2-D PSTD Simulation of optical phase conjugation for turbidity suppression

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Abstract: Turbidity Suppression via Optical Phase Conjugation (TS-OPC) is an optical phenomenon that uses the back propagation nature of optical phase conjugate light field to undo the effect of tissue scattering. We use the computationally efficient and accurate pseudospectral time-domain (PSTD) simulation method to study this phenomenon; a key adaptation is the volumetric inversion of the optical wavefront E-field as a means for simulating a phase conjugate mirror. We simulate a number of scenarios and demonstrate that TS-OPC deteriorates with increased scattering in the medium, or increased mismatch between the random medium and the phase conjugate wave during reconstruction.

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1. Introduction

In general, elastic optical scattering dominates over other light-matter interactions in light transmission through biological tissues. As a point of reference, consider light propagation in chicken breast tissue at wavelength 630 nm; the scattering coefficient is $\sim 23 \text{ mm}^{-1}$, the reduced scattering coefficient is $\sim 0.8 \text{ mm}^{-1}$, while the mean absorption coefficient is only $\sim 0.01 \text{ mm}^{-1}$ [1]. While characterization of tissue scattering or tissue turbidity can provide valuable information about the tissue for diagnostic applications [2, 3], tissue turbidity is generally regarded as a formidable obstacle for optical tissue imaging and other related applications. A significant fraction of the popular optical tissue imaging techniques relies on some ways to minimize the impact of tissue turbidity. For example, Optical Coherence Tomography [4, 5] preferentially detect ballistically propagating light and screen out multiply scattered light to enable optical imaging at a relatively deep tissue depth of ~ mm's. Two photon fluorescence microscopy relies on the lower tissue turbidity at longer optical wavelengths to achieve deeper imaging depth penetration [6]. Multiply scattered light is generally regarded as being random and stochastic in their trajectories. Though scattering may appear random and stochastic, it is actually a causal and time reversible process. This fact can be better appreciated from the view point of light as a wave. As an analogy, a wave that is propagating on the surface of a lake may break up into a complicated pattern when it encounters a collection of moored boats. If we can record, re-create and reverse the propagating direction of this complicated pattern, we can reasonably expect to be able to recover the original wave after this 'time-reversed' re-creation retraces its steps through the collection of moored boats. The same type of reasoning applies to light scattering in tissues as well

The idea of tissue turbidity suppression via some form of time reversal is appealing and can potentially lead to interesting biomedical applications. As an obvious example, one may potentially apply this idea to more accurately and more directly determine tissue absorption coefficient, which in contrast to tissue scattering coefficient, is able to reveal much more about the tissue's biochemical content. Applications for deep tissue imaging are less obvious, but one promising avenue is to use tissue turbidity suppression method to enable enhanced light transmission through tissues for more uniform contrast agent illumination in photoacoustic tomography methods [7].

Optical phase conjugation (OPC) offers a possible way to affect turbidity suppression [8]. Briefly, a phase conjugate mirror (PCM) acquires light field information impinging on its interface and generates a phase conjugate version that propagates in the reverse direction. Depending on the method employed, the output of the phase conjugate wave can be instantaneous or delayed. Strictly speaking, OPC is like a time-reversal technique for propagative waves but it is incapable of time reversing evanescent waves [9]. The exact impact of this subtlety on turbidity suppression deserves more detailed future studies. We will also like to note that the concept of using OPC to eliminate scattering is not a new one—in fact, Leith *et al.* demonstrated that OPC could reverse optical scattering induced by a ground glass slide in 1966 [10]. In the case of tissue scattering, the extent of scattering is much higher (average scattering per photon can rapidly range upwards of tens beyond a tissue thickness of 1 mm). In the experiments reported in Ref. [8], the average number of scattering

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per photon reached as high as 29. One can reasonably expect the turbidity suppression via OPC is an exacting process. The perceived difficulty is likely a major reason that tissue turbidity suppression via OPC has not been experimentally demonstrated until recently.

We recently implemented an OPC based tissue turbidity suppression experiment and demonstrated that the use of OPC for turbidity suppression is surprisingly robust despite the inherent practical limitations that prevent generation of an exact phase conjugate light field [8]. We termed this newly observed biophotonics phenomenon—turbidity suppression optical phase conjugation (TS-OPC). The experiment also revealed several interesting features—notably, the extent of turbidity suppression decreases as a function of tissue thickness, and the mismatch between the OPC wave and the random medium. The decrease as a function of tissue thickness appeared to follow a Beer's Law trend for thin tissue sections (up to 0.46 mm thick chicken breast tissue section).

