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Monte Carlo Simulations of Light Scattering by Composite Particles in a Planetary Surface

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Composite particles containing internal scatterers have been proposed as an explanation for the fact that most photometric studies of planetary surfaces based on Hapke's bidirectional reflectance model have found the planetary particles to exhibit moderately backscattering phase functions. However, an implicit assumption made in this explanation is that the scattering by composite particles containing multiple internal inclusions in a planetary surface can still be adequately computed using standard radiative transfer theory assuming the composite particles to be the fundamental scattering unit even though the particles are necessarily in close proximity to each other. This assumption was explored by J. K. Hillier (1997, *Icarus* 130, 328–335) using a Monte Carlo routine. However, in this initial study several simplifying assumptions were made. The internal scatterers were assumed to be isotropic and scattering off of the surface and absorption within the composite particle were ignored. While these assumptions are not very realistic, it was believed that the study could still provide insight into the light scattering by such surfaces. Here we relax these assumptions in order to examine the light scattering by more realistic particles. Almost all of the conclusions reached in the earlier paper remain valid. As before, we find that classical radiative transfer (assuming a random distribution of scattering particles) coupled with the assumption that the composite particle is the fundamental scatterer provides a good approximation in the high porosity limit. However, even for porosities as high as 90% the effects of close packing are clearly seen with the radiative transfer calculation underestimating the scattering by ∼10% at high phase angles. In contrast to the earlier study we find that the radiative transfer calculation tends to overestimate, not underestimate, the scattering at high emission but moderate phase angles. As the porosity is lowered further, the discrepancy becomes more severe and can reach 100% or greater. In particular, our main conclusion remains intact: the parameters derived using the classical radiative transfer theory will yield results intermediate between those of the composite as a whole and those of the internal scatterers and thus one should exercise caution in interpreting the results of models based on classical radiative transfer theory in terms of the physical properties of the surface particles.

Key Words: **radiative transfer; photometry; surfaces, planets; surfaces, satellites; regoliths.**

INTRODUCTION

Hapke's photometric model (1981, 1984, 1986) has been widely used to describe the light scattering properties of numerous Solar System bodies with particulate surfaces (e.g., Bowell *et al.* 1989, Buratti 1985, Domingue *et al.* 1991, Hapke 1984, Helfenstein *et al.* 1988, Helfenstein and Veverka 1987, 1989, Hillier *et al.* 1994, Verbiscer 1991, Veverka *et al.* 1987). The vast majority of these studies have found the surface particles to exhibit negative asymmetry parameters. In contrast, most laboratory studies suggest that particles should exhibit strong forward scattering lobes (Zerull *et al.* 1977, Giese *et al.* 1978, Weiss-Wrana, 1983). Using Hapke's model, Verbiscer and Veverka (1990) and Domingue *et al.* (1997) found that terrestrial snow does exhibit forward scattering behavior, in contrast to the planetary observations, which led them to suggest that the backscattering behavior of the planetary particles is due to a complex particle structure and texture such as particles containing internal scatterers including inclusions, microcracks, and bubbles (Hapke 1996). The McGuire and Hapke (1995) laboratory measurements show that nonabsorbing or weakly absorbing particles containing a large number of internal scatterers (optical thickness of the scatterers at least several tens) may indeed be backscattering even if the internal scatterers are forward scattering.[2] In contrast, Mishchenko (1994) argues that the planetary particles may in fact be forward scattering but that the approximations used in Hapke's model are not appropriate for a

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[2] It should be noted that McGuire and Hapke's results exclude the diffraction peak. However, as Hapke (1993) argues, the diffraction by a particle will be altered by its neighbors in a close packed surface. In addition, for large particles any diffracted light will be highly concentrated in the forward scattering direction and, in practice, will be indistinguishable from unscattered light. Therefore, in a planetary surface, it is appropriate to ignore the diffraction peak (in essence approximate any diffracted light as unscattered) while noting that the phase function and albedo derived for a particle is that of the nondiffracted component only.

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close packed medium (such as a planetary surface) and lead to erroneous findings.

Hillier (1997; hereafter Paper 1) used a Monte-Carlo scattering model to examine the light scattering from composite particles in a planetary surface. This paper showed that the effects of close packing modify the scattering by composite particles in a complicated way. Classical radiative transfer, whether assuming the composite as a whole or the individual scatterers as the fundamental scattering unit, provides only a rough approximation of the actual scattering particularly at high incidence, emission, or phase angles. However, several simplifying assumptions were made in Paper 1. The internal scatterers were assumed to be isotropic. In addition, all scattering was assumed to occur off of the internal scatterers; scattering from the surface of the composite particle or absorption within the particle was ignored. Neither of these assumptions are very realistic. In this follow-up study we relax these assumptions to examine the light scattering from more realistic composite particles.

