Discrete element method to model cracking for two layer systems

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ABSTRACT: Cracking at the fold is a serious issue for many grades of coated paper and coated board. Some recent work has suggested methods to minimize this problem by using two or more coating layers of different properties. A discrete element method (DEM) has been used to model deformation events for single layer coating systems such as in-plain and out-of-plain tension, three-point bending, and a novel moving force picking simulation, but nothing has been reported related to multiple coating layers. In this paper, a DEM model has been expanded to predict the three-point bending response of a two-layer system. The main factors evaluated include the use of different binder systems in each layer and the ratio of the bottom and top layer weights. As in the past, the properties of the binder and the binder concentration are input parameters. The model can predict crack formation that is a function of these two sets of factors. In addition, the model can predict the flexural modulus, the maximum flexural stress, and the strain-at-failure. The predictions are qualitatively compared with experimental results reported in the literature.

Application: Mills can use the results of this study to formulate the base and top coats and minimize the risk of cracking.

Coated board grades are typically double or triple coated, but the number of coating layers applied for standard coated paper grades often varies with mill location. North American coated papers typically are single coated; similar papers in Europe can have multiple layers of coating applied. The mechanical properties of all coating layers are critical to the paper and board passing through the various post coating application steps without experiencing any quality problems. These process steps include calendering (compression), printing (z-direction tension), and folding (bending). The potential quality problems that can result from these processes are cracking, picking, and cracking-at-the-fold (CAF).

The two main computer modeling techniques used for modeling free-standing coating layers has been the discrete element method (DEM) and the finite element method (FEM). The DEM approach has been used for modeling coating layers under tension [1-4], under compression [5-7], and during bending [8,9]. FEM has been used to model all three types of events [10-12].

The works of Salminen et al. [12,13], of Alam et al. [10], and of Yang et al. [14] were different because they looked at the effects of multiple coating layers on coating mechanical properties. All three groups were trying to optimize the balance between stiffness and CAF for multiple coated papers. The work of the first two groups involved modeling and pilot laboratory trials (comparing double and triple coating). The third team scaled up this work to the commercial level. The chief findings were that the optimal balance between stiffness and CAF was the case of a triple coated paper. This "ideal" paper was determined to consist of a thin, stiff bottom coating layer; a thick, lower-stiffness middle coating layer; and a thin, stiff top coating layer.

Oh et al. [15] conducted a series of laboratory experiments to evaluate the folding response of double-coated heavyweight papers and the relationship of tensile to CAF. They looked at the effect of styrene butadiene (SB) latex glass transition temperature (T_g) in the topcoat, of starch levels in the precoat, and of ground calcium carbonate (GCC) particle size. While not commenting on the effect of the pigments, they pointed out the negative effect of starch and of higher latex T_g on cracking tendency. An important finding was that, as starch levels and latex T_g increased, the number of cracks decreased, but their length and area increased.

Because the finite element method normally treats the coated paper as a composite material, it does not make the "connection" between events on the micro-scale and the responses on a macro-scale, whereas DEM can make the connection. FEM can be used to develop particle-level models [16], but the computational complexity and the computing time increase significantly as the number of particles goes up.

Our study builds on the recent work of Varney and Bousfield [8,9]. The three-point bending model of these papers will be expanded from one to two coating layers. The effects of the latex-to-starch ratio and of top layer to bottom layer thickness ratios (i.e., coat weight ratio) are assessed. The model results are compared with those of previous work where multiple coating layers were applied to a variety of paper substrates (Salminen et al. [12,13], Alam et al. [10], Oh et al. [15], Yang et al. [14], and Hashemi-Najafi et al. [17]).

MODEL DEVELOPMENT

Previous work by Varney and Bousfield [4,8,9] discussed an equation that fits well with the non-linear stress-strain results seen in prior tension experiments (Prall et al. [18], Raman et al. [19], and Zhu et al. [20]). The force equation had the following form:

