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Accurate and robust characterization of volume scattering materials using the intensity-based inverse adding-doubling method

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ABSTRACT

In several different research disciplines, modelling and simulating light propagation through volume scattering materials is a key necessity. Simulating diffusing and fluorescent materials in solid-state lighting and the interactions between intense light and skin tissue in biomedicine are just some examples of the widespread need for accurate volume scattering models. Although modelling volume scattering materials is important for several research fields, there is still no widespread reporting of model properties or of accurate and robust tools to estimate them, especially for lighting research. Most often, researchers estimate the scattering model properties, i.e. the absorption and scattering coefficients and the anisotropy factor, using Mie solutions. These are generally based on rough estimates of the scattering particle's properties and assume that the particle is perfectly spherical or cylindrical. This approach is not well suited for the myriad of volume scattering materials available for illumination research. Our work uses the intensity-based inverse adding-doubling (i-IAD) method to estimate the volume scattering model properties of samples. In this work, we investigate the feasibility of this method in an experimental scenario by studying samples made with two different scattering particles embedded in a transparent polymer with different scattering particle concentrations and sample geometries. The light scattered by the samples is measured and their volume scattering properties estimated with i-IAD. We show the accuracy and robustness of i-IAD by extrapolating the scattering parameters obtained for low concentration samples to higher concentrations and comparing simulations with experiments for these higher concentrations. Furthermore, measurements of samples that contain both types of scattering particles were also accurately simulated using the model parameters estimated from low concentration samples. This work demonstrates that the intensity-based inverse adding-doubling method provides accurate estimates for the volume scattering model parameters and that they can be generalized for different concentrations, geometries and scattering particle mixtures.

Keywords: Volume scattering, solid-state lighting, inverse problem, adding-doubling

1. INTRODUCTION

The redistribution of light in terms of position and direction because of optical inhomogeneities in a sample is called volume or bulk scattering.¹ In lighting this typically takes the form of a transparent matrix, usually made from a polymer such as PMMA or polycarbonate, to which particles of a material with a different refractive index are added. These materials are a crucial component of many devices in lighting. Mainly they are applied to diffuse or broaden the radiation pattern of light sources. It is usual to find diffusing elements in display backlights and luminaires.¹⁻³ Fluorescent materials are another relevant example of a material that exhibits volume scattering. Fluorescent materials, in the form of phosphors, are ubiquitous in lighting as they provide the most efficient way to create white light with solid-state sources such as LEDs. The scattering properties of phosphors greatly influence the colour conversion efficiency and colour mixing properties of fluorescence based white light sources. The importance of volume scattering however is not limited to lighting research: fields such as astronomy⁴ and biomedicine^{5,6} are active areas of research where volume scattering is a crucial phenomenon.

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The radiative transfer equation (RTE) provides a very efficient way to model light propagation through optically opaque materials, which includes volume scattering. To simulate light propagation through a specific volume scattering material, the RTE requires three parameters. The first two, the scattering and absorption coefficients, μ_s and μ_a , define the proportion of light that is redistributed due to scattering and absorption, respectively, per path length. The third parameter is the single-event phase function, $p(\theta)$, which describes the angular redistribution or deflection at each scattering event. In other words, at every scattering event the phase function defines the probability of each new direction that the light ray can take. The phase function can take an arbitrarily complex shape, but in practice some simplifications are typically employed. In most cases in lighting, the scattering is assumed to be rotationally symmetric, which is generally true for non-birefringent samples with random orientation of the scattering particles. Furthermore, in most cases a phase function model is used, which permits defining the phase function with a single, or a small set of parameters. The Henyey-Greenstein phase function model and the Gegenbauer kernel model are the two most widely used phase function models in lighting which are described by Equation (1) and Equation (2), respectively.

$$p(\theta) = \frac{1 - g^2}{4\pi (1 + g^2 - 2g \cos(\theta))^{3/2}} \quad (1)$$

$$p(\theta) = \frac{\alpha g}{\pi} \frac{(1 - g^2)^{2\alpha}}{(1 + g)^{2\alpha} - (1 - g^{2\alpha})} (1 + g^2 - 2g \cos \theta)^{-\alpha-1} \quad (2)$$

