Computer Simulation of Particle Packing in Acrylic Latex Paints

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Computer simulation of the random close packing of hard pigment particles and deformable latex particles in acrylic latex paint systems is described. The simulation requires only the particle size distribution of the pigment, the particle size distribution of the latex, and the deformation or softness of the latex. If these data are known, the packing density can be determined from the simulation. If paints with a range of pigment volume concentrations (PVC) are simulated, the critical PVC can be predicted from plots of packing density against PVC. The predicted values are in good agreement with experiment.

INTRODUCTION

Since the seminal work of Asbeck and Van Loo in 1949,[1] the critical pigment volume concentration (CPVC) has been recognized as being of fundamental importance in paint formulation. Many film properties change abruptly at the CPVC, and it is a true transition point.[2] The CPVC has been defined[1] as the volume percentage of pigment in the film which has just sufficient binder to completely fill the voids left between the pigment particles. This CPVC is seldom aimed for by a formulator but rather it is a reference point. Paints may be formulated below the CPVC to minimize air voids and optimize film properties or formulated just above the CPVC to take advantage of the increased opacity due to air voids. To maintain similar film properties when alternate pigments and binders are substituted in a formulation, substitutions should be made in a way which maintains the same reduced pigment volume concentration (PV).[2]

Bierwagen[3] has shown that, for solvent-based paints, the CPVC can be determined by assuming random close packing of the pigment particles plus adsorption of the oil or polymer onto the surfaces of the pigment particles. The total volume of oil plus pigment at the end of an oil adsorption test was assumed to be the sum of the pigment volume, the interstitial oil volume, and the adsorbed oil volume. The adsorbed oil was assumed to increase the effective size of the pigment particles. The CPVC was then the random close packing density of the pigment plus adsorbed oil. For uniformly sized, spherical pigment particles with no surface adsorption of oil, this reduces the packing density of uniform spheres at 64% PVC.[4] Surface adsorption of polymer, pigment porosity, and irregular shape would tend to lower this figure, while a broad particle size distribution would tend to increase the CPVC.

In water-based latex paints, the latex particles are not infinitely deformable, as is the solvated polymer in solvent-based paints. Therefore, surface adsorption in a manner which increases the effective particle size of the pigment is not expected. Adsorption of low molecular mass components, such as surfactant, is also not expected to increase the effective particle size of the pigment significantly. Hence, as pointed out by Rowland and Steig,[5] this results in both the pigment particles and the latex particles packing together to form the film from their dispersed state in the paint. In the film the pigment particles are held apart by the latex particles to various extents depending on the relative sizes of latex and pigment and also the deformation of the latex particles. The deformation of latex particles will depend on properties and conditions such as the minimum film forming temperature (MFFT) of the polymer, temperature of film formation, and amount and type of coalescing agents. Thus, the CPVC of a latex paint will generally be lower than a solvent-based paint with the same pigment formulation. In the limit of zero relative size of latex to pigment particle size and/or infinite deformability of the latex particles, the CPVC of the latex paint would be expected to be the same as a solvent-based paint with the same pigment formulation and no oil adsorption.

The CPVC of a latex paint can be determined by observing the variation of some property in a PVC ladder. Virtually any property can be used. Asbeck and Van Loo[1] measured gloss, blistering, rusting, and permeability. Schaller[6] measured enamel holdout, scrub resistance, tensile strength, contrast ratio, and corrosion. Hesler[7] measured gloss, stain porosity, and recommended contrast ratio. Anwari et al.[8] used contrast ratio and 85° sheen as well as other methods. To make the number of paints required for a PVC ladder and measure the properties is a tedious process. However, Berardi's binding

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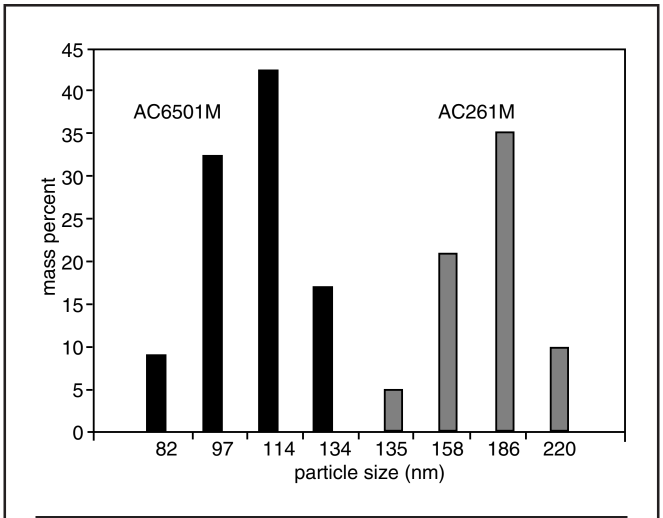

