlap. To encourage particles to settle (under the influence of gravity), the upward component of any such trial moves were only realized with a probability of 0.3 (called rebounding probability). For rotation, at each step and for each particle, a random rotation axis and angle was generated, and the particle was trial-rotated. If the trial move and rotation did not result in overlap(s), it was accepted.

Popcorn flakes were introduced into the container in random orientations at the rate of five pieces per one hundred Monte Carlo steps. The total number of flakes required to fill the tub and the packing fraction (ρ), or the fraction of the total interior container volume that was occupied by popcorn, were obtained from the DigiPac software. For all treatments except the binary mixtures, five simulations with identical setup but different random number sequences were performed for each popped shape type. Binary mixtures were run in duplicate. For each simulation, runtime on a Dell 15z laptop with Intel i7-2620M quad-core 2.7 GHz CPU and 8 GB RAM was 5-7 h for packing, using 1.4 GB of RAM.

2.3. Data analysis

All data were analyzed using SAS Software (version 9.2, SAS Institute, Cary, NC USA). Relationship between number of flakes to fill the tub for laboratory and simulated experiments was calculated using least squares regression. Modeling the number of flakes required to fill the tub using combinations of multilateral, bilateral, and unilateral flakes was calculated using

ANOVA in which the proportion of the three flake shapes were treated as part of a mixture design that summed to 100%. The design started with the full cubic model (%unilateral*%bilateral*%multilateral) with backward elimination at $\alpha=0.1$ to eliminate non-significant factors from the model. A contour plot was generated from the final model using Design Expert (version 8.0, Stat-Ease, Minneapolis, MN). Data for flake aspect ratio, geometric mean diameter, and packing fraction were compared using a generalized linear model analysis of variance (GLIMMIX) followed by Fisher's least significant difference test with $\alpha=0.05$.

3. Results and discussion

The number of popcorn flakes required to fill the tub agreed well between laboratory and simulated experiments (Fig. 2). Notably, laboratory and modeling experiments were performed independently by different researchers at different institutions.

Two factors contribute to density: inter-particle gaps and intra- particle pores. The manuscript focuses on the number of popcorn pieces required to fill a container, which is influenced by inter-particle gaps. However, popcorn pieces have a lot of internal pores as well, which would influence density. Our recent publication has shown that internal pores in popped popcorn flakes are 30-60 μm in diameter (Hoseney et al., 1983; Schwartzberg et al., 1995). CT scans were performed at a resolution of 50 $\mu\text{m}/\text{pixel}$. Pores of similar or smaller sizes than resolution were missed in the simulations (thus pieces were treated as solid particles). Because of this, counting the number of pieces for a given tub was the best way for comparison.

Using these data, statistical modeling of the number of flakes required to fill the tub using combinations of each of the three flake shapes was performed. The final model showed good fit to experimental data (Table 1; $R^2=0.99$). Parameter estimates for the linear mixture, unilateral, bilateral, and multilateral, were 637 ± 7 , 346 ± 7 , and 339 ± 7 , respectively; the parameter estimate

for the one interaction that was significant, unilateral*bilateral, was -140 ± 37 . The model estimated that fewer popcorn pieces were required to fill the tub as the proportion of unilateral-shaped popcorn decreased (Fig. 3). It may be that the low aspect ratio and limited appendages on the unilateral flakes facilitated denser particle packing. The model estimated that minimum number of pieces needed to fill the packaging (335) would be expected using a combination of 63.1% multilateral and 36.9% bilateral popcorn pieces.

Packing fraction (ρ) is one of the most important characteristics measured and reported in packing studies. It is defined as the ratio of physical space occupied by the solid particles to the total container volume.