MODEL

As was done in Paper 1, the planetary surface is assumed to consist of spherical particles containing randomly positioned internal scatterers. In Paper 1, all the scattering was assumed to occur from the internal scatterers and the internal scatterers were assumed to scatter isotropically. In this paper, these assumptions are relaxed. Scattering from the surface of, and absorption within, a composite particle are now both accounted for in the model. Further, the internal scatterers are now assumed to scatter light according to a Henyey-Greenstein phase function. With these refinements the individual particles in the surface are now described by a total of six parameters: the real and imaginary index of refraction of the composite particle (n_r and n_i), the optical depth of absorption across a diameter of the particle, τ_abs, the asymmetry parameter of the internal particle phase function, g, and the two parameters used in the original model—the internal particle single-scattering albedo, $\tilde{\omega}_0$, and the optical depth of internal scatterers across a diameter of the particle, τ_sc. It should be noted that the absorption optical depth and imaginary refractive index are related to each other through the (unspecified) particle size. In the model the absorption within the composite particle is determined from the absorption optical depth. n_i (along with n_r) only comes into play in determining the reflection coefficients and direction of refraction within a particle. For most materials of interest here, the imaginary refractive index has little influence on these factors. Thus, in practice, the imaginary index of refraction was ignored (set to 0). In addition to the parameters describing the composite scatterers the model contains one additional parameter: the porosity of the surface, P. The model parameters and their physical significance are summarized in Table I.

TABLE I
Summary of Model Parameters and Their Physical Significance

Parameter	Definition	Description and physical significance
$\tilde{\omega}_0$	Internal particle single-scattering albedo	Fraction of light scattered to light incident upon a single particle. It is related to the particle composition, size, and microstructure.
g	Asymmetry parameter	Describes the directional scattering properties of individual particles. g is the asymmetry parameter of a Henyey–Greenstein phase function. $g < 0$ indicates a backscattering particle while $g > 0$ indicates a predominately forward scattering particle.
τ_sc	Scatterer optical depth	Optical depth of internal scatterers across a diameter of the composite particle.
τ_abs	Absorption optical depth	Optical depth for absorption within the composite particle. Measured across a diameter of the composite particle.
nr, n_i	Index of refraction	Real (nr) and imaginary (n_i) indices of refraction of the composite particle.
P	Porosity	Fraction of space within the surface that is not occupied by particles.

A surface of such particles was generated randomly as described in Paper 1. Summarizing briefly, for highly porous surfaces (porosity >80%) it is possible to place the particles randomly within a square cell one at a time. However, as the porosity decreases much below 80% it becomes more and more difficult to find room for all the particles using this procedure. For these porosities an alternate procedure was employed. Initially, 175 particles were set in a regular $5 \times 5 \times 7$ square cubic close-packed lattice. The particles were then moved, in random order, one at a time by a random amount up to the initial distance between particles in the lattice being sure there was no overlap between particles after each move (if there was, the procedure was repeated until a valid spot was found for the particle). This procedure was then repeated four times to obtain a random distribution of paticles. Periodic boundary conditions were used to handle any rays that left the cell.

Once a random surface is generated, a Monte Carlo scattering routine is used to calculate the light scattering from the surface. The basic procedure is as follows. Photons are shot into the surface at random points and from random directions. The photon is then followed as it is scattered by the particles it encounters until it either is absorbed or escapes from the surface. This process is then repeated until adequate statistics are built up to describe the scattering in all desired directions.

Each run following a single photon is performed as follows. First, a random azimuth angle and intercept point with the surface is determined (for each calculation the incidence angle is given as an input to the model). The photon is then followed into the surface until it hits a particle. Whether the photon is reflected off the particle (at which point its interaction with the particle is done) or refracted into the particle is determined randomly using the Fresnel reflection coefficient. If refracted, three fates may befall the photon: It may be absorbed by the composite particle, encounter an internal scatterer, or make it through to the far boundary of the composite particle. A random distance, based upon the probability (as a function of the input absorption or scattering optical depth) of the photon traveling a given distance before being absorbed or encountering an internal scatterer is calculated. These distances are then compared with the distance to the far boundary of the particle and the smallest of these distances determines the photon's fate. If it is absorbed the run is complete. If it encounters an internal scatterer, it will either be absorbed (and again the run is complete) or be scattered with the probability being determined from the particle single-scattering albedo. If scattered, a new direction for the photon is determined randomly, weighted by the phase function. The calculation within the particle is then repeated starting from the location of the internal scatterer. If the photon reaches the far boundary, it can either be refracted out of the particle (at which point its interaction with the particle is complete) or be reflected back into the particle in which case the calculation within the particle is repeated. If the photon escapes from the composite particle, it is again followed until it encounters another particle or (if it is now traveling upward) it escapes from the surface. If it escapes, its phase angle and emission angle are recorded and placed in the appropriate bin so that the reflectance as a function of phase and emission angle can be calculated once adequate statistics are built up.

In addition to calculating the scattering from the surface, the above Monte Carlo routine was adapted for use in calculating the scattering properties (phase function and single-particle scattering albedo) of a single composite particle. These results, interesting in their own right, are needed to calculate the reflectance predicted by classical (low density) radiative transfer theory for comparison with the Monte Carlo results. These results are presented in the next section.