Figure 1—Particle size distribution of latices.

power index,[9] once known for a given latex, allows the CPVC of any formulation using this latex to be determined.[10, 11]

Experimentally, the CPVC of latex paints has been found to decrease with increase in size of the latex particles,[6,12,13] to decrease with increase in MFFT or glass transition temperature(T_g),[6,13] and to increase with amount of coalescing agent.[6,13] However, Becker and Howell[12] found no change in CPVC with amount of plasticizer in polyvinylacetate latices. Anwari et al.[14] found that dry hiding above the CPVC in acrylic latex paints, and by inference, the size and number of air voids, decreased with decrease in latex particle size, decrease in T_g, and increase in amount of coalescent. These results are mostly consistent and support the ideas of Rowland and Steig[5] that small soft latex particles allow pigment particles to pack together with minimum air voids and large hard latex particles introduce air voids at a lower PVC.

The aim of this paper is to present an algorithm which simulates the packing of pigment and latex particles in a paint film. The algorithm uses only three pieces of information. These are the particle size distributions of both pigment and latex and a deformation which is related to the MFFT or softness of the latex particles. This allows the CPVC to be predicted without making PVC ladders, provided the required information is known.

EXPERIMENTAL

The CPVCs for some titanium dioxide/acrylic latex paints and some calcium carbonate/acrylic latex paints were determined using acrylic latices and pigments for which particle size distributions were supplied by the manufacturers. The CPVCs were estimated from PVC ladders using 60° gloss versus PVC. In the case of the calcium carbonate pigmented films, we were able to visually observe the increase in opacity due to air voids at the CPVC and to confirm this observation by light transmission of the films.

The titanium dioxide was RHD2 (Tioxide Australia Pty. Ltd., Burnie, Tasmania, Australia). A typical particle size distribution, determined by a sedimentation method, was provided by the suppliers, and this was used in the simulations. The calcium carbonate used was Omyacarb 1 (Omya Southern Pty. Ltd., Melbourne, Victoria, Australia). The nominal particle diameter was 1 um. A typical particle size distribution, determined by a sedimentation method, was provided by the suppliers, and this was used in the simulations. The latices used were Primal AC6501M and Primal AC261M (Rohm and Haas Australia Pty. Ltd., Geelong, Victoria, Australia). The MFFT and particle size distribution of each latex were provided by the supplier. The MFFT of both latices was 16°C. The mean particle diameters of each of these latices were 119 nm and 193 nm, respectively. Particle size distributions of the two latices and titanium dioxide are shown in *Figures* 1 and 2. The particle size distribution, by mass and by number, of the calcium carbonate used is shown in *Figure* 3. Sixty percent PVC paints at 40% volume solids were made by dispersing the required amount of pigment in water with a recommended surfactant system.[15] This was 1% Orotan 731SD (Rohm and Haas Australia Pty. Ltd.), 0.5% Triton CF10 (Rohm and Haas Australia Pty. Ltd.), and 0.5% Teric N40 (ICI Australia Pty. Ltd., Ascot Vale, Victoria, Australia) based on weight of pigment. The pigment was dispersed using a Sardik Hi-Speed Dissolver (Sardik Engineering, Gladesville, NSW, Australia). The PVC ladder was prepared by diluting this dispersion with latex at 40% volume solids. The pH was kept at 8-9 with ammonia. No coalescing aids or other additives were used, excepting a viscosity control additive at one percent volume solids based on total volume solids. This was RM5 (Rohm and Haas Australia Pty. Ltd.). The paints were drawn down in films of 0.38 millimeter wet film thickness and allowed to dry at 30°C for 24 hr. Further drying at 25°C for one week took place before 60° gloss readings on the films were taken (Micro TRI Glossmeter, Byk-Gardner, Silver Spring, MD). Visible light transmissions, at a wavelength of 550 nm, of the calcium carbonate pigmented films were measured by a Hitachi U-3200 spectrometer (Hitachi Ltd., Tokyo, Japan).