Packing fraction ranged from 0.14 to 0.28 among simulations (Fig. 4). Notably, as mentioned, popcorn pieces were treated as solid particles in the simulations. Therefore, these packing fractions do not include the empty spaces within pores of individual popped flakes; it only includes the empty space surrounding popcorn pieces. Others have reported $\rho=0.68-0.71$ for predicted modeling of oblate spheroids such as M&M's® candies (Donev et al., 2004; Chaikin et al., 2006) and $\rho=0.34-0.50$ for extruded, puffed, or flaked cereals and snacks (Sandoval et al., 2008). The packing fraction of popped popcorn was lower than for these materials. This is not surprising, since interacting particles create an excluded volume effect (Chaikin et al., 2006) and it is likely that the multiple expansion appendage arms (Fig. 1) found in popcorn gave rise to more bridging, leading to larger interstitial void spaces than found in packing of geometrically-shaped particles.

Packing fraction was correlated with number of flakes required to fill the container ($p<0.001$), but the coefficient of determination was only moderate ($R^2=0.60$), suggesting other factors in addition to the number of flakes required to fill the tub play a role in packing fraction.

For example, bilateral and multilateral shapes required similar numbers of flakes to fill the tub (Fig. 2), yet the packing fraction for bilateral flakes was significantly lower than multilateral flakes (Fig. 4). The lower packing fraction for the bilateral shape compared to the multilateral was likely due to the higher aspect ratio for the bilateral shape (1.7 ± 0.4 versus 1.1 ± 0.2 for bilateral versus multilateral, respectively), resulting in a bridging effect for the bilateral polymorphism. This provides experimental evidence to support simulated packing research, which has shown that increased aspect ratio decreases packing density (Sherwood, 1997; Zou and Yu, 1996; Jia et al., 2007), even when the objects are irregularly shaped.

Another factor that influences packing fraction is flake size (Dofing et al., 1990). Though medium-sized pieces of each shape type were selected to minimize the effects of flake size, the flake shapes did show different mean geometric diameters: unilateral (18.8 mm), bilateral (22.8 mm), and multilateral (24.0 mm). The reduced number of flakes required to fill the tub for multilateral compared with unilateral (Fig. 2) was therefore likely due to the larger flake size since both multilateral and unilateral flakes had the same aspect ratio (1.1 ± 0.2 versus 1.1 ± 0.3 , respectively).

The interaction among particles of different shapes is yet another important consideration that describes packing fraction. Packing fraction decreased when comparing binary mixtures of each shape combination with the corresponding packing fraction of each shape individually. For example, when a 50:50 mixture of unilateral and bilateral shapes was used, the packing fraction was significantly lower than when either of the shapes was used alone (Fig. 4). This trend was true for all comparisons between single shapes and 50:50 mixtures. Thus, the binary mixtures must have created more opportunities for bridging among particles, creating an excluded volume effect.

Regarding the ternary mixtures, u10_b75_m15, which was selected based on the natural distribution of polymorphic shapes in a bag of microwave popcorn (Sweley et al. 2011), resulted in the lowest packing fraction among all flake combinations tested. This shape distribution was found using hybrid YPK-213(ConAgra, Omaha, NE USA), which is a popcorn being used in commercial markets. One of the major criteria that popcorn breeders use to select new hybrids is low bulk density (usually referred to as high expansion volume). Perhaps in this pursuit breeders have inadvertently selected for a shape distribution that minimizes bulk density. Indeed, we have previously shown that the distribution of polymorphisms can be manipulated through genetics and production practices (Sweley et al., 2012b).

While the design of this experiment used flakes with similar size, popcorn found in uncontrolled settings (such as purchased at a movie theatre or made at home in microwave) would be expected to contain a mixture of popcorn flakes with different sizes as well as shapes (Sweley et al., 2012a). Linear packing models predicts loose pack density often increases in multi-sized mixtures of nonspherical geometric particles due the increased chance of particles fitted together more tightly (Stovall et al., 1986; Yu and Zou, 1996). Thus, further investigation to characterize the relationship between heterogeneous mixtures of different shaped popcorn flakes in bulk packing would be meaningful.

4. Conclusions

Packing characteristics of popcorn pieces in a rigid container were accurately predicted using a digital-based algorithm. The packing fraction and number of pieces required to fill a container varied significantly depending on the shape of particles added. In particular, packing fraction and number of pieces required to fill a container was decreased by increasing the proportion of bilateral and multilaterally-expanded popcorn flakes.