COMPOSITE PARTICLE PROPERTIES

In Paper I, it was found that internal scatterers within a composite particle could indeed make the particle as a whole backscattering even if the internal scatterers were isotropic. However, isotropic scatterers are not very realistic. For more realistic forward scattering particles Mishchenko and Macke (1997) and Lumme *et al.* (1997) have found that the composite particle, while less forward scattering than the individual internal scatterers, is nevertheless still forward scattering. Due to the assumptions made in Paper 1, we could not address this question but here we can examine the scattering properties of composite particles containing more realistic forward scattering particles. A typical internal scatterer would be a void within the particle or an inclusion of a material of significantly different index of refraction. A void would have an effective index of refraction of $1/n$, where n is the index of refraction of the composite particle as a whole, while an inclusion would have an index of refraction equal to m/n, where m is the index of refraction of the inclusion in a vacuum. As typical internal scatterers two cases are examined. As an example of a void, an internal scatterer with an index of refraction of $1/1.55$ (1.55 was chosen as a typical refractive index of silicates in the visible) was examined. A second case with an index of refraction of $2/1.55$ was examined as an example of an inclusion. The scatterers were assumed to be on the order of a wavelength in size (three cases were examined with a size parameter of $x = \pi/2$, π, and 2π corresponding to diameters of 1/2, 1, and 2 times the wavelength). Mie theory was used to determine the scattering properties of these scatterers. While the internal scatterers are likely not spherical and recent results (Lumme and Rahola 1998) do suggest some dependence of the light scattering properties on particle shape at size parameters of a few, Mie theory should still be a sufficient approximation at these small particle sizes (Pollack and Cuzzi 1980) at least for our purposes. The results are shown in Fig. 1. Also shown is the Henyey-Greenstein phase function employed in this study. As can be seen, a Henyey-Greenstein phase function with an asymmetry parameter ranging from 0.4 to 0.75 provides a reasonably good fit to the actual phase function of these inclusions. Thus, the Henyey-Greenstein phase function with an asymmetry parameters in this range should be a good approximation of actual internal scatterers and this function is employed throughout the rest of this paper. In our nominal models we have assumed an asymmetry parameter of $g = 0.6$.

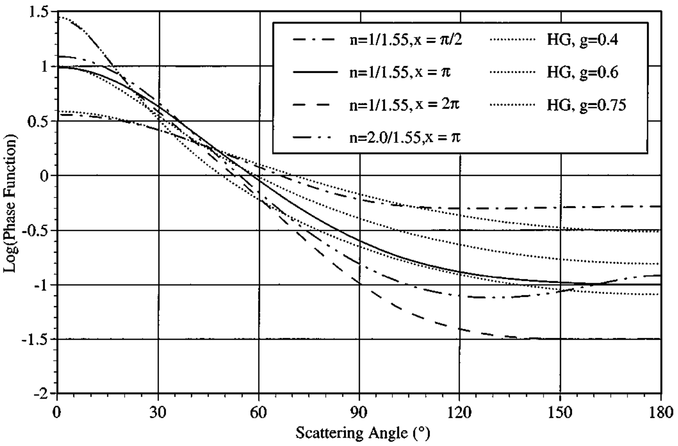

FIG. 1. Comparison of near wavelength size inclusion phase functions based on Mie theory to the Henyey-Greenstein phase function. The Henyey-Greenstein phase function with asymmetry parameter 0.4–0.75 provides a reasonable fit to the phase function expected for typical wavelength size inclusions.

Our results for the phase function and albedo of the composite particle, assuming no absorption within the composite particle, are shown in Figs. 2 and 3. With no internal scatterers, the distinctive rainbow and glory features associated with scattering from transparent spherical particles are seen. It should also be noted that as a test of our code our Monte Carlo results agree well with the predictions based on geometric optics (van de Hulst 1981) in the case of no internal scatterers. As expected, these features decrease as the optical depth of scatterers increases. They are still visible at an optical depth of one but are almost completely eliminated for optical depths greater than three. The asymmetry parameter and single-particle