THE ALGORITHM

The algorithm is based on previous work by the authors concerned with the random packing of spheres[16-18] and

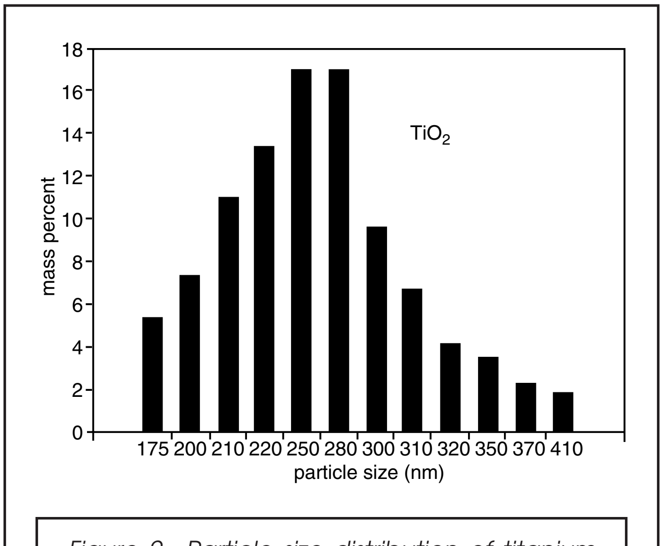

Figure 2—Particle size distribution of titanium dioxide.

nonspherical particles.[19] Coated titanium dioxide particles were approximated as hard spheres with a known size distribution. It is known[19,20] that broad particle size distributions have different random close packing densities to uniformly sized particles and so distributions were used in preference to average particle sizes, especially as the extra program coding required is trivial. Latex particles were approximated as deformable soft spheres with a known particle size distribution. The deformation D, of a latex particle, is defined as

D = mean radius lost due to coalescence/
original radius of latex particle.

A latex particle is also considered to be deformed by an equivalent amount when in contact with adjacent pigment particles. The deformation can have a value ranging from 0 (hard) to 1 (infinitely soft). The deformation of a latex is determined by its MFFT and different latices with the same MFFT are considered to have the same deformation value D. Ideally, the deformation would be able to be estimated from the MFFT and the CPVC determined from just three experimentally known values. However, insufficient data were available to determine the relationship between deformation and MFFT.

A latex particle is considered to be slightly compressible. For ease of simulation, it was assumed that the particle absorbs the volume associated with its deformation when coalescence occurs and does not redistribute this volume in the form of bulges or a greater sphere radius. For an assembly of latex spheres with a deformation value of 0.13 (the value estimated for the latices used in these simulations), the volume of the latex deformation in each sphere was calculated to be approximately four percent of the sphere volume. This was regarded as sufficiently too small to neglect. The photographs by Kendall and Padgett of coalesced latex particles[21] show no indication of "bulging" as a result of deformations.

A simulated packing comprised of spherical particles of both latex and pigment in the correct numbers to give the required PVC and which obey the specified size distributions is randomly generated within a spherical container. These particles can initially exist in overlapping configurations due to the random placements, but are gradually transformed by an iterative process which causes the packing to converge to an overlap free state. Within each iteration, every particle is moved a small increment under the net action of the forces resulting from its overlaps with neighboring particles. This type of simulation has successfully modeled random packings of hard, equal sized spheres,[16] hard spheres with sizes that obey a lognormal distribution,[17] and hard, nonspherical particles.[19] A packing comprised of pigment and latex particles was considered to be overlap free when the pigment particles had an insignificant mean overlap (less than one percent of mean pigment radius), and the mean latex overlap was less than or equal to its deformation D.