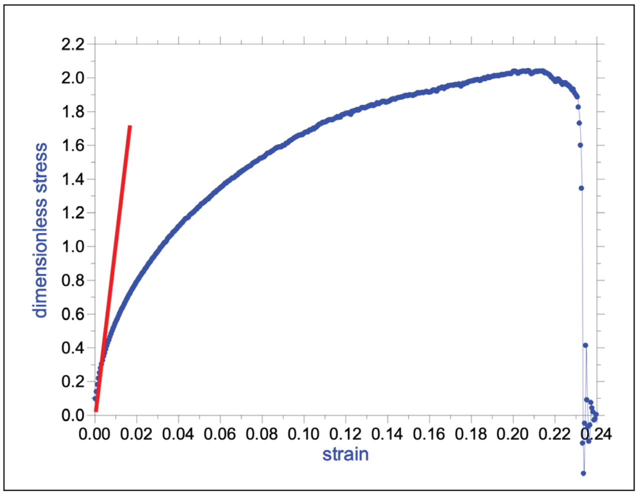
$$F = A(1-e^{-B\varepsilon})\pi R_b^2 \quad (1)$$

where F is the tensile force between particles, A and B are parameters that depend on the pure binder, ε is the local strain between particles, and R_b is the radius of the binder bridge between particles. The bridge radius and the spacing of the particles depends on the pigment volume concentration (PVC), which is defined as the ratio of total volume of pigments to the volume of pigments plus the volume of binder. When the local strain between particles is larger than the strain-to-failure of the pure binder, the binder is assumed to fail cohesively and the force is set to zero. Using data from Zhu et al. [20], the model provides a non-linear response, as depicted in **Fig. 1**.

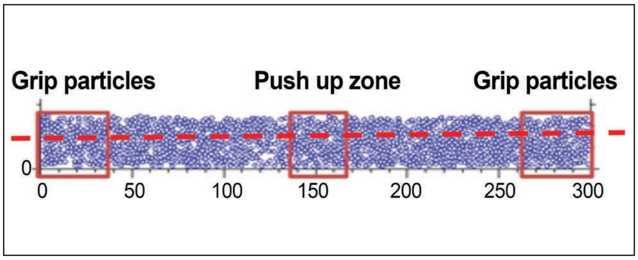
For compression, the repulsive force equation was established as:

$$F = \frac{Eh_i}{h}\varepsilon\pi R_b^2 \quad (2)$$

where h and h_i are the current and initial gaps between particles, respectively, and E is the elastic modulus of the binder. The ratio of initial to current gaps is needed in this expression to give a large force as the current gap goes toward zero. This large force would come from the compression of high points on the particles and is important to keep particles from overlapping. The difference between tension and compression is that, in compression, with a small gap, the force must go to a large value to keep particles from overlapping each other, whereas in tension, the force follows the behavior seen in tensile tests and goes to zero when the critical strain is reached.



1. Typical non-linear response from tension simulation [6].



2. Boundary conditions for a bending simulation. Particles in push up zone are set to move upward. The distance from the zero-y position to the red broken line is the height of the bottom layer.

The bending simulation is done by holding two groups of particles in place, not allowing motion, while another group of particles is set to move upward (**Fig. 2**). This arrangement simulates a three-point bending test. Other types of deformation are possible with the model, such as moving a group of particles at one end upward and not allowing some particles on the other end to move, as in a cantilever. Particles in the "push up" zone are moved upward with a dimensionless velocity of 1. The grip particles can be either not allowed to move at all or not allowed to move vertically. This latter condition lets the particles in the grip zones slide and simulates a three-point bending test where the sample is supported loosely with a support structure. For the simulations conducted for this paper, the grip particles were allowed to slide.