A simulation approach suitable for modeling OPC based tissue turbidity suppression is greatly desired at this point in time for three reasons. First, such a simulation can help us to better understand and interpret the experimental findings. Second, it can provide an easier means for realizing certain experimental schemes and geometries, and thereby allow us to design experiments that are better optimized. For example, the scattering coefficient (μ_s) and anisotropy (g) can be easier varied in a simulation. The angle dependent scattering profile of the scatterers can also be arbitrarily tailored—a flexibility that is difficult to implement experimentally. Specific spatial arrangements of scatterers can also be easier accommodated in simulations than in experiments. The third, and perhaps the most important, advantage for using simulation is that it allows access to details that cannot be readily observed/detected in the experimental context. The behavior of near-field components is an excellent example of a feature in TS-OPC that simulation can easily allow us to study, but which direct experimental study is difficult to implement.

This paper reports on the adaptation of a simulation method—the pseudospectral timedomain (PSTD) method to model TS-OPC. In Section 2, we briefly outline the PSTD method and the adaptation of the method to study the turbidity suppression phenomenon. We also go through the challenges posed by OPC simulation and turbidity modeling and point out the advantages associated with PSTD that makes it better at tackling these challenges in comparison with some other modeling methods out there. In Section 3, we report on the implementation of the method to simulate the interaction of light with random medium and PCM, and demonstrate the capability of the method to model TS-OPC. This section also contains details of 4 sets of simulation studies that demonstrate some of the features of this phenomenon. In Section 4, we discusses the ways by which the simulation model can be improved and the limits of this model. We summarize our results in Section 5.

2. Method

Simulations can provide useful information to guide experiments and allow us to better understand experimental results. The Monte Carlo technique is a stochastic simulation that is widely applied in various fields. It has also been commonly employed to simulate light propagation in random media [11, 12]. The Monte Carlo method approximates light propagation in random media as a collection of optical paths of independent "photons." Based upon a heuristic scattering model, light scattering is treated as a billiard ball collision problem—the optical path of each "photon" is determined by random numbers and each scattering event is treated independently. This heuristic approach to simulate light scattering is relatively simple to implement and computationally efficient. However, without the complete knowledge of the electric and magnetic fields, the Monte Carlo simulation of light falls short in accounting for dependent scattering and near-field effects. As a result, it is not suitable for modeling the interaction of an OPC light field with a random medium as the tracking of the exact wavefront evolution and coherence of light are critical in such a situation [13].

Simulation of the OPC effect of PCM requires accurate accounting of the coherence of light. In order to properly account for coherent interference effects, it is necessary to employ a rigorous and high-accuracy numerical technique based on solving Maxwell's equations over the entire volume of interest. The finite-difference time-domain (FDTD) technique is a simulation technique that fits this bill well. This widely used approach is a numerical solution of Maxwell's equations, and it can accurately account for coherent effects. However, FDTD is very computationally intensive—it is infeasible to model a macroscopic electromagnetic problem with currently available computer resources using the FDTD technique.

In this paper, we report the implementation of a PSTD technique to model TS-OPC. Pioneered by Q. H. Liu [14], the PSTD technique is a variant of the finite-difference time-domain (FDTD) technique [15]. The PSTD technique is advantageous for simulating electromagnetic problems of macroscopic dimensions. For large electromagnetic wave interaction models in D dimensions that does not have geometric details or material inhomogeneities smaller than one-half wavelength, PSTD reduces the computer storage and the running-time by approximately 8^{p} : 1 relative to the conventional FDTD while achieving comparable accuracy [14]. This numerical technique permits a rigorous simulation of a *macroscopic* light scattering problem based on Maxwell's equations, and enables accurate modeling of the PCM optical characteristics.