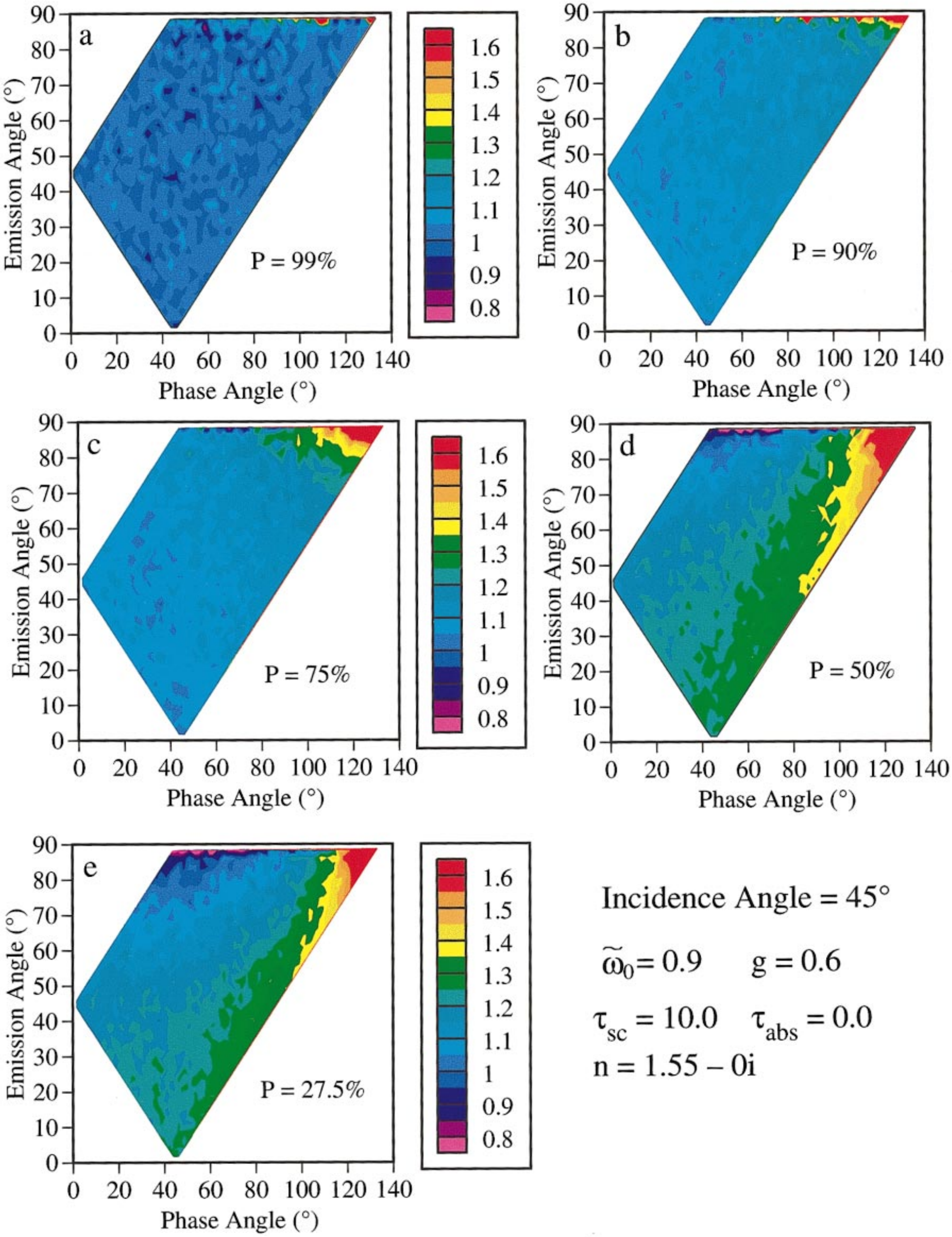

FIG. 5. Ratio of Monte Carlo calculations to predictions of classical radiative transfer as a function of porosity, emission angle, and phase angle at an incidence angle of 45°.

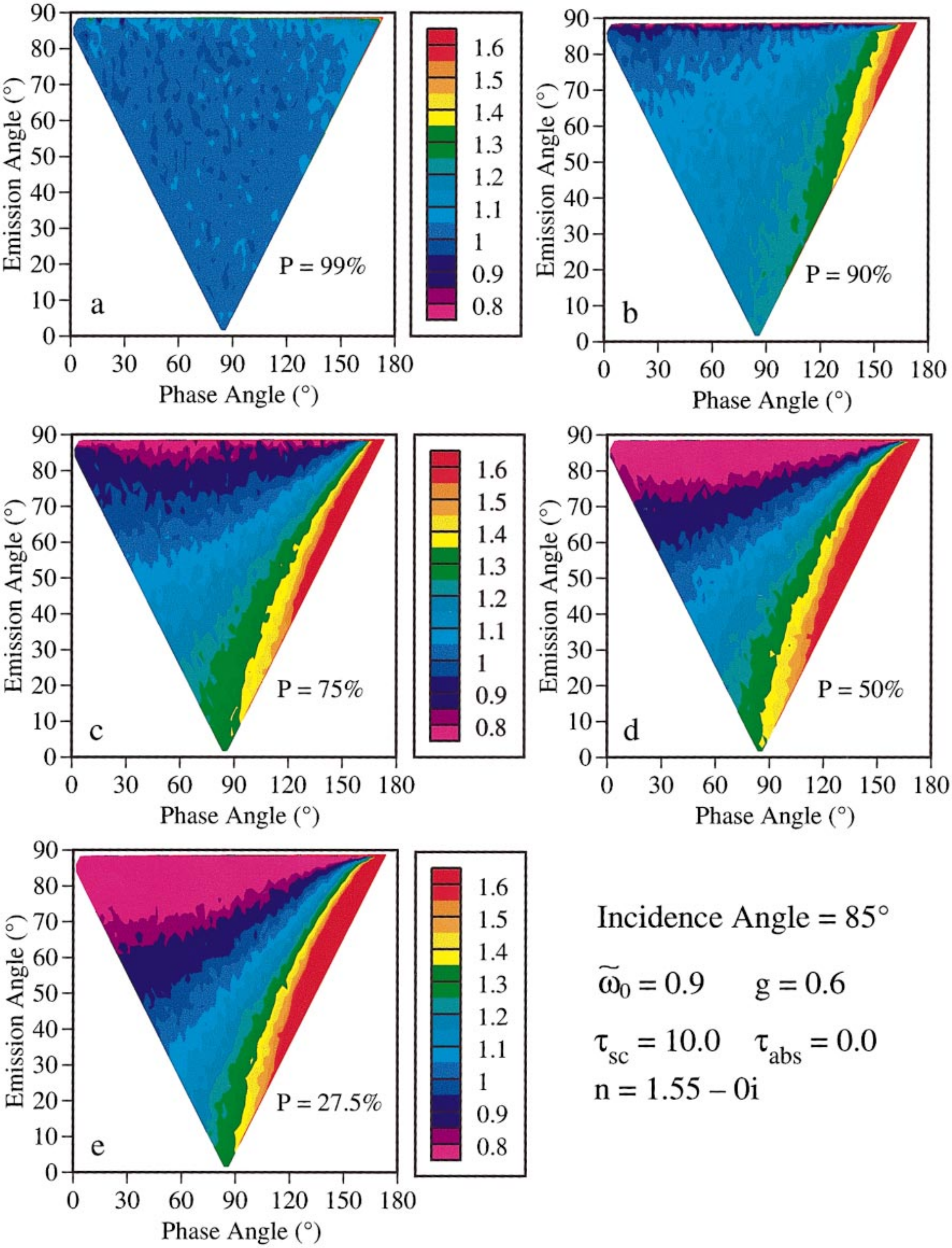

FIG. 6. Ratio of Monte Carlo calculations to predictions of classical radiative transfer as a function of porosity, emission angle, and phase angle at an incidence angle of 85°.