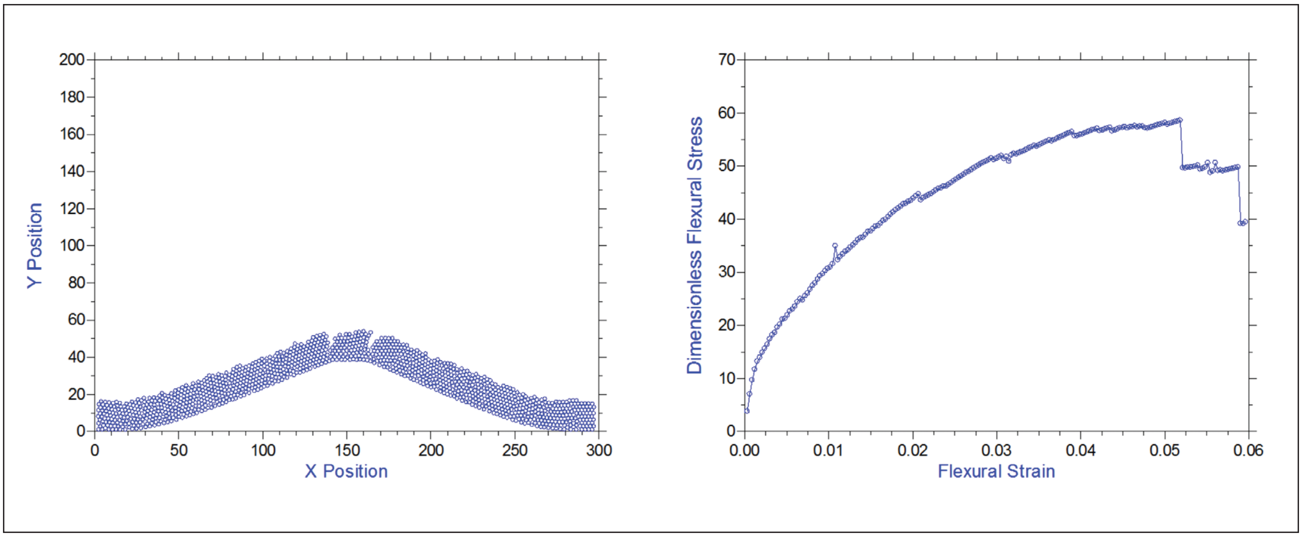
The flexural force on each particle is calculated as it moves relative to its neighboring particles. If particles move away from each other, Eq. (1) is used to calculate the tension force between these particles. If particles are pushed together, then a repulsive force is applied to keep the particles from overlapping, as in Eq. (2). The net vertical force on the left and right grip particles are summed. This upward force should equal the net downward force on the particles that are moving upward to balance the forces. The flexural stress and strain are defined respectively as:

$$\sigma_f = \frac{3PL}{2bd^2} \quad (3)$$

$$\varepsilon_f = \frac{6Dd}{L^2} \quad (4)$$

where P is the sum of the forces on the grip particles (or the load force), L is the distance between grips, D is the displacement of the upward moving particles at the center of the sample, b is the width of the sample, and d is the thickness of the sample. The strain, σ_f, is made dimensionless with the elastic modulus of the binder. The goal is to predict the bending behavior of these systems and to predict the crack propagation.

The key difference between this study and those presented by Varney and Bousfield [8,9] on three-point bending is the modeling of two layers in the present case. This "splitting" of the layers is performed by setting the particles below a certain height to have the properties of one binder system and the



3. Typical results for 62 PVC (20 pph binder) with binder properties that resemble 60% latex and 40% starch in the top layer and 80% latex and 40% starch in the bottom later. The ratio of bottom layer height to top layer height was 75:25. Left are the particle positions near the end of the simulation and right is the stress-strain prediction.

particles above this height (up to the top of the particle matrix) to have the properties of a different binder system. As such, data from two binder systems and the intermediate height (the bottom layer height) are inputs to the two-layer model. For this study, an 18 × 300 particle matrix was used, with the bottom layer heights being 4.5, 9.0, and 13.5 (thus establishing bottom layer to top layer ratios of 25:75, 50:50, and 75:25, respectively). The binder systems used in these simulations were based on the data of Hashemi-Najafi et al. [21] and were 60% latex/40% starch, 80% latex/20% starch, and 100% latex/0% starch. These binder systems would represent typical latex-to-starch ratios used in the paper industry.

The length scales for the bending simulations are scaled with pigment radius. If the particles have a radius of 1 μm, then the length in Fig. 2 would represent a 300 μm × 20 μm; the height of this region would be typical of a paper coating layer thickness. The length scale is much smaller than typical bending tests or production scale, but representative paper and board deformations of these sorts can be modeled by increasing the number of particles in the matrix. Regardless of the length scale, the results should be similar because the parameters input into the model would be the same.