To simulate the coalescence of latex particles, the mean latex overlap was required to equal the deformation D. When the aforementioned iterative process was used alone, the mean latex overlap was always less than the deformation due to the large starting volume. An increase in the mean latex overlap was accomplished by compressing the latex. In this process the centers of all particles were moved closer together vertically. This caused more overlaps to occur which were removed by allowing it to reconfigure, using the same iterative technique, until the pigment particles again had an insignificant mean overlap, and the latex particles had a mean overlap equal to the deformation D. The simulated formation of the paint film was a product of both the iterative technique and the compression process. These operations were performed in conjunction with two constraints. First, the initial packing was constructed so that it was less dense than the final packing. This simulates the compression of particles in the film formation process as described by Vanderhoff and Bradford.[22] Secondly, the PVC of the initial packing was uniform. The uniformity in concentration was maintained throughout the compression process by selectively allowing migration of particles into and out of the region used for analysis. Once the simulated film formation process had been completed, many of the geometric properties of the packing could be determined from the coordinates and radii of the particles. These properties include the packing density and coordination numbers. The packing density is that fraction of the total volume of the film occupied by the latex and pigment particles. The remaining fraction is assumed to be air. Coordination numbers are the number of particles surrounding a given particle. For example, the latex to latex coordination number is the average number of latex particles surrounding a given latex

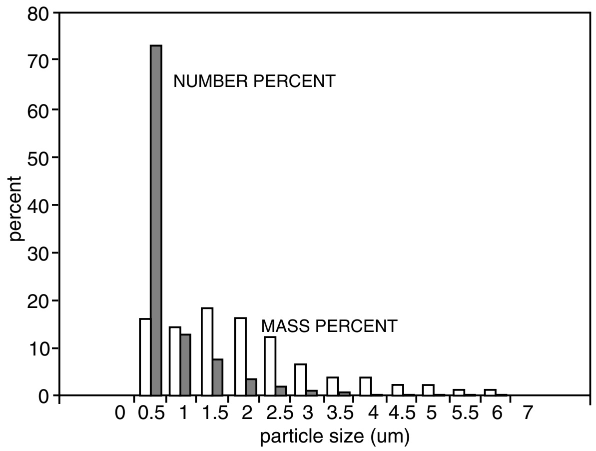

Figure 3—Size distribution of calcium carbonate by particle mass and particle number.

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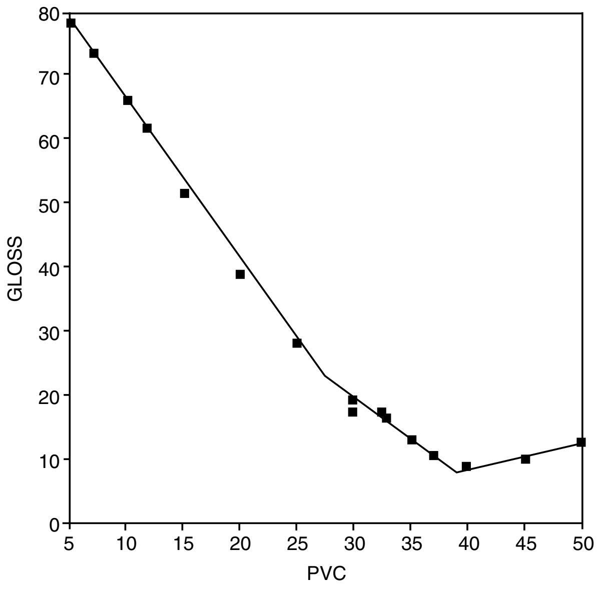

Figure 4—60° gloss against PVC for 119 nm latex/titanium dioxide paint.

particle. Simulations of paints comprised of hard pigment particles and soft latex particles were performed with packings of approximately 1000 particles made up of the required number of latex and pigment particles to give a particular PVC. A separate simulation was performed for each PVC. PVC values ranged from 0 to approximately 70%. The size distribution of each set of particles was modeled on the distributions described in *Figures* 1-3.