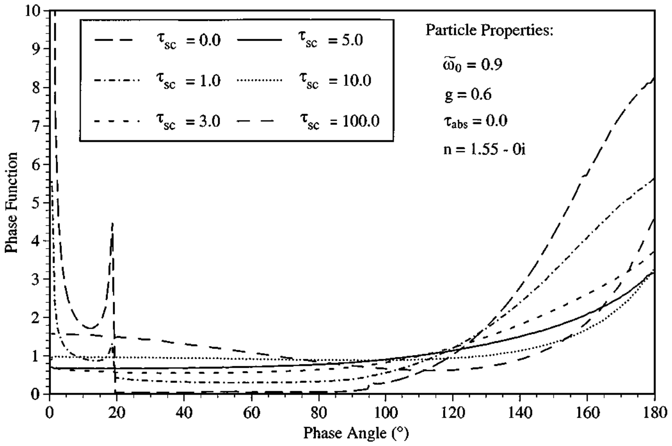

FIG. 2. Particle phase function for the composite particles as a function of internal scatterer optical depth. $g = 0.6$ for the individual scatterers is assumed.

scattering albedo of the composite particles are given in Table II. While the asymmetry parameter of the composite particles may approach zero, the composite particles remain forward scattering except at very high internal scatterer optical depths. For low albedo internal scatterers the composite particle remains significantly forward scattering for all optical depths (Table III). This is due, at least in part, to the fact that most of the reflected light in this case comes from reflection off of the composite particle surface. If we remove this contribution (by setting the index of refraction to 1) the degree of forward scattering is reduced but is still larger than that seen for the higher albedo internal scatterers (Table III). Thus, while it is possible to reduce the degree of forward scattering to nearly isotropic particles, composite particles containing realistic internal scatterers remain forward of isotropic scattering. Only for very large numbers of internal scatterers may the composite become significantly backscattering. These results are in full agreement with the conclusions of Mishchenko and Macke (1997) and Lumme *et al.* (1997).

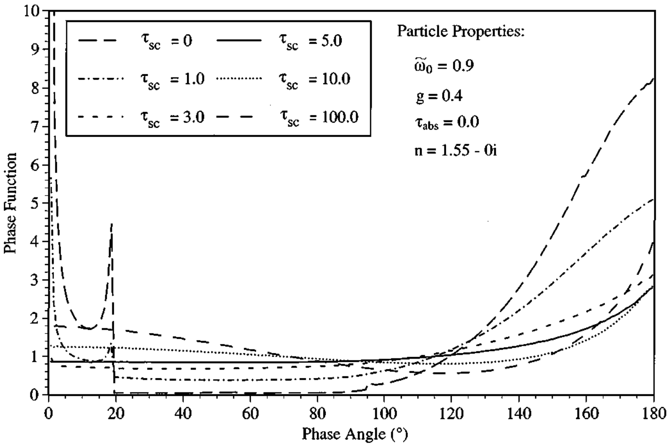

FIG. 3. Particle phase function for the composite particles as a function of internal scatterer optical depth. $g = 0.4$ for the individual scatterers is assumed.

TABLE II

Asymmetry Parameter and Albedo of a Transparent (τ_{abs} = 0.0) Composite Particle

τ_{sc}	g	$\tilde{\omega}_0$
	$\tilde{\omega}_{0_{int}} = 0.9$; $g_i = 0.6$	
0.0	0.619	1.000
1.0	0.472	0.874
3.0	0.293	0.680
5.0	0.199	0.548
10.0	0.071	0.372
100.0	−0.038	0.210
	$\tilde{\omega}_{0_{int}} = 0.9$; $g_i = 0.4$	
0.0	0.619	1.000
1.0	0.414	0.871
3.0	0.210	0.676
5.0	0.112	0.547
10.0	−0.020	0.387
100.0	−0.107	0.249

Note. $n = 1.55$ is assumed.

SURFACE SCATTERING PROPERTIES

Results for two nominal models representing a dark ($\tilde{\omega}_0 = 0.1$; $g = 0.6$; $\tau_{sc} = 10.0$; $\tau_{abs} = 0.0$; $n = 1.55 - 0i$) and bright ($\tilde{\omega}_0 = 0.9$; $g = 0.6$; $\tau_{sc} = 10.0$; $\tau_{abs} = 0.0$; $n = 1.55 - 0i$) surface were calculated for porosities of 27.5, 50, 75, 90, and 99% at three representative incidence angles of 5°, 45°, and 85°. The results were then compared to the predictions of classical radiative transfer theory assuming the single particle scattering albedo and phase function calculated above. Following our previous paper, a shadow hiding opposition surge following Hapke's (1986) formulation was included with width parameter, $h = -3/8\ \ln(P)$, where P is the porosity and amplitude parameter $B_0 = 0.75$ in the radiative transfer calculation (because our modeling does not

TABLE III

Asymmetry Parameter and Albedo of a Transparent (τ_{abs} = 0.0) Composite Particle

τ_{sc}	g	$\tilde{\omega}_0$
	$\tilde{\omega}_{0_{int}} = 0.1$; $g_i = 0.6$	
0.0	0.619	1.000
1.0	0.627	0.475
3.0	0.516	0.172
5.0	0.424	0.115
10.0	0.071	0.372
100.0	0.393	0.100
	$\tilde{\omega}_{0_{int}} = 0.1$; $g_i = 0.6$; $n = 1$	
1.0	0.583	0.072
3.0	0.512	0.039
5.0	0.415	0.025
10.0	0.236	0.015
100.0	0.018	0.009

Note. $n = 1.55$ is assumed.