The task of numerically solving Maxwell's equations requires a numerical substitution of the spatial and temporal derivatives. Towards this end, the PSTD method calculates the temporal derivatives using a 2nd-order finite-difference scheme as employed in the FDTD method. For the spatial derivatives, the PSTD method calculates the spatial derivatives in the frequency domain via discrete Fourier transform: Let {**E**_i} denote values of the electric field or magnetic field, and { $(\partial \mathbf{E}/\partial x)_i$ } denote the spatial derivative of **E** along the x-direction. Based on the differentiation theorem of Fourier transform, we can write:

$$\left\{\frac{\partial \mathbf{E}}{\partial x}\Big|_{i}\right\} = -\mathbf{F}^{-1}\left(i\tilde{k}_{x}\mathbf{F}\left\{\mathbf{E}_{i}\right\}\right)$$
(1)

where **F** and **F**⁻¹ denote, respectively, the forward and inverse discrete Fourier transforms, and \tilde{k}_x is the Fourier transform variable representing the *x*-component of the numerical wave vector. The spatial derivatives in each direction can be obtained numerically. According to the Nyquist sampling theorem, the spatial derivatives calculated in (1) is of spectral accuracy (meaning as accurate as it can get with the given information), allowing the PSTD technique, with a coarse grid of two spatial samples per wavelength, to achieve similar accuracy as the FDTD technique (FDTD requires 20 spatial samples per wavelength.) Finally, an anisotropic perfectly matched layer absorbing boundary condition [16] is implemented to absorb all outgoing wave. If all outgoing waves never re-interacts with the medium, then the optical simulation can be considered as being practically isolated in vacuum.

There are several approaches that we can take to implement a PCM simulation. The specific nature of the PCM also factors into the consideration. Of particular importance is whether the PCM in question is an instantaneous reflector or a time delayed one. For example, a PCM based on a four wave mixing scheme is an instantaneous reflector while a PCM based on holography will likely be time delayed. As the experiment reported in Ref. [8] is holographic in nature, we will presently focus on implementing a time delayed PCM.

Our strategy for implementing a time delayed PCM is as follows. In the scenario where the incoming light pulse crosses the PCM interface from left to right, we implement a simulation region to the right of the PCM interface (hereby named the inversion region) that is sufficiently large enough to accommodate the profile of the pulse after it has completely passed the interface. When the pulse has completely passed the interface and is wholly in the

inversion region, we manually invert the E-field and D-field components throughout this region:

$$\mathbf{E} \to -\mathbf{E}, \ \mathbf{D} \to -\mathbf{D}$$
 (2)

The magnetic field **H** and magnetic induction **B** remain unchanged. The inversion of **E** and **D** in the inversion region causes the poynting vector $\mathbf{S} = \mathbf{E} \times \mathbf{H}$ to reverse direction without changing the amplitude. As a result, light with inverted phase will propagate in the opposite direction, exit the PCM interface from the right and effectively become an OPC wave that travels back towards the random medium. The inversion region must be large enough as to enclose the entire pulse when it has passed wholly through the PCM interface from the left to avoid discontinuity of the field components. If the OPC region only encloses a fraction of the light pulse, the discontinuity of the **E**-field and **D**-field will excite non-physical field oscillations as a result of the Gibb's phenomenon.

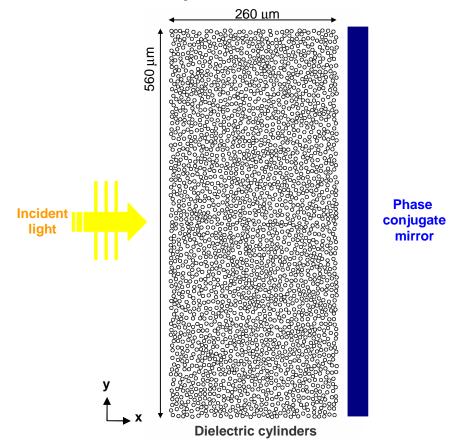


Fig. 1. Simulation of a PCM using the PSTD technique. A 260μ m-by- 560μ m cluster of N = 2500 randomly-positioned, dielectric cylinders is illuminated on the left by a light pulse. Light is multiply scattered as it propagates through the cluster, and impinges the PCM. The phase and propagation direction of the light that impinges the PCM is inverted, causing light to propagate in the reverse direction and back-trace to where it originated.