The average time for each simulation and subsequent analysis of a paint with a specified PVC was of the order of four hours. At the present time, the simulations are limited to pigments and latices with relative particle size differences of less than the same order of magnitude. This is because the volume of a particle depends on the cube of the radius and hence, particles which differ in radius by a factor of 10, differ in number by a factor of 1,000. For example, the introduction of a single extender particle with large diameter would require thousands more of small latex and/or titanium dioxide particles which would not allow the simulation to finish in reasonable time. Because of this, it was necessary to truncate the size distribution used in the calcium carbonate simulations. The maximum diameter in the distribution used for simulation was 800 nm. As can be seen from *Figure* 3, this represented approximately 90% of the particles by number but considerably less by mass. It was assumed that the missing number of larger particles were spread randomly throughout the film and would not affect the results in a major way. We expect this deficiency will be overcome in time, with the advent of more powerful computers. The programs were written in Turbo Pascal (Borland International, Scotts Valley, CA) and run on an IBM compatible 386 with a math coprocessor. Executable versions of the programs used in these simulations are available to researchers and can be obtained by writing to the authors. A pseudocode listing of the algorithm is given in *Appendix* 1.

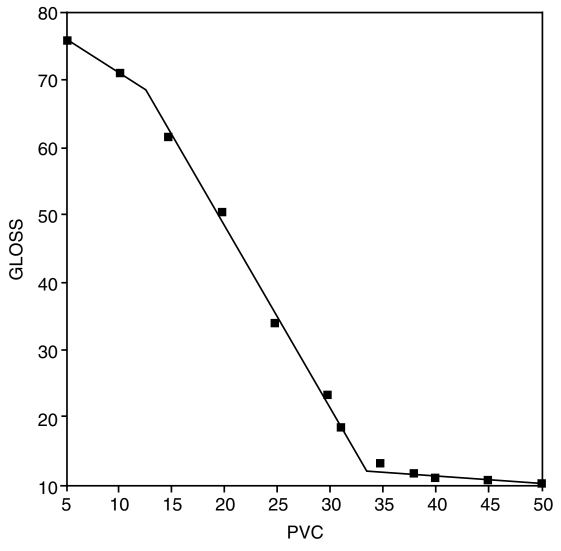

Figure 5—60° gloss against PVC for 193 nm latex/titanium dioxide paint.

RESULTS AND DISCUSSION

The experimental results of gloss versus PVC for the 119 nm latex/titanium dioxide system are shown in *Figure* 4. From this graph it can be seen that the CPVC is about 40%. The experimental gloss results of the 193 nm latex with titanium dioxide are shown in *Figure* 5 and with calcium carbonate in *Figure* 6. Percentage transmissions of visible light at 550 nm are also shown in *Figure* 6. The rapid fall off in percent transmission at a PVC of 53% is a better indicator of the CPVC in these films than the gloss readings. The difference in CPVC due to latex particle size is small and of the same order as the experimental error. However, it agrees with the work of Schaller[6] who found a change of about 15% in PVC per micron change in latex particle size. The difference in CPVC on changing from titanium dioxide pigment to calcium carbonate pigment is more significant due to the larger difference in particle size. The calcium carbonate is about five times the diameter of the titanium dioxide pigment and the experimental CPVC of this formulation is 53%. In comparison, the CPVCs for the 119 nm latex/titanium dioxide and the 193 nm latex/titanium dioxide paints are 40 and 35%, respectively.

The shape of our experimental graphs at low PVC does not agree with the shape obtained by Asbeck and Van Loo[1] for solvent-based paints. The shape obtained by Asbeck and Van Loo shows a small slope at low PVCs, a change to a larger negative slope before the CPVC, and small slope after CPVC. This curve has been reproduced by Floyd and Holdsworth[23] and used by them to tentatively assign another transition point, called the percolation threshold (PT), at the PVC below the CPVC where this change in slope occurs. Only the 193 nm latex/titanium dioxide paints show any similarity to this curve. The 119 nm latex/titanium dioxide and the 193 nm latex/calcium carbonate systems both show a rapid fall off in gloss with increase in PVC below the PT and less slope between the PT and the CPVC. Hesler[7] and Anwari et al.[8] have shown similar experimental curves to the 119 nm latex/

titanium dioxide and 193 nm latex/calcium carbonate curves reported here.