A model of this nature involves a number of assumptions. The results presented here are limited to equal-sized spheres that are confined in a monolayer (true three-dimensional simulations currently are in progress). The spheres are assumed to be rigid particles, and all of the deformation is either compression or tension of the latex bridges between the particles. The model in this current form neglects the rotation between particles, which can be included if it is deemed to be important. In addition, the failure between the particles is assumed to be cohesive in nature, so any failure that takes place is within the binder bridge and not at the interface between the binder and the particles (recent work has incorporated adhesive failure in to the model, but it was not included in this paper). Lastly, the model does not take the Poisson's ratio (the absolute ratio of the transverse strain to the longitudinal strain) in to account, as the pigment particles and the binder are assumed not to compress. As such, the ratio is presumed to be about 0.5 in all cases.

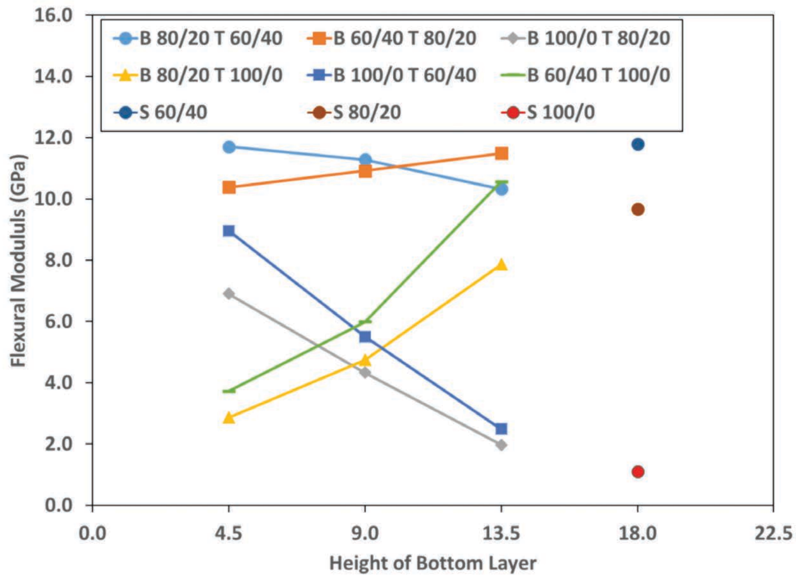
Figure 3 shows the results of a bending simulation in which the bottom layer was comprised of 80% latex and 20% starch (80L/20S) and the top layer consisted of 60% latex and 40% starch (60L/40S). The ratio of the bottom layer to the top layer heights (i.e., the coat weight ratio) was 75% bottom layer and 25% top layer. The PVC for the simulations was kept to a constant value of about 62. The pure binder data used as inputs for the model came from the work of Hashemi-Najafi et al. [21], where the PVC was 62 (20 pph binder). The particle position plot on the left shows the formation of cracks taking place in the top layer, which has a higher amount of starch in it, but the crack does not propagate through the second layer.

SIMULATION RESULTS

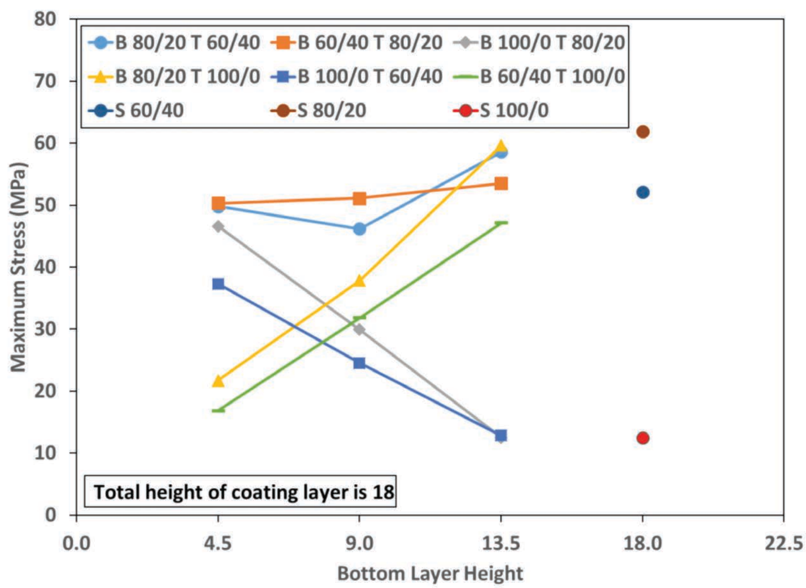
Of the 21 simulations conducted for this study, 18 represented various combinations of bottom layer/top layer thicknesses and binder systems and three represented single coating with the three individual binder systems (60L/40S, 80L/20S, and 100L/0S). **Table I** shows the model inputs for the pure binder data of Hashemi-Najafi et al. [21].