A schematic of the PSTD simulation is shown in Fig. 1. The physical dimensions of the simulation region are 320 μ m by 600 μ m with a spatial resolution of 0.33 μ m. The simulation is performed with a temporal resolution of $\Delta t = 0.05$ fs. A macroscopic random medium consisting of a cluster of randomly positioned dielectric cylinders is placed in space. The random medium is illuminated by an incident light pulse; the light pulse is multiply scattered

as it propagates through the cluster of cylinders. At time t, the **E**-field of the region to the right of the random medium is inverted, simulating OPC light field generation from a PCM that is placed adjacent to the random medium. Based on our understanding of the TS-OPC phenomenon, we expect the OPC light field to travel back through the sample and reconstruct the original incident light pulse. Depending upon the choice of the inversion region, a different placement of PCM can be simulated. The time t should be chosen such that the pulse has left the random medium and has passed completely through the PCM interface. Each simulation takes typically ~12 hours with 4 computing cores of a Xeon Woodcrest 3.0GHz processor.

To quantify the extent of TS-OPC effect that is achieved, we compare the energy of the reconstructed light pulse with the original incident light pulse energy. The PSTD simulation yields field information everywhere in space; the refocused light energy is determined by integrating the energy in the area of the original incident pulse

refocused energy =
$$\iint_{\text{area of original light pulse}} \left[\frac{\varepsilon \mathbf{E}^2}{2} + \frac{\mathbf{H}^2}{2\mu}\right] dxdy$$
(3)

If the TS-OPC effect is perfect, we will not expect to see a loss in energy, and the reconstructed light pulse would be identical to the original incident light pulse (with a 180-degree phase difference). The ratio of refocused energy to the original incident energy is a good measure and definition of the TS-OPC efficiency.

3. Results

Four simulation studies of the PCM are presented. First, a simulation of light impinging a PCM in vacuum is presented in Section 3.A; and as a comparison, a simulation of light propagating through a random medium then impinging a PCM is presented in section 3.B. Next, we study the extent by which the TS-OPC effect is affected by the scattering coefficient μ_s , and the mismatch of the random medium and the OPC wavefront. These results are presented in Sections 3.C. and 3.D., respectively.

3.A. Light impinges a PCM in vacuum

We first model light impinging a PCM in vacuum as a validation of the PSTD simulations. Six still images of the simulation are shown in Fig. 2 to illustrate the time evolution of the wavefront. The initial light pulse is a Gaussian pulse with a cross-sectional width of 42.4 μ m and temporal duration of 0.141 fs. As the light pulse propagates through space, the wavefront expands to a width broader than 360 μ m prior to impingement on the PCM, as shown in Fig. 2(c).

As the light pulse reaches the PCM, the E-field is manually inverted to simulate the OPC effect. After phase inversion, the light with an inverted E-field reverses its original propagating direction and travels back towards its source. We can also see that the back-propagating wave reverses the diffractive spreading as it retraces its previous optical path. Eventually, the backward propagating light converges back to a narrow pulse of light at the original location where the incident pulse was initially located, as shown in Fig. 2(f).

From the figures, we can see that the OPC inverted light propagation in vacuum is practically equivalent to a time-reversal of the light propagation process. Since no energy is lost, the total energy of the refocused light pulse should equal the original incident pulse. As shown in Figs. 2(a) and 2(f), it is clearly seen that the refocused pulse profile is perfect and the amplitude of 2(f) matches very well with 2(a). The ratio of refocused energy to initial energy is measured to equal 1.000—another clear indication that the simulation worked as predicted in this scenario.