The computer simulation of these paints, using the method outlined in the algorithm section, required the deformation value of the latices. To estimate the deformation of the latices, a series of simulations were performed with mixtures containing titanium dioxide pigment and Primal AC6501M latex particles (119 nm latex particle size) with varying deformation values and various PVCs. The packing density at each PVC was determined from each simulation and plotted against PVC. The CPVC for a paint using a latex with a particular deformation value was predicted from inflection points on this graph. The CPVCs predicted for each deformation value of the latex were plotted against the deformation and shown in *Figure* 7. Thus, *Figure* 7 allows the unknown deformation D to be estimated for one latex (AC6501M) by finding the deformation required to give the experimental CPVC found from a PVC ladder. This deformation D was then used to predict the CPVC of paints made with a different particle size latex (AC261M) but same deformation, with titanium dioxide and with calcium carbonate as separate pigments. Agreement of the predicted and experimental CPVCs for these last two paints should indicate the validity of the algorithm. From *Figure* 7, the deformation required to give the experimental CPVC of 40% is 0.13. This deformation was taken to be the deformation of both the 119 nm latex and the 193 nm latex and used in all subsequent simulations. This method of determining the deformation of a latex detracts somewhat from the ability of the algorithm to estimate the CPVC of a formulation from first principles; however, it is the only method available. Once the deformation of a latex with a particular MFFT is known, that deformation should apply to all latices with the same MFFT. *Figure* 7 can also be used to show the simulated effect of softness or deformation of the latex particles on the CPVC. For the given particle size distributions of the AC6501 latex and RHD2 titanium dioxide pigment, this graph shows that the CPVC increases with deformation in agreement with known experimental results.[6,13]

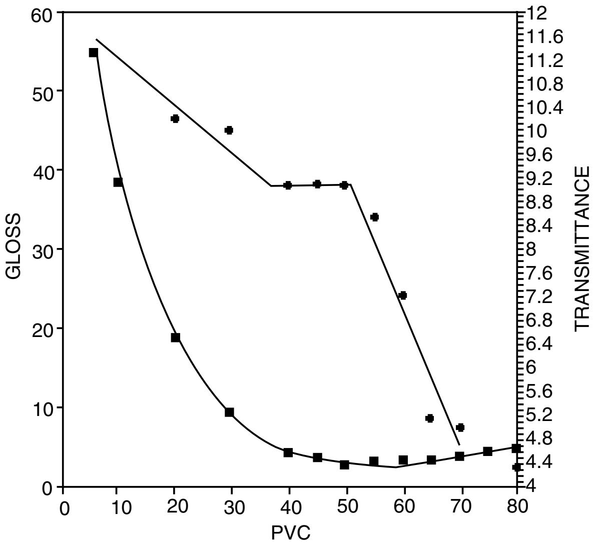

Figure 6—60° gloss and percentage transmission against PVC for 193 nm latex/calcium carbonate paint.

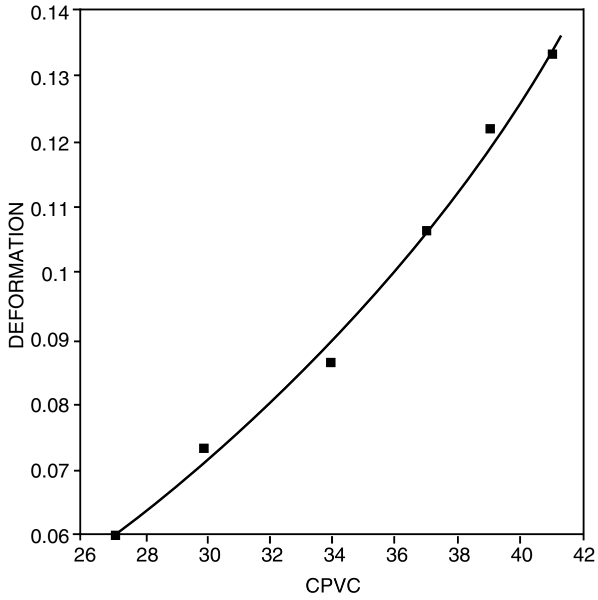

Figure 7—CPVC dependency on deformation.