Having shown here the influence of popcorn shape on flake packing characteristics, future studies will address how flake size may affect popcorn packing, since loose pack density of other materials tends to increase when heterogeneous mixtures of multi-sized particles are used due to the increased chance of fitting together more tightly (Yu and Zou, 1996; Stovall et al., 1986). We expect that these results, together with our previous paper on factors affecting popped popcorn morphology (Sweley et al., 2012b), will be useful for popcorn breeders and purveyors of popcorn to create the “lighter and fluffier” popcorn that is desirable to consumers.

5. Acknowledgements

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Table 1. Analysis of variance for number of pieces to fill popcorn tub.

Sources of variation	DF	Sum of squares	Mean Squares	F Value
Model	3	222169	74057	385 ^a
Linear Mixture	2	219347	109674	570 ^a
Unilateral x Bilateral	1	2822	2822	15 ^a
Lack of Fit	4	970	243	1.35
Error	16	2879	180	
Corrected Total	23	226018		

^asignificant at $p < 0.01$

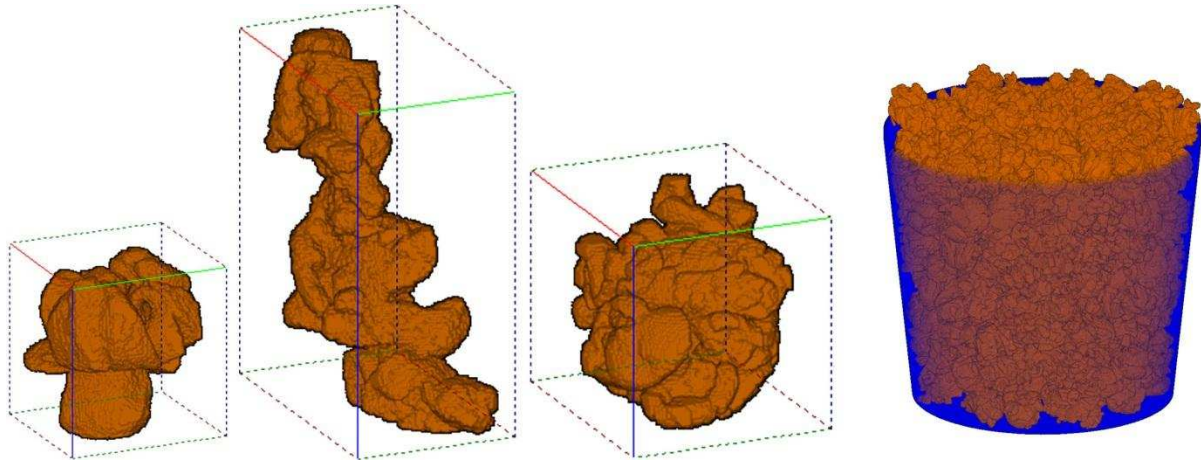


Figure 1. 3D view of popcorn digitized using x-ray tomography at $240\ \mu\text{m}/\text{voxel}$ resolution and resultant packing in movie theatre-style packaging tub. From left: unilateral polymorphism (18.0 x 19.4 x 20.6 mm), bilateral polymorphism (28.6 x 16.3 x 35.0 mm), multilateral polymorphism (23.1 x 19.2 x 19.7 mm), and packing tub (14.0 cm bottom rim diameter, 17.0 cm upper rim diameter, and 15.4 cm tub height). Note: orange indicates popcorn pieces, blue empty space.