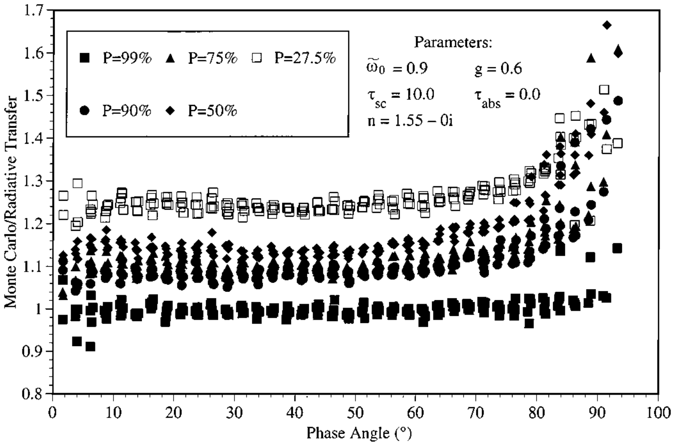

FIG. 4. Ratio of Monte Carlo calculations to radiative transfer results as a function of porosity at an incidence angle of 5°.

account for coherence the effects of coherent backscatter do not appear). As before, these parameters provide a good fit to the opposition surge found in the Monte Carlo results.

The ratios of the Monte Carlo calculations to the predictions of classical radiative transfer assuming the composite particle phase function for the bright surface are shown as a function of porosity and phase and emission angle in Figs. 4–6. A ratio of one indicates that classical radiative transfer provides a good fit to the data while significant deviations from one indicate where the radiative transfer approximation starts to break down. As expected, radiative transfer provides a good approximation at high porosities: at a porosity of 99% the ratio remains near one at all phase, emission, and incidence angles. However, even for porosities as high as 90% significant deviations are seen with classical radiative transfer calculations underestimating the scattering at phase angles $>60°$ by 10% or more. As the porosity is reduced further, these discrepancies increase. In general, compacting the surface tends to brighten the surface at most viewing and illumination geometries, but especially so at high phase angles where the discrepancy can reach 100% or more for a highly compacted surface. This is the same behavior suggested by the simpler model employed in Paper 1 and suggests that using a model based on classical radiative transfer will yield more forward scattering particles than the true composites. However, while more forward scattering than the composites, they are, as found in Paper 1, less forward scattering than the internal scatterers.

While the underestimation of the scattering by radiative transfer increases as the phase angle is increased, the opposite effect is seen with the emission angle. The ratio of the Monte Carlo to radiative transfer results decreases as the emission angle is increased. In fact, the general trend for the surface to brighten reverses and radiative transfer theory overestimates the scattering at very high emission angles as long as the phase angle remains moderate. The opposite trend was found in Paper 1 where it was found that the underestimation of the scattering by radiative transfer increased with increasing emission angle. However, the data were binned in 2.5° wide bins in emission (and phase) angle and thus data from a variety of phase angles were included in each emission angle bin. Because the highest phase data would be included in the highest emission angle data, this might tend to skew the results toward higher ratios at higher emission angles. A reexamination of the data (assuming isotropic particles) shows that it indicates a similar trend with the ratio decreasing as the emission angle increases, though less severely than seen in the current paper. This observation may also provide an alternative explanation for the earlier paper's finding that the ratio falls off near opposition at high incidence angles. At high incidence angles, data near 0° phase angle will necessarily be at grazing emergence, and the fall off seen at low phase angle in this case may in fact be due to the high emission angle rather than the low phase angle.

Why is the scattering relatively lower than expected at high emission angle? One possible explanation is that light that escapes from a particle heading nearly straight upward toward the planet's surface will tend to come from the upper regions of a particle while light that leaves at higher emission angles (or is scattered back down into the surface) will generally come from regions of the particle more deeply imbedded in the surface. For a close-packed surface, a particle will occupy a significant fraction of an optical depth in the surface. Thus, though the light may emerge from the same particle, that which is scattered at low emission angle will generally exit the particle higher in the surface than light scattered at higher emission angles. Therefore, light scattered at more grazing emergence, generally exiting at points deeper in the surface, will have less of a chance of escaping before being absorbed or rescattered by another particle, leading to a reduction in the reflectance at high emission angles. If this explanation is true, then the magnitude of the effect should be greatest for the spherical particles assumed here and may be reduced for the more irregularly shaped particles one would expect to find in a typical planetary surface. However, it seems likely to occur at some level for such particles as well.

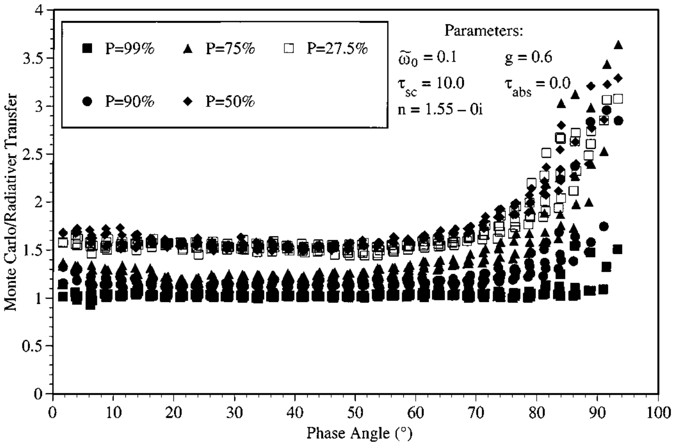

FIG. 7. Ratio of Monte Carlo calculations to radiative transfer results as a function of porosity at an incidence angle of 5°.