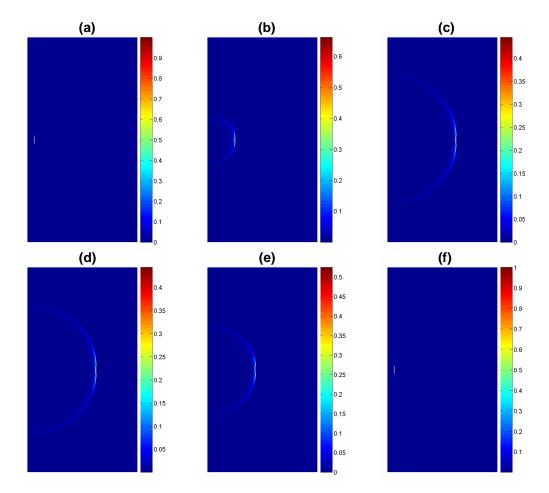


Fig. 2. PSTD simulation of the OPC effect of a PCM in vacuum. The physical dimensions of the simulation region are 320 μ m by 600 μ m. An initial light pulse with a cross-sectional width of 42.4 μ m and temporal duration of 0.141 fs propagates through vacuum is shown in (a)-(c): (a) t = 0 fs, (b) t = 200 fs, and (c) t = 600 fs. At t = 1200 fs, the phase of the E-field is inverted, simulating the effect of a PCM. Then the light pulse propagates backward and refocuses to the original location where it first emerged, as shown in (d)-(f): (d) t = 1200 fs, (e) t = 1400 fs, and (f) t = 1800 fs. Notice that the initial light pulse (a) and the refocused light pulse (f) both bear an amplitude of 1.

3.B. Light propagates through a random medium then impinges a PCM

Here we simulate light scatter through a macroscopic random medium and reflect off a PCM. The random medium consists of 2500 randomly-positioned dielectric cylinders in a 260µmby-560µm region with a grid resolution of 0.3 µm and temporal resolution $\Delta t = 0.05$ fs. Each cylinder has a diameter of 2.5 µm with a refractive index of 1.2. Three still images of the simulation movie clip (584KB movie) are shown in Fig. 3. The incident light pulse is a Gaussian pulse with a cross-sectional width of 13.4 µm. As the light pulse propagates through the cluster, it is multiply scattered by the randomly located dielectric cylinders, resulting in a reverberant wavefront, as shown in Fig. 3(b).

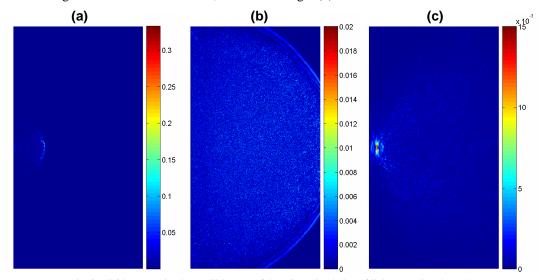
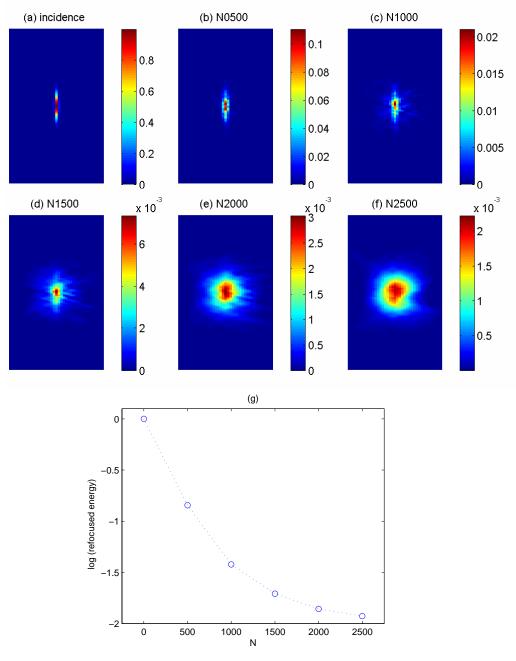


Fig. 3. (2.34MB movie) three still images of the PSTD simulation of light scattering through a macroscopic cluster of dielectric cylinders and reflected back by a PCM. The physical dimensions of the simulation region are 320 μ m by 600 μ m. The initial light pulse is a Gaussian pulse with a cross-sectional width of 13.4 μ m and temporal duration of 4.472 fs. The electric fields at various time-steps throughout the evolution are shown: (a) 200 fs, (b) 1000 fs, and (c) 2400 fs. As light scatters through the cluster of dielectric cylinders, the wavefront gradually spreads out due to diffraction. After the OPC effect of the PCM, light back-traces and refocuses back to the original location where it first emerged. Some light is lost as it scatters into other directions, resulting in a wider and reverberant wavefront profile.

A PCM is positioned on the right side of the cluster of dielectric cylinders, as depicted in Fig. 1. Light emerging on the right end of the cluster impinges the PCM where OPC occurs. After phase inversion, the light pulse propagates backward and back-traces its previous optical path through the random medium. The backward propagating light is again multiply scattered through the cluster of dielectric cylinders and refocuses back to an incident pulse at the original location where the incident pulse was initially located via the TS-OPC effect (Fig. 3(c).)

