Raytracing is the standard method to simulate optical systems. For many decades, raytracing has been used to design imaging systems. Especially for radiometric analyses, so-called non-sequential ray tracers are used, in which the order of physical objects that are hit by a ray is not pre-defined, but computed during ray propagation. Due to the relatively high computational requirement, non-sequential ray tracers were established only with the advent of modern, powerful computers. Since then, they have conquered practically all branches of industry in which light is used creatively. Software packages such as ASAP (Advanced Systems Analysis Program) from Breault Research Organization are able to perform wave-optics simulations and can interoperate with other optics programs. Most all phenomena of classical optics can be modeled within a uniform user interface.

Simulation of tissue

The simulation of light scattering materials, particularly biological tissue, is one of the key topics of biophotonics. Light propagation in biological tissue is dominated by absorption and multiple scattering, in which both elastic and inelastic scattering processes play a role. The distances between neighboring scattering centers in the tissue (entire cells, cell membranes, organelles) are small, which causes a coherent near-field interaction. This interaction makes the ab-initio calculation of scattering properties difficult. For practical applications, one therefore mostly uses phenomenological models. The required experimental tissue parameters can be found in literature [1] and in databases.

Because of the diversity of preparation, measurement and evaluation methods used for data acquisition, the resulting tissue parameters are often hardly comparable and associated with considerable measurement errors. Reproducibility of measurements is another critical issue, which is often not fulfilled because of the strong variability of the tissue samples. Sometimes tissue phantoms offer a way out: these are artificial, well characterized materials whose scattering properties resemble natural tissue. In summary, we can state that a thorough and critical evaluation of the tissue parameters is essential before starting with the optical simulation.

Monte Carlo raytracing

The theoretical basis for light propagation in scattering media is the radiative transport equation [2]:

\[
\frac{dI(r, \omega)}{ds} = -\left(\mu_a + \mu_s\right)I(r, \omega) + \\
\mu_s \left( \frac{\mu_a}{4\pi} \int \frac{p(\omega', \omega)I(r', \omega')}{4\pi} d\omega' \right)
\]

1 Principle of Monte Carlo radiative transfer
In this equation, $I$ is the radiance (specific intensity) at position $r$ directed towards the solid angle $w$, and $dI/ds$ is its directional derivative; $\text{mabs}$ is the absorption coefficient, $\text{msca}$ is the scattering coefficient, and $p(w,w')$ is the phase function which determines the angular distribution of the scattered light. The authors refer to literature for a more detailed discussion [2].

A standard method for the numerical solution of the radiative transport equation is Monte Carlo raytracing. The ray path in the scattering medium is represented by an alternating sequence of straight propagation and scattering (Figure 1), which is repeated until the ray leaves the medium or until another stop criterion is met. Upon scattering, the direction and – in case of absorbing media – also the flux of the ray changes. Monte Carlo raytracing has a wide range of applicability, excluding only optically thick media, for which the method becomes impractical due to excessive computation times.

ASAP optical software implements Monte Carlo raytracing, making it well-suited for the simulation of light scattering media. The input quantities for the radiative transport equation – mabs, msca, and $p(w,w')$ – can be computed in the framework of Mie theory. Alternatively, the Henyey-Greenstein model, which is frequently applied in biophotonics, and arbitrary user-defined models are available. Even inelastic scattering, for example, fluorescence or Raman scattering, can be modeled in ASAP. Breault Research Organization offers an application-specific tutorial »volume scattering and biomedical optics«, which presents and discusses these capabilities of the software in detail.

**Advantages of commercial software**

One considerable advantage of commercial ray tracers is their comprehensive built-in analysis tools. We exemplify this in the case of a tissue phantom inside a cuvette, illuminated by a laser beam (Figure 2). The simulation was performed with ASAP, and the following quantities were determined:

- irradiance distribution on a detector,
- volume distribution of the absorbed power,
- time-of-flight spectrum of the transmitted light,

In ASAP, all radiometric (and photometric) quantities can be computed on all surfaces and, if it makes sense, also inside the volume. Using the scripting language of ASAP, user-defined distribution...
functions, such as the time-of-flight spectrum in the previous example, can be determined from the ray data.

Originally, non-sequential ray tracers were developed for the simulation of complicated opto-mechanical systems. Their strength in modeling complex geometries is advantageous also in bio-optics. Figure 3 shows a detailed model for the simulation of the reflection/absorption properties of human skin with hair. The implementation of blood vessels in the model is currently under development.

Light scattering materials are usually only one part of a larger optical system that needs to be modeled. A considerable value of commercial ray tracers comes from their compatibility with other software packages. For instance, ready-to-use light source models can be imported from databases, optical components can be imported from lens-design programs, and mechanical components can be imported from CAD programs. Because ray tracers can model entire optical systems, it is getting more and more popular using them for virtual prototyping in the field of biophotonics. Virtual prototyping means that most of the development work takes place in the computer. A hardware prototype gets assembled only after having already fixed most design details in the computer model. In the ideal case, the hardware prototype is then needed only for fine-tuning of the design. Virtual prototyping saves development costs and time as it becomes more and more established.

Summary:

Non-sequential ray tracers such as ASAP are suitable for virtual prototyping in biophotonics, because they are able to model both biological media and their technical environment – from the light source to the detector – in an accurate and reliable way.

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LITERATURE

1. »Biomedical Photonics Handbook«, Tuan Vo-Dinh
   Editors, CRC Press, New York 2003
The design of a light applicator for photodynamic therapy (PDT) is one example how raytracing software can be used to assist and speed up the development of medical devices. Photodynamic therapy is a method of treating tumors and other neoplasias by a photosensitizer in combination with light irradiation.

The patient receives the sensitizer, which accumulates selectively only in the tumor tissue. Then, tumor and surrounding healthy tissue are irradiated with light of a certain wavelength. The induced photochemical processes occur only within the tumor due to the tissue selectivity of the photosensitizer. Thus, the resulting phototoxic substances damage only tumor cells. A very promising application for PDT is the treatment of benign penis condyloma. The challenge of this application is to irradiate two surfaces simultaneously, that is, the outer surface of the penis and the inside of the urethra. Therefore, a special light applicator is needed for this application that has to meet the following requirements: the applied irradiance should be uniform on all irradiated surfaces, and the overall efficiency should be sufficiently high.

The resulting complex geometry of the applicator would make a trial-and-error development very time consuming and expensive. The benefit of a raytracing program such as ASAP is to implement many different geometrical configurations, simulate the light propagation and analyze the results within a short time.

One possible configuration of such a special light applicator is shown in figure 4. A light-guiding fiber couples light from a light source into the applicator. One part of the treatment light is coupled into the round diffuser cap serving as a light source for the outer surface of the penis. The other part of the light is guided into the thin tube of the cylinder diffuser. This part of the applicator is placed into the urethra delivering light to this treatment area. A model of the light applicator created in ASAP is shown in figure 5. Both, geometry and optical properties of the model can be parameterized in ASAP. Powerful algorithms are available for systematic optimization. As an example, the optimization process for the cylinder diffuser is explained in more detail: a scattering medium is used within the cylindrical diffuser to obtain a diffuse radiation of the light. The characteristics of the resulting radiation pattern depend on the scatterer concentration of the scattering medium. Figure 6 shows a typical set of ray paths after the simulation. The radiation profile as a function of the scatterer concentration is shown in figure 7. The simulation program can assist in finding the optimum concentration by varying the concentration until a uniform radiation profile is achieved. Very similar procedures were conducted to determine in all details the optimum characteristics of other applicator components.