Parameters	Pure Latex	80L-20S	60L-40S
a	1.5	4.9	4.8
B	2.0	15.0	35.0
E, MPa	3.0	73.5	168.0
STF, %	200.0	80.0	22.0

I. Properties of the pure binder films from tensile tests. Strain-to-failure (STF) is given as a percent. 80L-20S is 80% latex and 20% starch on a weight basis from companion paper.



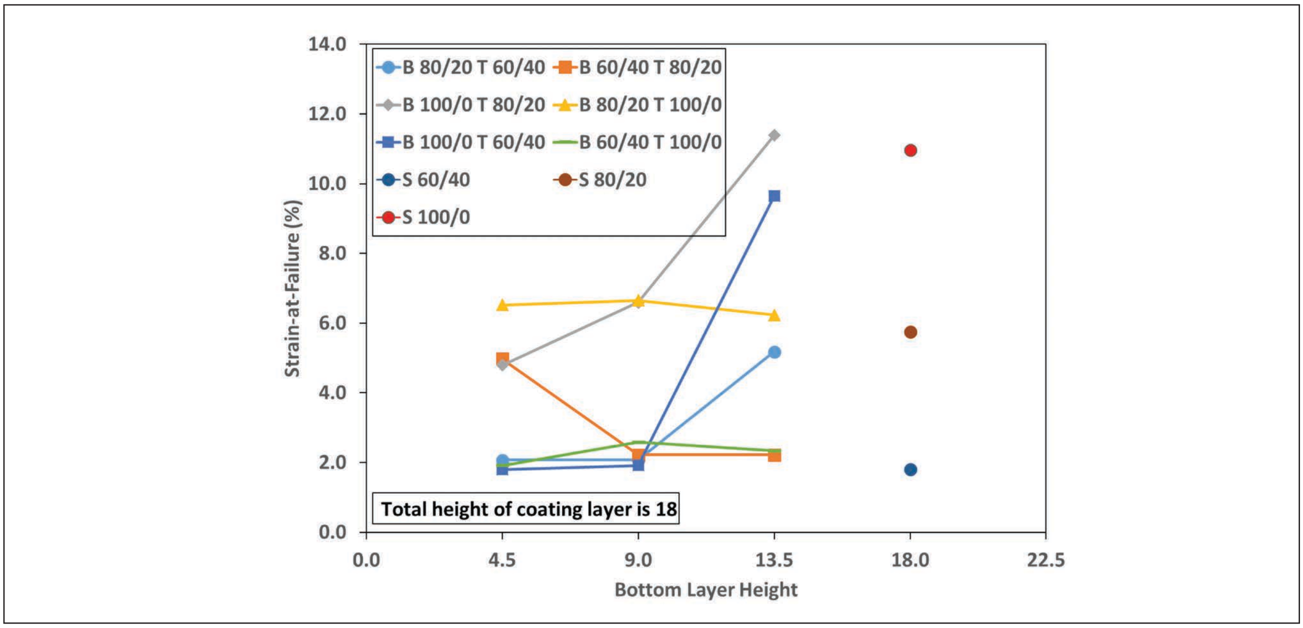
4. Simulated flexural modulus as a function of the bottom layer height and various bottom layer/top layer binder systems. B 80/20 T 60/40 stands for bottom layer with an 80% latex/20% starch binder system and a top layer with a 60% latex/40% starch binder system. S 60/40 stands for single layer with a 60% latex/40% starch binder system.



5. Simulated maximum stress as a function of the bottom layer height and various bottom layer/top layer binder systems. B 80/20 T 60/40 stands for bottom layer with an 80% latex/20% starch binder system and a top layer with a 60% latex/40% starch binder system. S 60/40 stands for single layer with a 60% latex/40% starch binder system.

Figures 4-6 show the results for flexural modulus, maximum stress, and strain-at-failure. Each property is plotted against the height of the bottom layer (with the total height being 18 in dimensionless form). A bottom layer height of 4.5, for example, gives a top layer height of 13.5, and the ratio of the bottom to the top layer heights is 25:75. A height of 18 indicates that the coating is comprised of one layer.