As shown in Fig. 3(b), light undergoes complex optical paths as it is multiply scattered through the irregular geometry. The wide-spread wavefront that is reflected by the PCM back-traces its previous trajectory and converges into a narrow light pulse at the original location of the incident pulse, as shown in Fig. 3(c). Unlike in the previous scenario, the reconstruction is not perfect as some of the original incident light is scattered at large angles and cannot be collected and reversed by the PCM. The loss is twofold—in addition to the net energy loss, there is also a loss in the wavefront information. This information loss implies that the reconstruction process will be imperfect and the TS-OPC effect will be diminished.



The extent of TS-OPC efficiency loss as a function of scattering extent is the subject of study reported in the next section.

Fig. 4. Effect of the number of cylinders (*N*) on the phase-conjugate refocusing of light. *N* is varied from 0 to 2500, whereas for $\lambda = 1 \mu m$, N = 500 corresponds to a scattering coefficient μ_s = 0.0258 μm^{-1} and N = 2500 corresponds to $\mu_s = 0.1291 \ \mu m^{-1}$. Light refocused by the PCM back-traces its optical path and refocuses at the original position where it first emerged. The refocused light pulse profile for various *N* is shown in (a)-(f), each is of dimensions: 13.3 μm by 180 μm . With a larger *N*, more scattering occurs, resulting in a blurred pulse profile. The ratio of the total refocused energy to the initial total energy is shown on a semi-log scale in (g).

3.C. Scattering coefficient (μ_s)

In this section, we investigate the effect of μ_s on the TS-OPC efficiency. The simulation setup is the same as described in Section 3.B, except that the number of scatterers, N, is varied among 500, 1000, 1500, 2000, and 2500. (For $\lambda = 1 \mu m$, N = 500 corresponds to a scattering coefficient $\mu_s = 0.0258 \ \mu m^{-1}$ and N = 2500 corresponds to $\mu_s = 0.1291 \ \mu m^{-1}$.) The scattering coefficient is calculated by multiplying the extinction coefficient of a single dielectric cylinder and the number density of the cluster of dielectric cylinders [17]. The extinction coefficient of a single cylinder is determined by an analytical solution of Maxwell's equations (Mie expansion), which also yields the phase function of a single cylinder [18]. The incident light pulse is a Gaussian pulse with a cross-sectional width of 94.86 μm and temporal duration of 4.472 fs. By changing N, the scattering coefficient (μ_s) of the random medium can be varied as desired.

As *N* is increased, the random medium becomes more complex; more scattering occurs and the TS-OPC efficiency drops. The refocused light pulse profile becomes blurry for larger *N*, as shown in Fig. 4(a)-(f). In order to quantify the degradation of the TS-OPC effect, we calculate the total refocused energy (eq. (3)) that is focused into the vicinity of the original light pulse at t = 0.

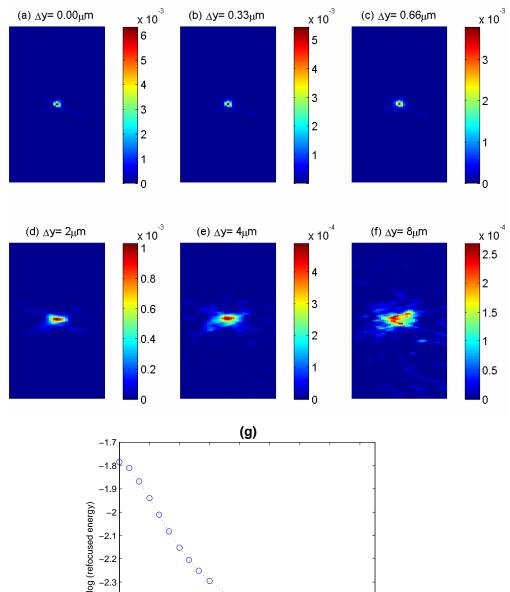
The total refocused energy compared to the initial light pulse energy is shown on a semi-log scale in Fig. 4(g). It can be readily seen that as N increases, the refocused energy decreases rapidly. This is anticipated since with more scattering, more light is lost as it scatters into other directions and never reaches the PCM, resulting in a less coherent refocused light pulse.