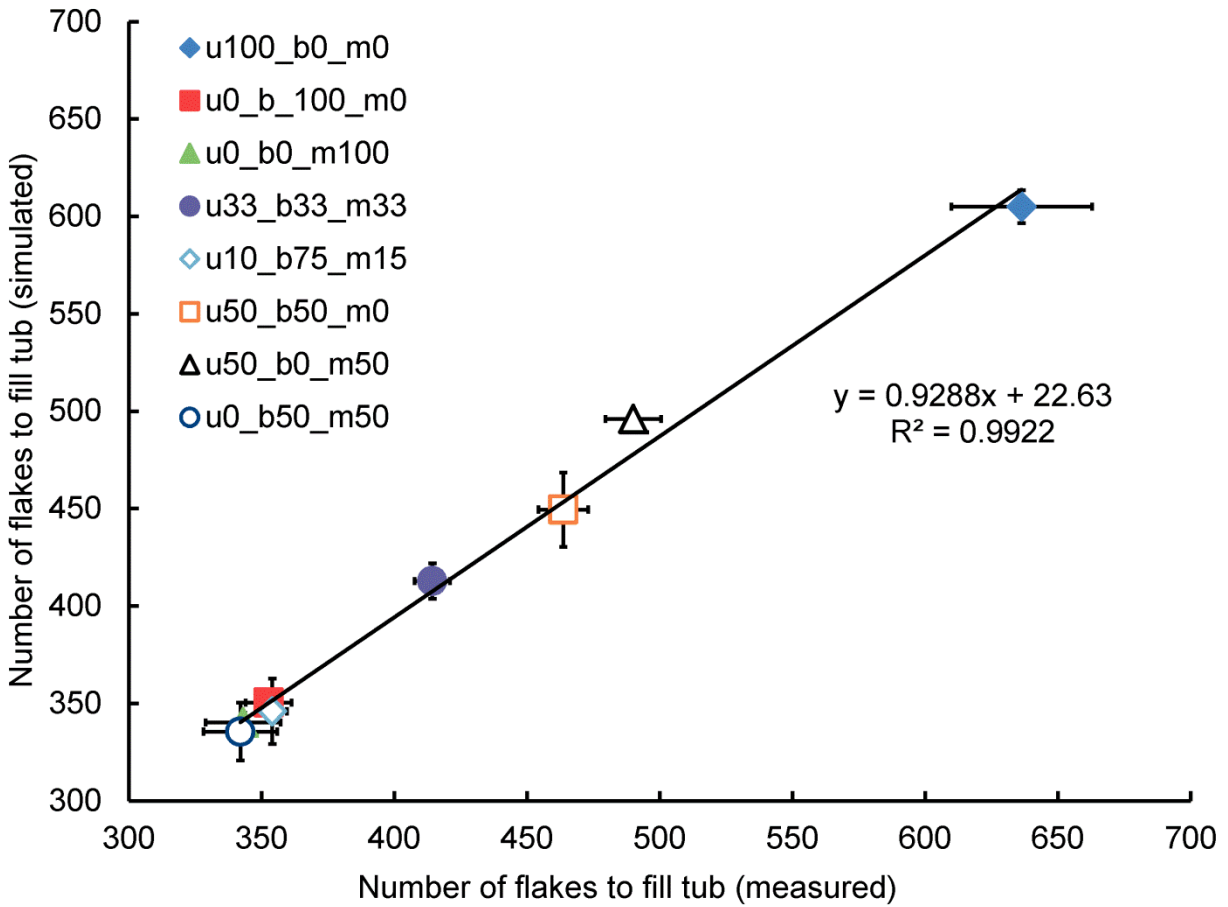


Figure 2. Comparison of measured and simulated number of popcorn flakes required to fill the packaging tub using combinations of unilateral (u); bilateral (b); and multilateral (m) flakes; flake combinations are abbreviated u100_b0_m0 for 100% u, 0% b, and 0% m and u0_b100_m0 for 0% m, 100% b, and 0% m, and so on; error bars show standard deviation; for simulated data n=5, except for binary mixtures (n=2); for measured data n=3.