For the flexural modulus, the simulations show the values to be highest with increased thickness of the starch-rich layer. This layer dominates the response and drives the flexural modulus to a value approaching the single layer condition with the same starch-rich binder system. The same trends were observed with the maximum stress. As for the strain-at-failure (STF), similar trends were observed, but in reverse. The values tend to decrease at higher thicknesses of the starch-rich layer, as is expected. The highest STF values were for increasing thickness of an all latex binder bottom layer (100L/0S), with either of the other two binder systems in the

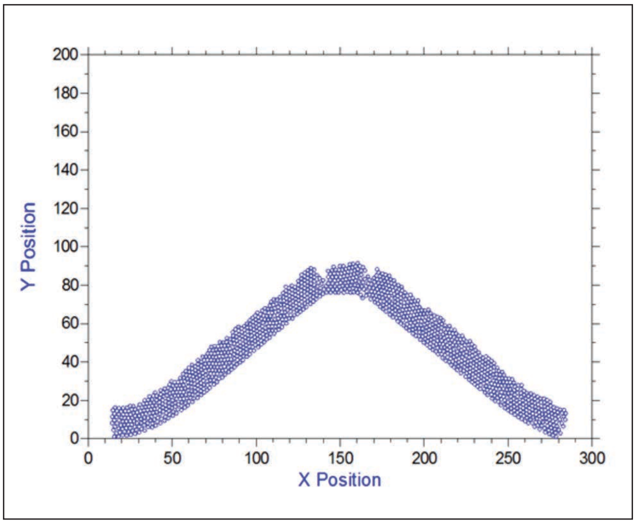


6. Simulated strain-at-failure as a function of the bottom layer height and various bottom layer/top layer binder systems. B 80/20 T 60/40 stands for bottom layer with an 80% latex/20% starch binder system and a top layer with a 60% latex/40% starch binder system. S 60/40 stands for single layer with a 60% latex/40% starch binder system.

top layer. When the 100L/0S binder is in the top layer, the STF values remain constant with the bottom layer height, regardless of the bottom layer binder system (80L/20S or 60L/40S). These constant values are similar to the single layer condition using the same binder package as the bottom layer.

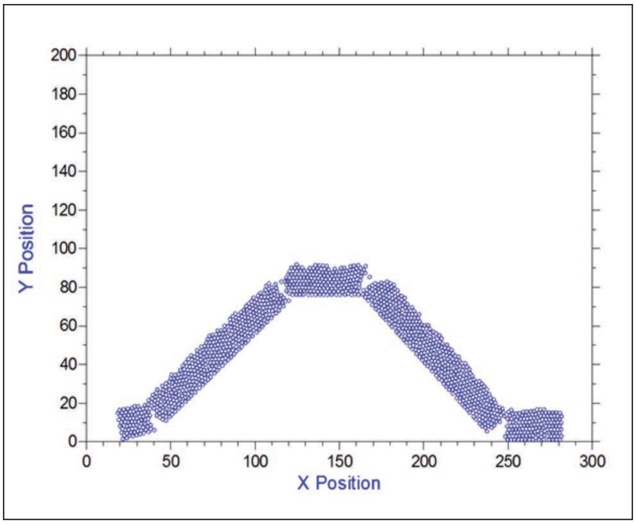
The position plots show cracking in all 21 cases if the simulation is allowed to run long enough to result in failure. Cracking would always occur in the starch-rich layer, regardless of whether it was in the top or bottom layer. The appearance of cracks in the bottom layer always occurred near the grips. Although cracks did appear in some cases for the all-latex binder system, this occurred infrequently and might have been a result of the length of the simulation. These durations were varied to achieve failure (and thereby obtain the stress/strain and modulus values) and might not correlate perfectly with a bending test, which is run for the same amount of time in all experiments.