The 119 nm latex/titanium dioxide, 193 nm latex/titanium dioxide, and the 193 nm latex/calcium carbonate paints were simulated at various PVCs using the algorithm described. The deformation found experimentally for the 119 nm latex was resubmitted to this simulation. The deformation for the 193 nm latex was assumed to be the same as the MFFT is the same. Hence, the simulation of the 193 nm latex used independently determined data. Two properties were determined from the three sets of simulated packings. The first was the packing density which should indicate the CPVC as the onset of air voids will cause a rapid lowering of the density. The second property was the latex to latex coordination number. This is one of a number of theoretical parameters, such as the latex to pigment coordination number, which can be easily estimated from the simulation. These numbers might be expected to have an important bearing on paint film properties such as tensile strength, scrubability, etc. Plots of the two properties in turn, versus PVC, are shown in *Figures* 8 and 9. The inflection points in these graphs are collected and compared with the experimental CPVCs in *Table* 1. The agreement between the two sets of results is good, especially considering the approximations made in the simulations. Not all graphs show an inflection point for the CPVC. The latex/latex coordination number plotted against PVC did not detect the CPVC for the 193 nm latex/titanium dioxide system. This is not unexpected that in this system both the latex and titanium dioxide particles have very similar particle sizes.

The effects of the approximations and assumptions made in these simulations are in general unknown. However, some comments can be made. First, all particles were assumed to be spheres. For pigments this is, at best, only approximate. Some pigments, such as mica, may not even be approximately spherical. For those pigments that are close to spherical, the errors are not expected to be large as it has been shown by simulation[19] that cylindrical and bean shaped particles, whose axial

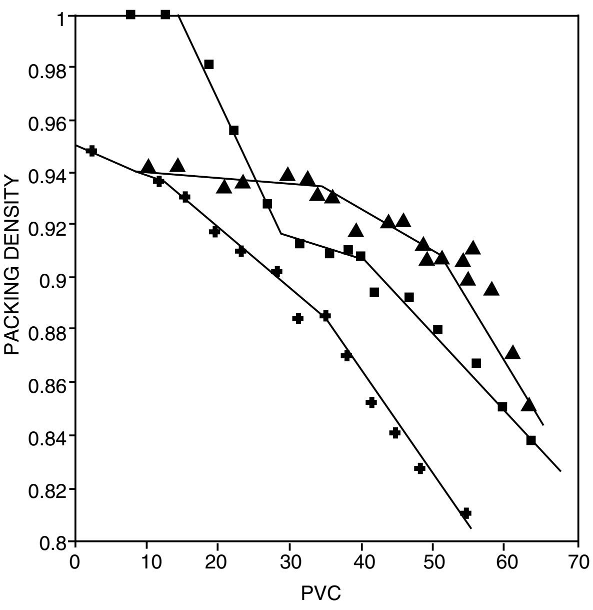

Figure 8—Simulated packaging density against PVC. (■) 119 nm latex/titanium dioxide; (+) 193 nm latex/titanium dioxide; and (▲) 193 nm latex/calcium carbonate.

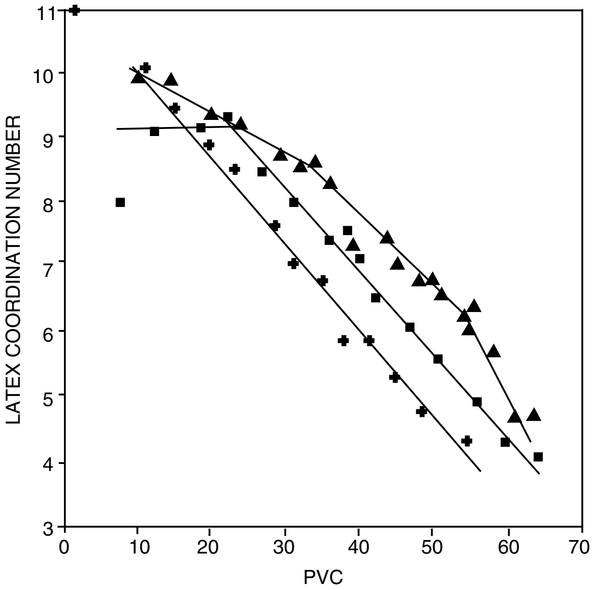

Figure 9—Simulated latex/latex coordination numbers against PVC. (■) 119 nm latex/titanium dioxide; (+) 193 nm latex/titanium dioxide; and (▲) 193 nm latex/calcium carbonate.

lengths do not vary greatly, have random close packing densities and coordination numbers not too different from those of spheres. Second, larger errors can be expected as the deformation of the latex increases. This is because the algorithm does not allow for a redistribution of that part of the latex volume which is lost in deformation. It has been shown that the lost volume is small for the deformation used in the simulations reported. However, the error in neglecting this volume increases as the deformation increases. It is expected to be able to reduce this error by increasing the complexity of the algorithm. Third, the effect of truncating the calcium carbonate particle size distribution and using only particles of less than 800 mm in the simulation is expected to be small, provided the small number of larger particles neglected are insuffficient to form a network and begin their own large particle packing. This appears to be the case as good agreement was found between the experimental and predicted CPVC for this system. The elimination of this approximation is a matter of computing power.