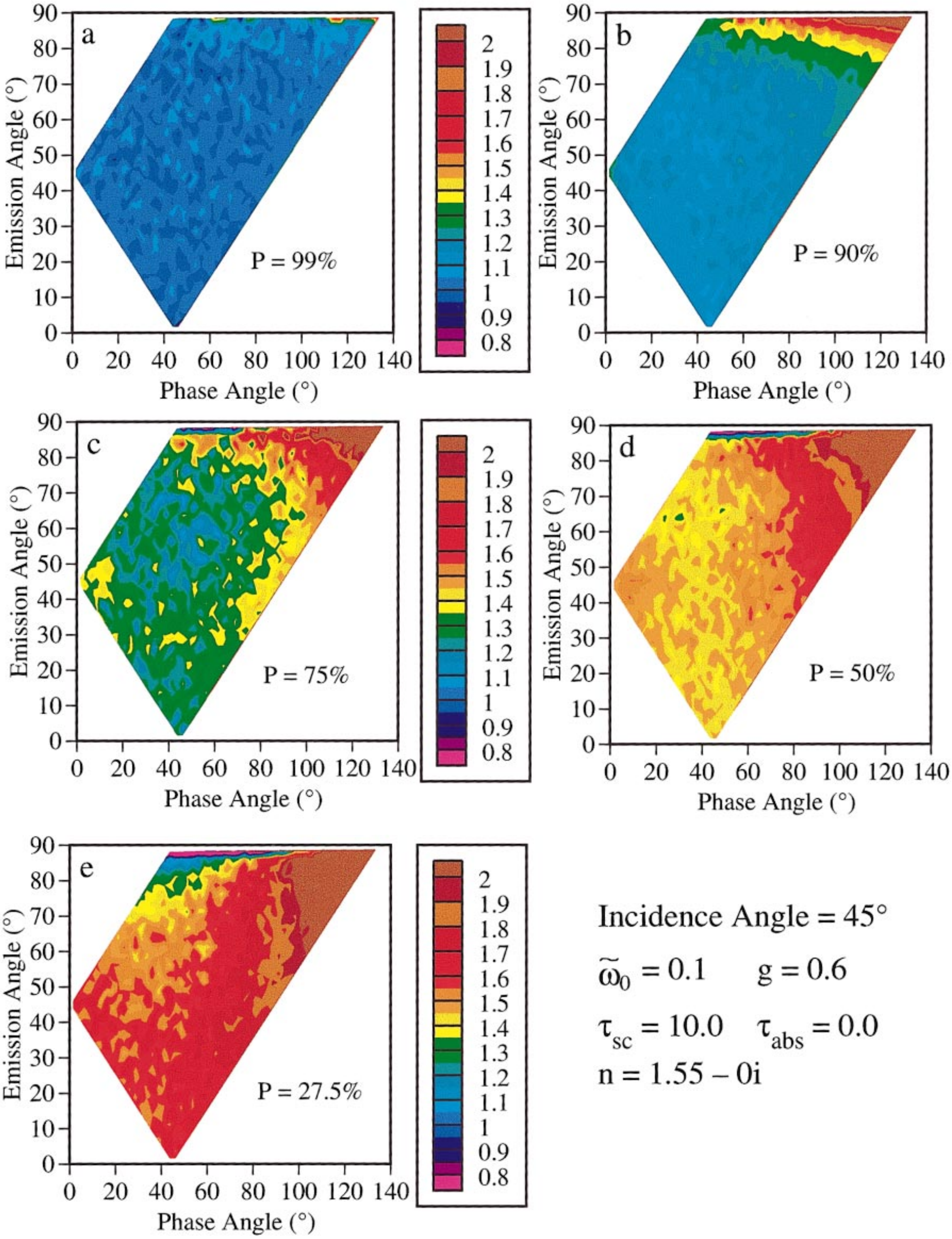

FIG. 8. Ratio of Monte Carlo calculations to predictions of classical radiative transfer as a function of porosity, emission angle, and phase angle at an incidence angle of 45°.