The position plots in **Figs. 7-10** depict some specific situations. The first three cases are for thick bottom layers with thin top layers (a 75:25 ratio of bottom layer to top layer heights). Figures 7 and 8 represent opposite scenarios. Figure 7 shows a thick latex only bottom layer with a thin starch-rich top layer. Figure 8 shows a thick starch-rich bottom layer with a thin latex-only top layer. In Fig. 7, the cracks appear only in the thin starch-containing top layer. The thick latex-rich bottom layer does not appear to crack, as might be expected. Figure 8 shows cracking in the bottom thick starch-rich layer, but it also shows cracks in the top latex-only thin layer. The appearance of cracks in this top layer is a bit confusing, but it could be the result of slippage out of the grips, as seen by the bottom cracks on the left and ride sides. In addition, the work of Salminen et al. [12,13] showed the case of Fig. 7 to be less

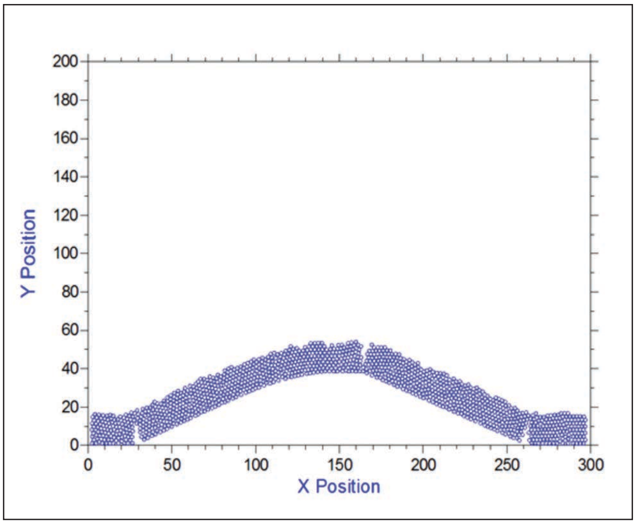


7. Position plot for 62 PVC (20 pph binder) with binder properties that resemble 100% latex in the bottom layer (100L/0S) and 60% latex plus 40% starch in the top layer (60L/40S). The ratio of bottom layer to top layer heights is 75:25 (i.e., a thick latex-rich bottom layer and a thin starch-rich top layer).

prone to cracking. Figure 9 shows a two-layer system with a 50:50 split of a 60% latex/40% starch bottom layer (60L/40S) and a 80% latex/20% starch top layer (80L/20S). In this case, more cracks occur in the higher starch-containing bottom layer, as might be expected. Lastly, Fig. 10 is a single layer (of equal thickness as the two-layer systems) with a binder system comprised of 60% latex and 40% starch. Cracks can be seen in the top and bottom of the single layer. As in the other cases, the bottom cracks appear near the grips, possibly indicating some slipping at these positions.



8. Position plot for 62 PVC (20 pph binder) with binder properties that resemble 60% latex plus 40% starch in the bottom layer (60L/40S) and 100% latex in the top layer (100L/0S). The ratio of bottom layer to top layer heights is 75:25 (i.e., a thick starch-rich bottom layer and a thin latex-rich top layer).

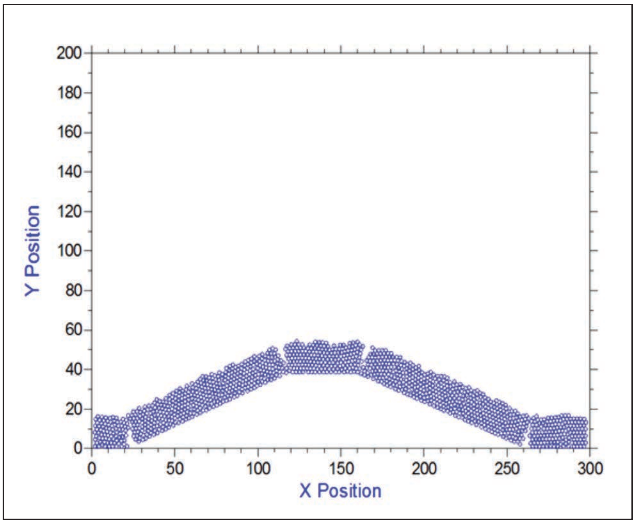


9. Position plot for 62 PVC (20 pph binder) with binder properties that resemble 60% latex plus 40% starch in the bottom layer (60L/40S) and 80% latex plus 20% starch in the top layer (80L/20S). The ratio of bottom layer to top layer heights is 50:50 (i.e., layers of equal thickness that both contain starch, with the bottom layer having twice as much starch as the top layer).