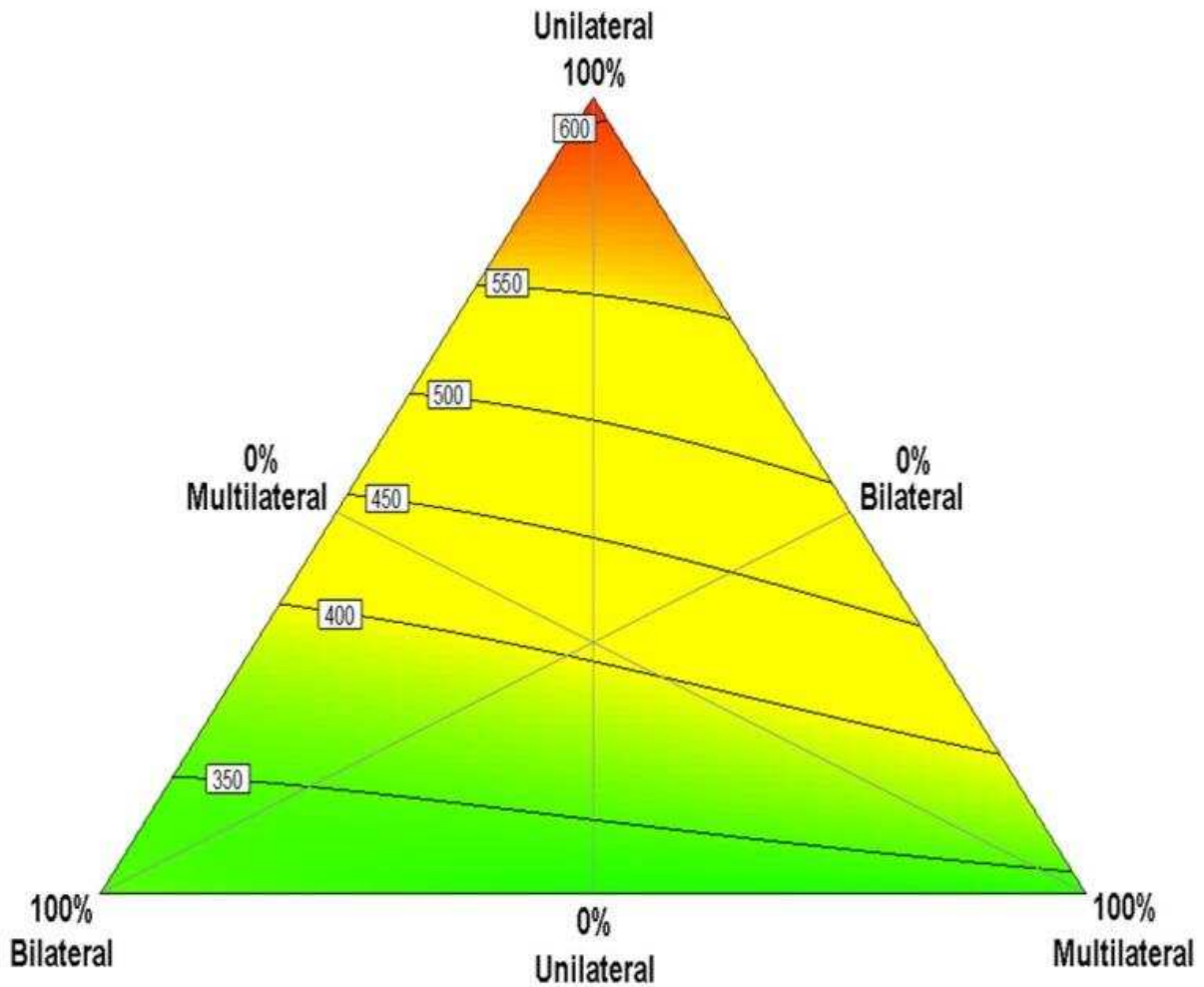


Figure 3. Predicted number of pieces to fill movie theatre style packaging tub; axes for each popcorn polymorphism indicate relative proportion in mixture; corners of figure represent 100% proportion of polymorphism; outside lines of triangle show binary mixtures; and interior of figure indicates ternary mixtures; the intersection of the three axes in middle of figure indicates an equal mix (33%/33%/33%) of the three shapes; contour lines are labeled to show expected number of pieces to fill package.