Any numeric method that implements the radiative transfer equation uses the volume scattering model described above. These methods allow predicting, or simulating, how light is scattered from volume scattering materials. Regardless of the numeric method chosen to perform the simulations, it is necessary to have accurate estimates for the volume scattering model parameters, which is true for all modelling work. Two main approaches are usually followed to estimate the model properties: direct and inverse approaches. In a direct approach the microscopic properties of a samples and its constituent particles need to be known. This includes, generally, the scattering particles' geometry and (complex) refractive index and the refractive index of the surrounding medium, usually a transparent binder.⁷ These properties are known for some standard materials, but generally have to be estimated with specialized equipment in an accurate way which can be experimentally challenging. With these microscopic parameters at hand, a numeric tool that solves Maxwell's equations can be used to estimate the (macroscopic) volume scattering parameters. Because it is generally time intensive to solve Maxwell's equations, simplifications such as Mie solutions are sometimes employed at the expense of the type of scattering geometries that can be modelled.

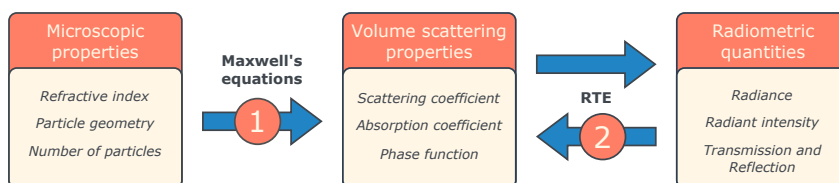


Figure 1: Illustration of the differences between direct (1) and inverse (2) approaches.

In the inverse approach it is not necessary to know the microscopic scattering properties or particle geometry. Instead, the macroscopic properties are estimated directly from experimental measurements of the behaviour of light when it interacts with the sample.² As the name indicates, in the inverse approach the consequence (change in the behaviour of light) is used to predict the cause (sample's scattering properties). In an inverse approach there are two requirements. First, it is necessary to have a way to experimentally measure the light scattered by a sample. The second is that it is necessary to have a method to simulate how the sample scatters light. The first requirement is easily satisfied. For instance, integrating spheres and goniometers are typically used to measure light scattering and can provide the type of data necessary as input for an inverse approach. Methods such as Monte Carlo ray-tracing and adding-doubling^{8,9} are usually available to simulate scattered light from samples when their volume scattering parameters are known. Having met the two requirements, the inverse approach is

usually framed as a numerical optimization problem. The goal is to find the set of scattering model parameters that minimizes the difference between the simulated and experimentally measured scattered light distribution. Depending on the numeric tool used to simulate the scattered light distributions, the inverse method takes a different name. Inverse adding-doubling (IAD)² and inverse Monte Carlo¹⁰ use the adding-doubling method and the Monte Carlo ray-tracing method, respectively, to perform the simulations. Depending on the method chosen to perform the simulations, it may be necessary to carefully consider which numerical optimization method is best suited for the inverse problem.

In most situations in lighting, inverse methods provide a much simpler way to obtain the volume scattering properties of material samples. But it is generally unknown how well the obtained parameters scale to other similar samples. That is, it is not clear if the volume scattering parameters obtained for a sample with a specific concentration of scattering particles can be used to predict the scattering properties of a more concentrated sample or a sample with a different geometry. This is, after all, one of the great advantages of estimating the scattering properties for a material: being able to predict its scattering effects in different conditions.

We tackle this question in this work for the inverse adding-doubling method. We extract the volume scattering parameters from experimental measurements of scattering samples with a low concentration of scattering particles and use those parameters to predict the scattering properties of more concentrated samples, which we also measured. Finally, we measure samples with two different types of scattering particles and combine the previously extracted volume scattering properties for each individual particle to predict the light scattering distribution of the hybrid sample.

2. METHODS

To estimate the volume scattering model parameters for a sample with inverse adding-doubling it is necessary to experimentally measure how the sample scatters light. The experimental procedure is described below, followed by some numerical aspects related to IAD.