An additional factor which reduces the usefulness of the algorithm in its present form is that most acrylic latex paint formulations include some coalescing agent. A coalescing agent will increase the deformation of the latex. Thus, the CPVC will vary depending on the type and amount of coalescing agent. This factor could be taken into account if the variation in deformation for a particular latex that the amount of coalescing agent varied was known.

Table 1—Experimental and Simulated CPVC

	Experimental		Simulated	
	60° Gloss	Percent Transmission	Packing Density	Latex/Latex Coordination
	CPVC	CPVC	CPVC	CPVC
119 nm latex/titanium dioxide	40%	—	41%	—
193 nm latex/titanium dioxide	35%	—	35%	—
193 nm latex/calcium carbonate	55%	53%	53%	55%

CONCLUSION

It has been shown that simulations of the packing of pigment and latex particles can predict the CPVC of simple latex paint systems. The simulations require the particle size distributions of both the latex and pigments. Also required is the deformation value of a latex. This deformation value, at the present time, has to be determined from a PVC ladder but should be the same for all latices with the same MFFT. New data such as latex to latex, latex to pigment, and pigment to pigment coordination numbers are able to be estimated from the simulations. These parameters might be expected to have strong influences on such properties as tensile strength, elongation, scrubability, etc. We have not pursued such relationships or the extension of the algorithms to extenders which have a much larger size than latex particles in this preliminary paper. However, we intend to investigate these possibilities at a later stage.

ACKNOWLEDGEMENTS

The authors would like to thank the following people and their companies for their help in producing this research: H. McEwan, Tioxide Australia Pty. Ltd., who donated titanium dioxide and who gave advice on pigment dispersion; J. Belousof, Omya Southern Pty. Ltd., who donated calcium carbonates; R. Gailius, Rohm and Haas Australia Pty. Ltd., who donated the acrylic latices and measured their particle size distributions and MFFT; and finally, W. Thiedeman, Rohm and Haas Australia Pty. Ltd., who measured all gloss readings.

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Appendix 1

```
Begin (program paint)

    if new packing then
    begin (if)
        input particle population and lattice size
        randomly place particles
    end else
    begin (if)
        load existing lattice
    end (if)

    analyze packing parameters
    begin (packing analysis)

        begin (packing density)

                for every lattice particle
                begin (loop)
                    find volume of particle within or
                    partially within analysis region
                    adjust volume of latex particles due
                        to deformations
                end (loop)

                packing density = aggregate particle
                        volume/analysis region volume

    end (packing density)

    begin (PVC)

        for every lattice particle
        begin (loop)
            find volume of particle within or partially
            within analysis region
        end (loop)

        PVC = pigment particle volume/
                analysis region volume

    end (PVC)

    begin (deformation)

        for every latex particle
        begin (loop1)
            for every overlapping particle
            begin (loop2)
                    latex deformation = overlap/particle radius
                    store in distribution array
                end (loop2)
            end (loop1)

            deformation = mean of distribution array

        end (deformation)

    end (packing analysis)

    set iteration = true
    while iteration = true
    begin (while)

        for every lattice particle
        begin (loop1)

            analyze particle
                begin (particle analysis)

                    set net restoring force to zero (fx,fy,fz)
                    for every contacting particle
                    begin (loop2)
                        find overlap between particle and contact
                        calculate magnitude and direction of
                            restoring force
                        add to net restoring force (fx,fy,fz)

                    end (loop2)

                end (particle analysis)

            move particle under action of net restoring force

        end    (loop1)

            analyze packing parameters
            (packing density, PVC, deformation)
            If iterations are a multiple of 100 and deformation
                 < desired value then compress lattice vertically.
            if deformation = desired value
            then set iteration = false

        end (while)

        store coordinated of packing

    end (paint)
```