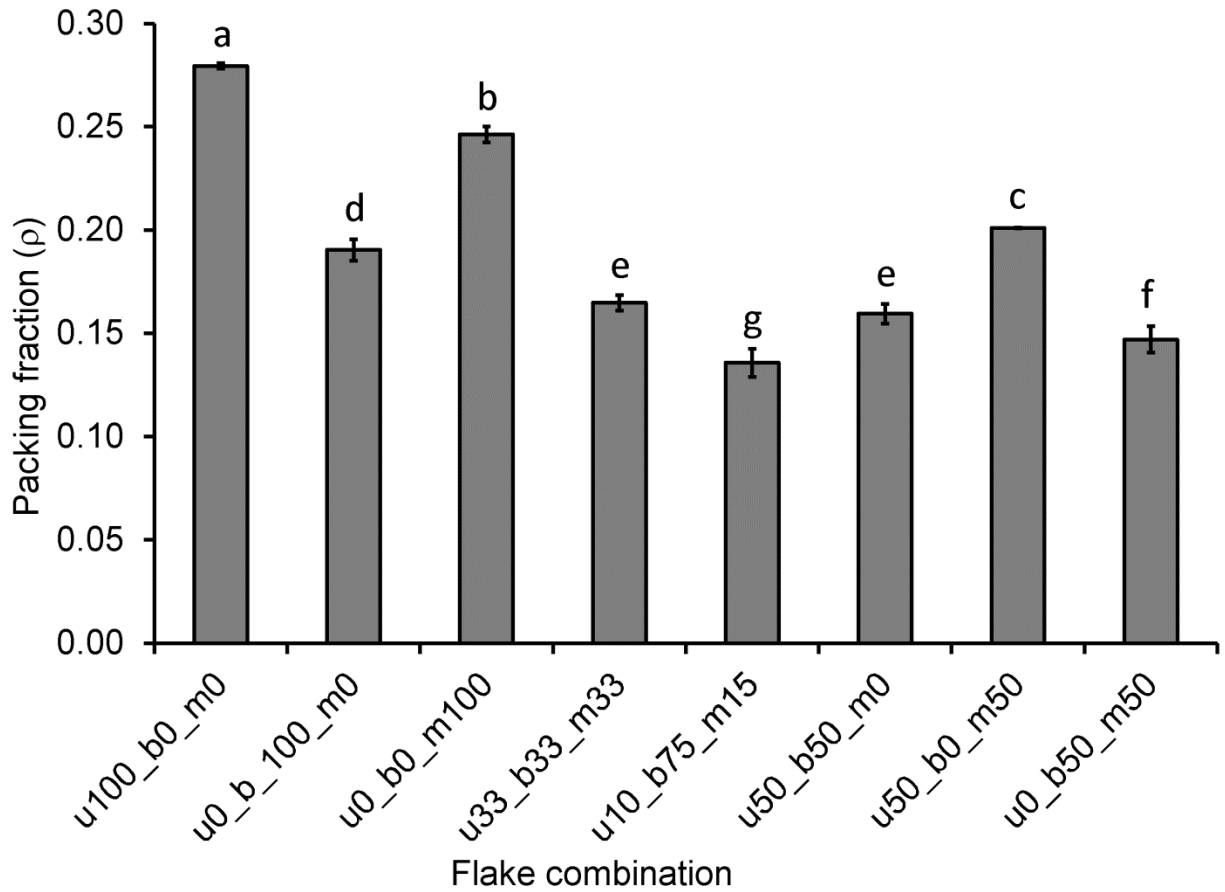


Figure 4 (version 1). Packing fraction obtained from simulated filling of popcorn tub with combinations of unilateral (u); bilateral (b); and multilateral (m) flakes; flake combinations are abbreviated u100_b0_m0 for 100% u, 0% b, and 0% m and u0_b100_m0 for 0% m, 100% b, and 0% m, and so on; error bars show standard deviation; n=5, except for binary mixtures (n=2); bars labeled with different letters are significantly different (p<0.05).