2.1 Experimental measurements and material samples

The inverse adding-doubling method fits to the radiant intensity of light scattered by a sample to estimate the volume scattering parameters. We measure this information with a bidirectional scattering distribution function (BSDF) measurement device built at our laboratory.¹¹ A schematic of the measuring setup is shown in Figure 2. The volume scattering sample is positioned in the center of rotation of the BSDF setup and it is illuminated, at a predetermined angle of incidence, by a collimated light source. The detector head moves around the sample and measures the captured spectral radiant flux at a predefined set of angles. More information about the setup can be found in the original publication.¹¹

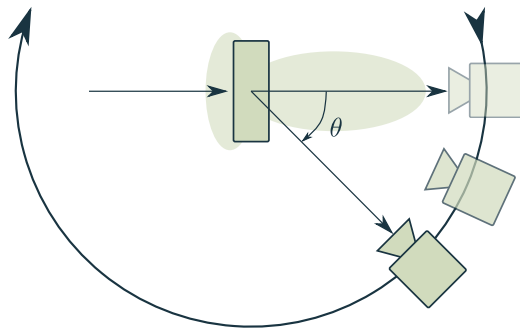


Figure 2: Depiction of a BSDF measuring device. Light is incident perpendicular to a sample positioned in the center of rotation of a spectral detector. The detector measures the spectral radiant flux at each angle θ to construct the BSDF. The scattering lobes for the sample are shown in transparent gray.

After some initial testing, we found that the samples used in this work scatter light in a rotationally symmetric way. Furthermore, we only consider the case where the scattering sample is illuminated with on-axis

incidence. This simplifies the calculation of the BSDF. First, the samples are only illuminated with on-axis light (perpendicular to their surface). But more importantly, the scattering can be fully described with a single angle θ , which means that the scattering only needs to be measured along a single axis of rotation instead of the usual two. Furthermore, because scattering in the range $\theta \in [-180, 180]^\circ$ is symmetric around 0° , only half of this range is considered, i.e. $\theta \in [0, 180]^\circ$.

The BSDF measurements obtained with the experimental setup can be converted to normalized radiant intensity, so that they can be used with inverse adding-doubling, by using the simple relation described in Equation (3). It is important to note that the full set of scattering angles was split into two ranges: one corresponding to transmitted (or forward) directions and another corresponding to reflected angles. This permits defining transmitted scattered radiant intensity and reflected scattered radiant intensity quantities which are useful for the inverse fitting process. In all graphical representations of these quantities in this work, e.g. Figure 3, 0° corresponds to light leaving the sample perpendicular to its surface for the transmitted radiant intensity while 90° corresponds to light reflected perpendicular to the sample's back surface for the reflected transmitted intensity. In other words, the transmitted radiant intensity peaks at 0° while the reflected radiant intensity peaks at 90° . Another relevant note is that while the BSDF device provides spectral measurements, all the work done uses only the measurements for a single wavelength $\lambda = 550$ nm.

$$I(\theta) = BSDF(\theta) \cos(\theta) \quad (3)$$

Two different materials were measured with the setup described, which for simplicity will be called material A and material B throughout this manuscript. Material A corresponds to polysiloxane polymer particles dispersed in a transparent polycarbonate binder, while material B corresponds to PMMA or acrylic particles also dispersed in polycarbonate. For each material, samples with different concentration of scattering particles and thickness were measured. All samples are 10 by 10 mm wide, while the thickness varies for each sample. Two sets of samples were measured: a low concentration set $\rho = \{0.05, 0.10, 0.20\}$ w/w % and a high concentration set $\rho = \{0.40, 0.80, 1.20\}$ w/w %, where w/w % is the weight by weight ratio, i.e. the ratio between the mass of the scattering particles and the total mass of the sample. For each concentration, samples with three different thickness values were measured: $d = \{1.0, 2.0, 3.0\}$ mm for the low concentration samples and $d = \{1.5, 3.0, 4.5\}$ mm for the higher concentrations. This results in a total of 18 different samples.