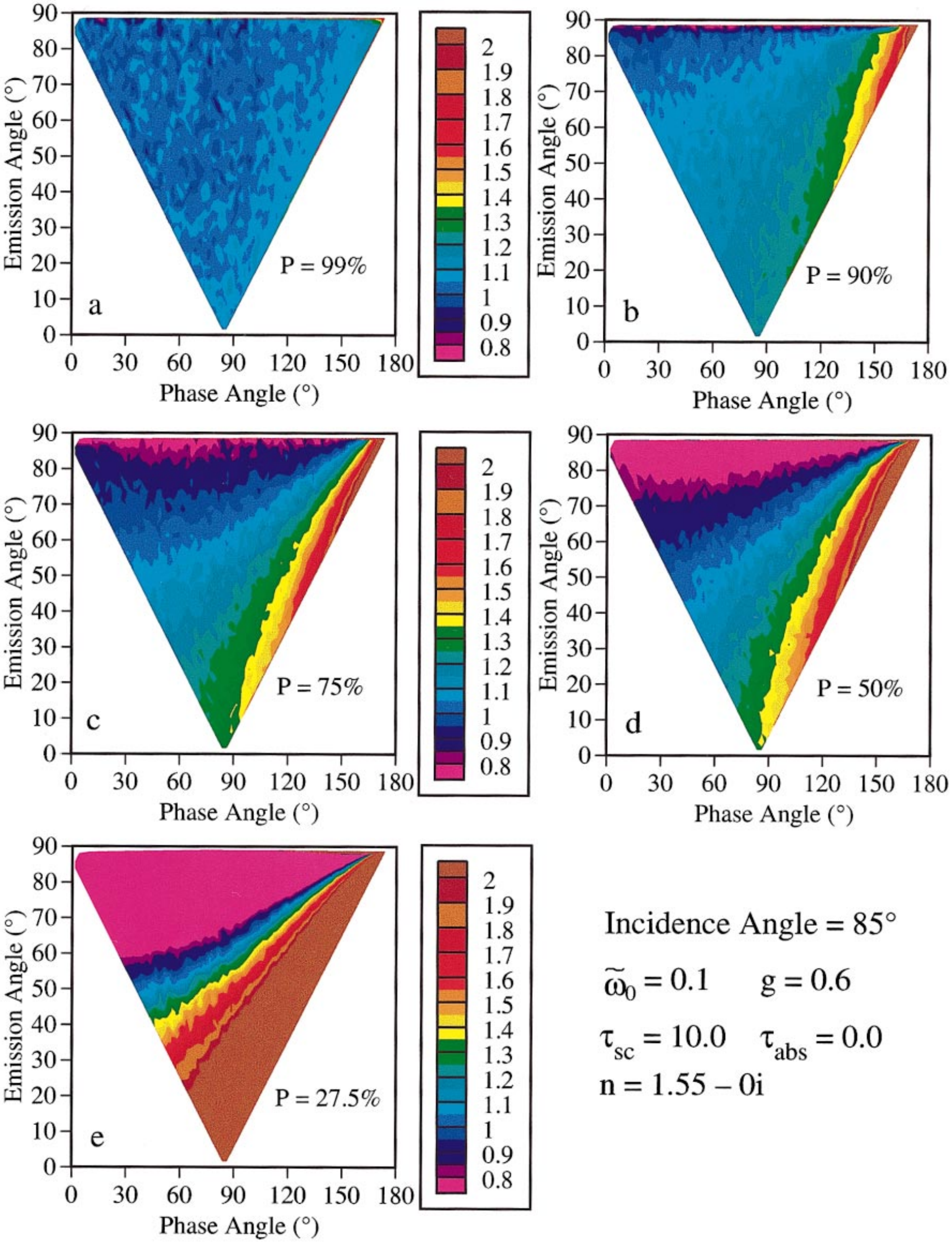

FIG. 9. Ratio of Monte Carlo calculations to predictions of classical radiative transfer as a function of porosity, emission angle, and phase angle at an incidence angle of 85°.

The ratios of the Monte Carlo to radiative transfer results for the dark surface as a function of porosity, phase angle, and emission angle are shown in Figs. 7–9. While trends similar to those found for the bright surface are seen, the discrepancies between the Monte Carlo and radiative transfer results are larger at lower albedos. As the albedo is lowered, the singly scattered component becomes more important. Thus the larger discrepancy at lower albedos can readily be explained by the fact that, as reported in Paper 1 and by Pelteniemi and Lumme (1992), the effects of compaction are seen most strongly in the singly scattered component of the scattering. In contrast to the singly scattered component, the multiply scattered light tends to lose memory of its original path in the surface, becoming more isotropic and thus it is less influenced by the compaction state of the surface.

CONCLUSIONS

In our original study (Paper 1) we studied the light scattering from a planetary surface consisting of composite particles. However, several simplifying assumptions (isotropic internal scatterers, no scattering off of, or absorption within the composite particle) were made in our initial study. In this follow-up study these assumptions were relaxed. While the model has been refined, most of the conclusions of the original paper remain valid.

Mishchenko and Macke (1997) found that, for realistic forward scattering internal scatterers, composite particles remain nearly isotropic to forward scattering except at very large internal scatterer optical depths. Our original study, which assumed isotropic internal scatterers, could not address this question. However, in this study we confirm Mishchenko and Macke's result.

As expected, classical radiative transfer provides a good approximation in the low density limit. However, even for porosities as high as 90% significant deviations from classical radiative transfer are seen, particularly at high incidence, emission, and phase angles. The effects of close packing are most pronounced at high phase angles where classical radiative transfer significantly underestimates the scattering. These results indicate that models based on classical radiative transfer will yield more forward scattering asymmtery parameters than the true composites, though still less than the individual internal scatterers. The effects of close packing modify the scattering by composite particles in a complicated way. Classical radiative transfer, whether assuming the composite particle as a whole or the individual scatterers as the fundamental scattering unit provides only a rough approximation of the actual scattering. Similar conclusions were reached in Paper 1. In a departure from our previous conclusions, however, we find that compaction decreases, rather than increases, the scattering expected at high emission but moderate phase angles. Despite this last disagreement, most of the conclusions of our original paper remain valid. In particular, our cautionary note that models based on classical radiative transfer should be avoided if possible and, where this is impractical, one should at least exercise caution in interpreting the derived parameters in terms of the actual physical properties of the surface remains in force.

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