3.D. Misalignment of optics

Lastly, we analyze the extent to which the TS-OPC effect is influenced by a position mismatch (Δy) of the optical alignment. Effective TS-OPC requires an accurate match between the OPC light field and the random medium. If the random medium is displaced, the OPC light field will not be able to accurately retrace its original light paths through the medium. We can expect the deterioration of the TS-OPC effect to be a function of the position mismatch; in fact, this prediction was experimentally verified in Ref. [8]. Our simulations offer us an alternate way to study this effect.

An optical misalignment is introduced by a displacement of the random medium, where the cluster of dielectric cylinders is displaced by Δy in the y-direction immediately after the OPC effect of the PCM. As we can see, the reconstructed light pulse becomes progressively blurrier as Δy increases (see Fig. 5(a-f)).

In addition to the broadening of the reconstruction, we also expect the TS-OPC efficiency to drop. Figure 5(g) shows this deterioration as a function of Δy . The research findings of this simulation are consistent with our experimental findings [8].



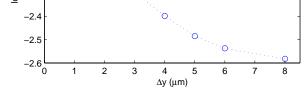


Fig. 5. Effect of displacement (Δy) of the random media on the OPC refocusing of light. The cluster of 2500 5- μ m-diameter dielectric cylinders is displaced by Δy in the y-direction immediately after the phase inversion of the E-field due to the PCM. The refocused light pulse profile for various Δy is shown in (a)-(f), each is of dimensions: 13.3 μ m by 180 μ m. The ratio of the total refocused energy to the initial total energy for various Δy is shown on a semi-log scale in (g). Notice that as Δy increases, the refocused light energy drops rapidly.

4. Discussion

The 2D simulation provides a way to compare and provide insight to better understand 3D experimental results. Most of the interesting 3D experimental geometries have good analogies in 2D geometries. The simulation described in this paper is well suited for TS-OPC simulation of scenarios where a pulsed light source is employed. This is because a pulse light source allows us to fairly easily choose a suitable time point to perform the **D**- and **E**-field inversion within the volume to the right of the PCM interface. Specifically, because the total duration of a light pulse is limited, such a time point can be chosen to be the time at which the bulk of the light pulse has passed through the random medium and the PCM interface. The task of simulating a CW light illumination is more complicated. In this case, it is difficult to assign a proper time point for the **E**-field inversion to occur.

As we expect a broad range of TS-OPC experiments to be performed with CW light source, it is highly desirable for us to be able to adapt this simulation approach to accommodate accordingly. One possibility is to implement a Fourier analysis of the PSTD simulation of PCM with a pulse illumination. A light pulse essentially contains a wideband of wavelengths; by means of a Fourier analysis [15], we believe a CW light source based TS-OPC scenario can be solved. This specific topic is worthy of more research and further evaluation.

Recently, Vellekoop and Mosk [19] reported the use of adaptive optics to achieve focusing light through strongly scattering media. This interesting and potentially very important approach is different from the approach of optical phase conjugation, as they modulate the incident light through an optimization process.

The phase conjugate light field represents a possible light field that is suited for focusing light through strong scattering media. In fact in the limiting case where the light collection efficiency during the recording process is unity, we can expect the phase conjugate light field to represent the optimal light field for focusing light through a scattering medium. Going forward, it will be interesting to experimentally verify and numerically simulate to see if there is a better light field pattern that can outperform a phase conjugate light field for enhancing light focusing through a strong scattering medium if the phase conjugate light field is incomplete. The simulation described in this paper is a suitable approach for conducting such a study.

5. Summary

We have adapted a PSTD simulation model to study a newly observed biophotonics phenomenon—TS-OPC. Our simulations show that our PSTD model is capable of modeling the inversion property of a PCM and is accurate enough to simulate the turbidity suppression effect of TS-OPC. In this paper, we report the use of the model to study the impact of 1) turbidity increase and 2) OPC light field to random medium mismatch, on the TS-OPC efficiency. The results are consistent with our experimental findings.

Going forward, we are convinced that the computational efficiency and flexibility of our PSTD model makes it well suited for simulation based analysis of TS-OPC as both a cross-check on TS-OPC experiments, and a means to reveal TS-OPC features that are hard to access experimentally.

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