Another set of samples was also measured, which have the same amount of both scattering materials included. The set of these hybrid samples is smaller, with $\rho = \{0.2, 0.4\}$ and $d = \{1.5, 4\}$ for a total of 4 samples.

2.2 Volume scattering characterization

The model properties that need to be estimated for each sample are the scattering and absorption coefficients and the phase function model parameters. The Gegenbauer Kernel (GK) phase function model was chosen for this work, as it was previously reported to provide good results for a similar problem.¹² The GK phase function model is defined by only two parameters as shown in Equation (2): g , the anisotropy factor, and α which is a shape factor.

The inverse adding-doubling method follows closely the approach described in the introduction: it iteratively tests new volume scattering parameters, simulates the radiant intensity with adding-doubling for those parameters and compares it to the experimental measurement to determine if the parameters are "correct" or if a new set of scattering parameters should be tested. This means that it is necessary to choose two aspects when implementing IAD: which objective function should be used to compare simulations and measurements and what numeric optimization algorithm should be used to find the best set of parameters in an accurate and efficient way.

The chosen objective function can determine the type of parameters found. For instance, if the sample scatters light strongly in the backwards direction, then the radiant intensity of light that is transmitted will be very low. This means that an objective function that only takes the absolute magnitude of the scattered light into account could end up ignoring the low contribution of the transmitted radiant intensity and fit, almost exclusively, to the reflected radiant intensity. In other words, the choice of objective function should be such that it takes advantage of all the information available in the measurements so that the numeric optimization can

best exploit it to find the best possible result for the problem. The objective function chosen for this problem can be seen in equation Equation (4). The objective function $F(\mathbf{x})$ for a set of scattering parameters \mathbf{x} is the combined root mean-squared error (RMSE) between the simulated and measured reflected radiant intensity, I_R^s and I_R^m , and transmitted radiant intensity, I_T^s and I_T^m , scaled by their average magnitudes, $\overline{I_R^m}$ and $\overline{I_T^m}$.

$$F(\mathbf{x}) = \frac{\text{RMSE}(I_T^s, I_T^m)}{\overline{I_T^m}} + \frac{\text{RMSE}(I_R^s, I_R^m)}{\overline{I_R^m}} \quad (4)$$

The other choice is related to the optimization algorithm. This is the algorithm that will choose the next set of test volume scattering parameters. The goal is to do so in a way that minimizes the amount of time or tests necessary to go from a random starting guess towards the global minimum of the objective function. In this case, this will correspond to the best set of volume scattering parameters for the measured sample, i.e. the volume scattering parameters that best reproduce the observed scattered radiant intensity. In this work, we use a combination of a metaheuristic algorithm with a local convex optimizer following.¹³ The genetic algorithm is used to explore the domain of volume scattering parameters and avoid possible multiple solutions or saddle points. When close to an optimum solution, a sequential quadratic programming is applied starting from the best solution estimated by the genetic algorithm to further refine it.

3. RESULTS

3.1 Volume scattering parameters

The volume scattering parameters obtained using IAD for the low concentration samples of each scattering particle type are shown in Table 1. The volume scattering parameters obtained for the samples with varying thickness were averaged. To understand the quality of the volume scattering parameters obtained with IAD, a comparison between the measured and simulated scattered radiant intensity for the best and worst match are shown in Figure 3 for both types of samples. The best match for material A corresponds to ($d = 1.0$ mm, $\rho = 0.05$ w/w%) and the worst to ($d = 2.0$ mm, $\rho = 0.20$ w/w%), while for material B the sample with the highest and lowest quality match are ($d = 3.0$ mm, $\rho = 0.05$ w/w%) and ($d = 2.0$ mm, $\rho = 0.05$ w/w%) respectively. The simulations and experiments generally agree very well. However, for certain samples there is a significant amount of surface scattering, which creates a near-specular peak, which can be seen on the top-right image in Figure 3. This surface scattering effect is not included in IAD, which only models volume scattering. While the effect is less visible in other samples, it is likely that it still has a subtle effect on the intensity distribution, which can impact the volume scattering parameters obtained with IAD.