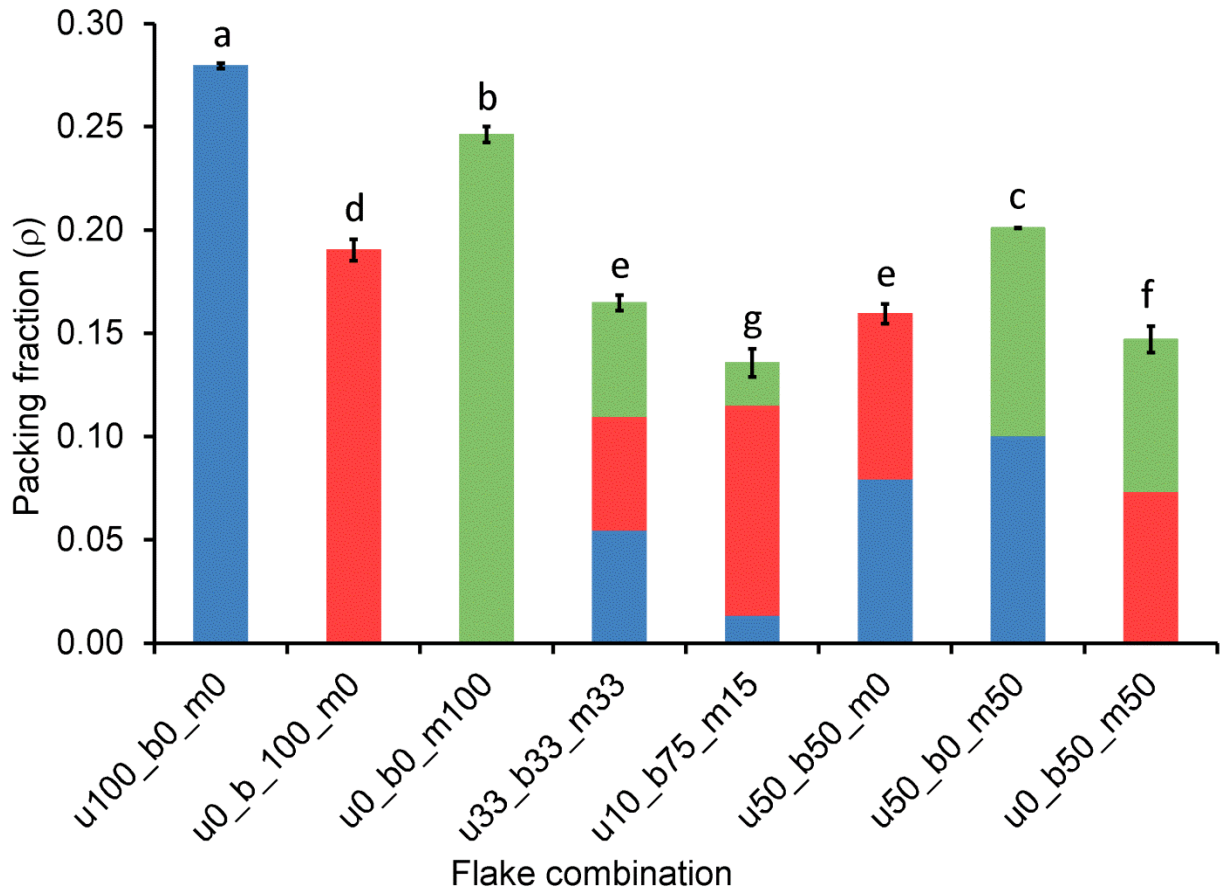


Figure 4 (version 2). Packing fraction obtained from simulated filling of popcorn tub with combinations of unilateral (u); bilateral (b); and multilateral (m) flakes; flake combinations are abbreviated u100_b0_m0 for 100% u, 0% b, and 0% m and u0_b100_m0 for 0% m, 100% b, and 0% m, and so on; shading is proportional to the percentage of the flake shapes used in each simulation (u=blue; b=red; m=green); error bars show standard deviation; n=5, except for binary mixtures (n=2); bars labeled with different letters are significantly different (p<0.05).