COMPARISON TO EXPERIMENTAL DATA

The simulations for this study show agreement with trends observed in the literature. The model was not concerned with finding the optimal balance between stiffness and CAF (as were Salminen et al. [12,13], Alam et al. [10], and Yang et al. [14]). The current simulations did show that cracking tendency would decrease with a thick, low-stiffness bottom layer and a thin, stiff top layer (i.e., conditions with an all-latex bottom layer and a top layer with some level of starch—the conditions with the highest strain-at-failure values). As noted earlier, the position plot of Fig. 7 is an example of how the simulations agreed with past work. These earlier investigators found their ideal paper to be a thin, stiff bottom coating layer; a thick, lower-stiffness middle coating layer; and a thin, stiff top coating layer. It might be that cracks form in the top coating layer in these systems, but they are not noticed because the middle coating layer either does not crack or dissipates the crack.

The tendency for the starch-rich layers in the model to be more prone to cracking was in accordance with Oh et al. [15]. Those authors commented on the negative effect on cracking tendency when adding starch to the precoat (the topcoat was an all-latex binder system in their study). They found that the length and area of the cracks would increase directly with starch level. In addition, their data agreed with the results of Zhu et al. [20] in that the strain-at-failure decreased and the maximum stress increased as more starch was added to the precoat. Because the model is concerned with two dimensions, at present, definitive comments about the size and number of cracks cannot be made. However, the model does show agreement with the stress-strain data from Oh et al. [15] for the simulations involving starch-containing precoats and an all-latex topcoat. The maximum stress goes up when the starch level is raised, be it from adding more to the precoat or from increasing the precoat weight. As for the strain-at-failure, this parameter drops with more starch, but remains constant with increasing precoat weight. However, the position plot of Fig. 8 shows the appearance of cracks in an all-latex top layer. These results are not in agreement with Oh et al. [15], even though the simulated stress-strain results follow the same trends as the prior experimental work.



10. Position plot for 62 PVC (20 pph binder) with binder properties that resemble 60% latex plus 40% starch (60L/40S) in a single layer (i.e., one starch-rich layer equal in height to the two-layer scenarios).

Hashemi-Najafi et al. [17] applied two coating layers to a couple of paper substrates. The coatings were formulated at two different PVCs and with the four binder systems used in the simulations previously mentioned. Following bending, the area of the cracks was found to be a strong function of the amount of latex in the topcoat. The area was lower at higher levels of latex in the top layer binder system, indicating that cracking became less of an issue in this case. These results concur with the model in that cracking, in general, did not occur in the layers with an all-latex binder system. However, the simulated strain-at-failure results for the case of an all-latex topcoat (100L/0S) were not the highest in all cases, thus indicating that these conditions did not show the lowest propensity of cracking.

CONCLUSIONS

A discrete element model was found capable of simulating bending for a two-layer system comprised of different ratios of two heights and of different binder systems in two layers. The model could predict cracking during the three-point bending event. The model was based on using the mechanical properties obtained from pure binder films.

The model shows direct relationship between starch level and height of a starch-rich layer on the flexural modulus and the maximum stress. For the case of strain-at-failure, the model shows the relationship to be the inverse case.

The trends shown by the model are in general agreement with the literature in that starch-rich coating layers of high coat weight were seen to be more prone to cracking. Additionally, the lowest tendency for cracking was seen for a thick layer of an all-latex binder system with a thinner layer of a starch-containing coating.

More work needs to be performed to improve the model's predictions relative to experimental results. This might include studies of the effect of starch on the mode of failure (cohesive vs. adhesive) and true three-dimensional packing. **TJ**

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ABOUT THE AUTHORS

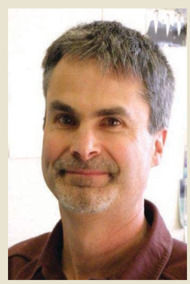
This study is part of my (Varney) Ph.D. thesis with Professor Bousfield. It is an extension of prior work modeling single layer coatings.

The biggest challenge in conducting this study probably was making the free-standing films, which Hashemi-Najafi [21] figured out how to do successfully. One of the more interesting findings was that the amount and location of the starch can have a big impact on cracking. One of the surprises was the appearance of cracks on the bottom layer – always by the grips.

The results of this study give mills a strategy for how to formulate the base coat and top coat and minimize the risk of cracking.

As a next step, this work could be expanded to encompass three dimensions.

Varney



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