Table 1: Volume scattering parameters estimated with IAD for the low concentration samples.

Parameter	Material A			Material B		
	$\rho = 0.05$	$\rho = 0.10$	$\rho = 0.20$	$\rho = 0.05$	$\rho = 0.10$	$\rho = 0.20$
μ_s (1/mm)	0.0012	0.0030	0.0034	0.0054	0.0095	0.0138
μ_a (1/mm)	0.7884	1.5036	3.0730	0.3036	0.5921	1.3199
g	0.8783	0.8450	0.8335	0.9373	0.9190	0.9290
α	1.1473	1.2870	1.4819	0.7633	1.0624	1.0922

The obtained scattering parameters follow the expected trend for the scattering and absorption coefficient. That is, as the concentration of scattering particles increases, both coefficients also increase. The phase function model parameters, however, vary with the concentration of scattering particles, which is generally not expected. It is possible that the observed variation of the phase function model properties does not correspond to a significant change in the actual phase function shape. To ascertain if this is the case, the phase function for the lowest and highest concentration for each material is shown in Figure 4. Clearly, the shapes are significantly different. There are two plausible justifications for this deviation between what was predicted and what was observed. The first is that the manufacturing process at higher concentrations altered the shape of the scattering

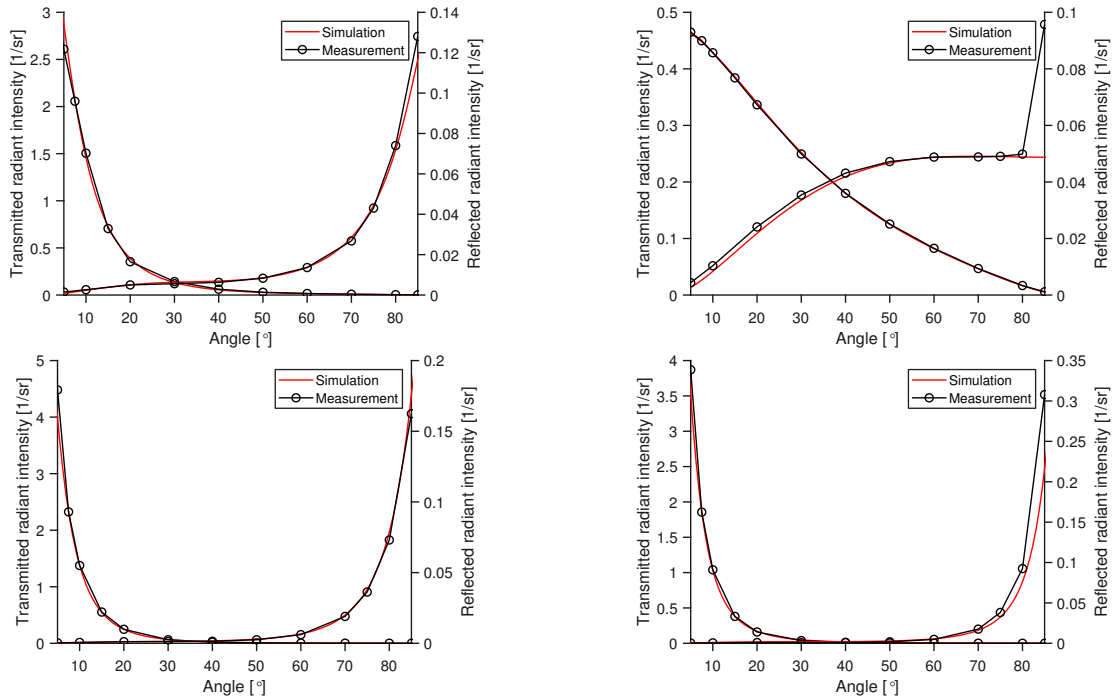


Figure 3: Comparison between measured and simulated scattered radiant intensity for the (left) best match and (right) worst match. The top row shows the results for material A and the bottom for material B.

particles. There is partial evidence for this, as one of the high concentration samples that was measured but not reported here, included scattering particles that scattered light anisotropically. Furthermore, the higher the concentration the more likely it is for scattering particles to clump together, also changing their optical geometry and thus the scattering properties. The second justification is related to the surface scattering effect discussed in the previous section. Surface scattering is not modelled with IAD, but it certainly has an impact on the light redistribution properties of a sample. Thus, the volume scattering properties estimated with IAD may deviate from their true value due to surface scattering.

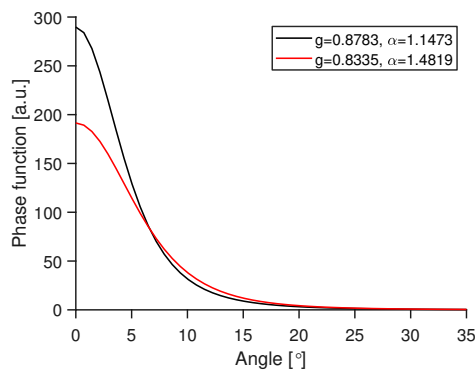


Figure 4: Comparison between the estimated phase functions for the lowest and highest concentration samples of material A.

3.2 EXTRAPOLATION TO DIFFERENT SAMPLES

The previous results show that the IAD method is capable of estimating the volume scattering parameters from the scattered radiant intensity of samples. But the usefulness of estimating the single-event volume scattering parameters for a certain sample is in using them to extrapolate the scattering properties of samples that were not characterized with IAD and simulate how they scatter light. This is a direct consequence of the fact that the volume scattering parameters only depend on the material properties and not on the geometry.

We perform two tests to investigate if the parameters obtained with IAD for the low concentration samples are robust enough to predict the scattering properties of samples that were not characterized. First, we test if they can predict the scattered radiant intensity that was measured for the higher concentration samples of material A. Then, we test a more complicated case, where samples with a mixture of both types of scattering particles, material A and B, were measured. The scattering characterization for each individual scattering material was combined and used to predict the scattering properties of the hybrid sample.

3.2.1 Higher concentration

The scattering properties of a sample depend linearly on the concentration of scattering particles, i.e., the number of particles per volume. This is generally true while the concentration is not too high. After a set point, the assumption that a scattering particle is isolated from surrounding scattering particles is violated and the estimated scattering properties are no longer appropriate.

This translates into a linear dependence of the extinction coefficient $\mu_t = \mu_a + \mu_s$ with concentration. A simple linear fit was performed on the volume scattering parameters obtained with IAD for each material type and is shown in Figure 5. The scattering parameters estimated from the measurements show a clear linear increase. It is important to note that this relationship is only for the scattering and absorption coefficients. These are bulk quantities and depend on the number of scattering particles per unit volume. The phase function parameters, g and α are single-scattering properties that only depend on the geometry and optical properties of the scattering particles and surrounding medium. For the remaining tests, these values were assumed to not depend on the concentration.

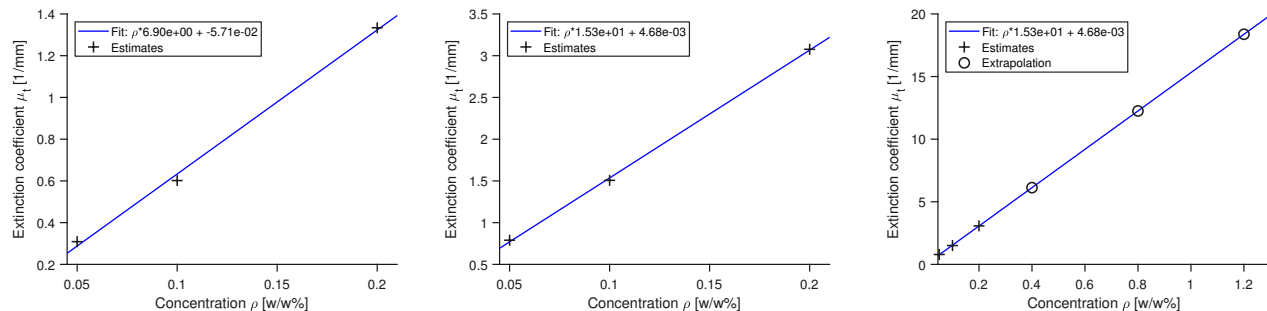


Figure 5: Extinction coefficient estimated with IAD for each scattering particle concentration along with a linear fit over concentration for (left) material B and (middle) material A. Extending the fit for material A (right) permits extrapolating the extinction coefficient to higher concentrations.

The linear fit is used to predict the scattering parameters for the higher concentration samples of material A, as shown in Figure 5 on the right. The values for the phase function parameters are taken to be the average of the ones collected from the lower concentration samples. With the extrapolated values for the extinction coefficient and the averaged values for the phase function, adding-doubling was used to simulated the reflected and transmitted scattered radiant intensity and the simulations were compared to the experimental measurements. The best ($d = 4.5$ mm, $\rho = 0.4$ w/w%) and worst comparisons ($d = 1.5$ mm, $\rho = 0.4$ w/w%) are shown in Figure 6.

As shown, the comparison between the simulations and measurements is very good using the extrapolated parameters directly. This shows that the parameters obtained with IAD from the lower concentration samples are robust enough to predict the scattering properties of higher concentration samples.

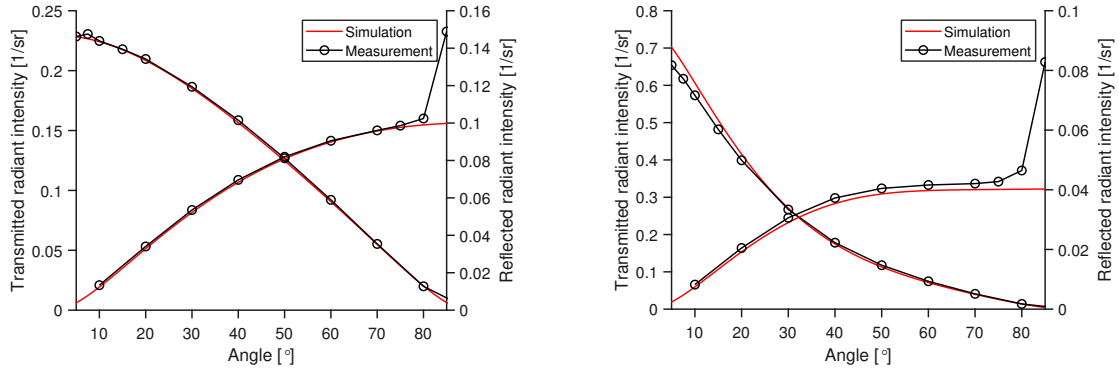


Figure 6: Comparison between the simulated and measured transmitted and reflected scattered radiant intensity obtained through extrapolation, showing the (left) best match found and (right) worst match.

3.2.2 Hybrid samples

For the remaining test, the scattering properties obtained for the low concentration samples of material A and B were used to predict the scattering properties of a hybrid sample that contains both material A and material B scattering particles. To calculate the properties of the hybrid sample from the individual scattering properties Equation (5) is used, where the superscript indicates material A or material B.

$$\begin{aligned}
 \mu_s &= \mu_s^A + \mu_s^B \\
 \mu_a &= \mu_a^A + \mu_a^B \\
 p(\theta) &= \frac{p(\theta)^A \mu_s^A + p(\theta)^B \mu_s^B}{\mu_s^A + \mu_s^B}
 \end{aligned} \tag{5}$$

The values estimated for the hybrid sample were then used to simulate the scattered radiant intensity distribution and the simulations were compared to the experimental measurements of the light scattered from the samples. The comparison between simulations and measurements are shown in Figure 7 for all hybrid samples that were measured.

As with the extrapolated case, the matches for the hybrid samples are also good. While many different reasons can plausibly explain the small deviations, we think that the uncertainty on the estimated phase function parameters, which was clearly observed for the low concentration samples, is the main cause. Nevertheless, these results indicate that the parameters obtained from low concentration samples can be used to confidently predict the volume scattering properties of samples with multiple types of scattering materials.

Taking the hybrid test and the extrapolation to higher concentration test together, it becomes clear that the volume scattering parameters estimated with inverse adding-doubling are both accurate and flexible, making it a valuable tool for volume scattering characterization.

4. CONCLUSION

In this work we have investigated the capabilities of the inverse adding-doubling method in extracting accurate and robust volume scattering properties from experimental measurements of scattering material samples. The scattered radiant intensity for several different samples was measured and inverse adding-doubling was applied to estimate their corresponding volume scattering properties, resulting in good matches between simulations and experiments.

To assess the robustness of the scattering parameters estimated with inverse adding-doubling, samples with higher concentration of scattering particles and multiple types of scattering particles were also measured but not

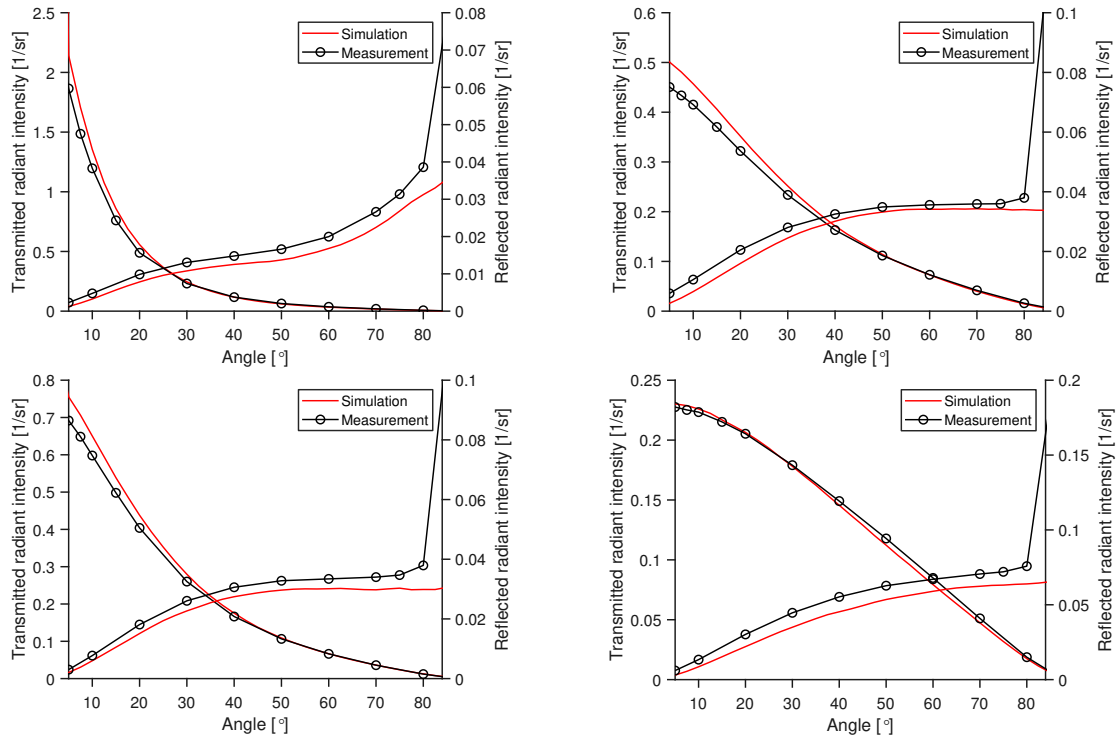


Figure 7: Comparison between the simulated and measured scattered radiant intensity for the hybrid samples for (left) $d = 1.5$ mm, (right) $d = 4.0$ mm, (top) $\rho = 0.2$ w/w% and (bottom) $\rho = 0.4$ w/w%.

supplied to inverse adding-doubling. Instead, the properties previously estimated were used directly with adding-doubling to simulate the scattered radiant intensity and this was compared to experimental measurements. An overall good match between experiments and simulations was found for both tests, demonstrating that inverse adding-doubling is capable of estimating the volume scattering properties of samples in an accurate and robust manner.

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