White light thermoplasmonic activated gold nanorod arrays enable the photothermal disinfection of medical tools from bacterial contamination

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![Figure SI 1](image-url) The spectral response of the glass substrate using air as the baseline. It is evident a very intense absorption below 300 nm.

1. **Theoretical model**

1.1. **AuNRs optical coefficients**

Optical cross sections, which are crucial to determining the absorption coefficient, are generally solved via two different methods – Mie-Lorentz theory and Rayleigh or Rayleigh-Drude approximation. The last one assumes that the light-nanoparticle interaction is described as dipoles carrying the charge whose arrangement is maximal if the nanoparticle and light frequencies are equal, which is called localized plasmonic resonance [1]. Mie-Lorentz's theory may be much more appropriate due to its enhanced accuracy, including multipole interactions. To define the nanoparticle's shape appropriately, however, this theory requires sophisticated mathematics whose solutions are generally followed with
long-time simulations unless it is a pure sphere. On the other hand, the Rayleigh-Drude approximation, although it imposes the conditions that \( \frac{\lambda}{2\pi} > d_{NP} \), where \( d_{NP} \) is the AuNR size, appears to be a perfect verification for a wide number of shapes in IR- and Vis-ranges [2][3].

On the other hand, Rayleigh-Drude-approximation offers simpler solutions that may be solved without using numerical methods. The optical cross sections are introduced as:

\[
C_{absi} = (C_{exti}) - (C_{scai}) = \left( 4\pi \left( \frac{2\pi}{\lambda} \right) \cdot \text{im}(\alpha_i) \right) - \left( \frac{8\pi}{3} \left( \frac{2\pi}{\lambda} \right)^4 |\alpha_i|^2 \right)
\]

(1)

where:

- \( C_{exti} \) – extinction cross section of the \( i \)-particle, \( m^2 \);
- \( C_{scai} \) – scattering cross section of the \( i \)-particle, \( m^2 \);
- \( C_{absi} \) – absorption cross section of the \( i \)-particle, \( m^2 \);
- \( \lambda \) – incident wavelength, \( m \);
- \( \alpha_i \) – total polarizability of the \( i \)-particle, \( m^3 \);
- \( \text{im} \) – symbol of imaginary part

For the standard approach, the light-AuNR interaction is represented via polarizability functions of the dipole configurations, where the double-layered ellipsoids with an anisotropic depolarization factor \( \delta_i \) follow the formulas [2][4]:

\[
\alpha_{ix} = \frac{V_i + V_2}{4\pi} \left( \frac{\varepsilon - \varepsilon_h}{\varepsilon_h + (\varepsilon - \varepsilon_h)\cdot J_{1,1i} \cdot J_{1,2i}} \right) \left( \delta_i \cdot e_x \cdot (e_1 - e_2) \right)
\]

(2)

\[
\alpha_{iy} = \frac{V_i + V_2}{4\pi} \left( \frac{\varepsilon - \varepsilon_h}{\varepsilon_h + (\varepsilon - \varepsilon_h)\cdot J_{1,1i} \cdot J_{1,2i}} \right) \left( \delta_i \cdot e_y \cdot (e_1 - e_2) \right)
\]

(3)

\[
\alpha_{iz} = \frac{V_i + V_2}{4\pi} \left( \frac{\varepsilon - \varepsilon_h}{\varepsilon_h + (\varepsilon - \varepsilon_h)\cdot J_{1,1i} \cdot J_{1,2i}} \right) \left( \delta_i \cdot e_z \cdot (e_1 - e_2) \right)
\]

(4)

\[
\delta_i = \frac{V_1}{V_1 + V_2}
\]

(5)

where:

- \( \alpha_{ix} \) – polarizability of the \( i \)-particle along the \( x \) axis, \( m^3 \);
- \( \alpha_{iy} \) – polarizability of the \( i \)-particle along the \( y \) axis, \( m^3 \);
- \( \alpha_{iz} \) – polarizability of the \( i \)-particle along the \( z \) axis, \( m^3 \);
- \( V_1 \) – volume of the \( i \)-particle’s core, \( m^3 \);
- \( V_2 \) – volume of the \( i \)-particle’s shell, \( m^3 \);
- \( e_1 \) – complex function of the electrical permittivity of the core, here: gold permittivities, \( \varepsilon \);
- \( e_2 \) – complex function of the electrical permittivity of the shell, here: CTAB permittivities, \( \varepsilon \);
- \( e_h \) – complex function of the electrical permittivity of the surrounding medium, here: air, \( \varepsilon \);
- \( J_{1,1i} \) – depolarization factor of the \( i \)-particle core along the \( x \) axis, \( \varepsilon \);
- \( J_{1,2i} \) – depolarization factor of the \( i \)-particle shell along the \( x \) axis, \( \varepsilon \);
- \( J_{1,1y} \) – depolarization factor of the \( i \)-particle core along the \( y \) axis, \( \varepsilon \);
- \( J_{1,2y} \) – depolarization factor of the \( i \)-particle shell along the \( y \) axis, \( \varepsilon \);
\[ J_{i,1,z} \] – depolarization factor of the \( i \)-particle core along the \( z \) axis, -;
\[ J_{i,2,z} \] – depolarization factor of the \( i \)-particle shell along the \( z \) axis, -.

The electrical permittivities are, in general, calculated via different Drude-model-based approaches. This work applies the Drude-CP model studied in \([5] \) because it corresponds to many experiments. For prolate (stretched) structures, however, the depolarization factor should be specified via \([2][4] \):

\[
J_i = \frac{1 - \phi_i^2}{\phi_i^2} \left( 1 - \frac{1 + \phi_i}{1 - \phi_i} \right),
\]

\[
\phi_i = \sqrt{1 - \left( \frac{d_{si}}{d_{li}} \right)^2}
\]

where:
- \( d_{si} \) – short diameter of the \( i \)-particle, \( m \);
- \( d_{li} \) – long diameter of the \( i \)-particle, \( m \).

Contrary to ellipsoids, rods possess the long flat dimension, which contributes to appear new dipole configurations. Therefore, the depolarization factor that determines the dipole arrangement in an AuNR may be claimed to be a perfect parameter to solve and establish the other dipole configurations. It was discovered by Fuchs \([51] \). In his work, edgy shapes (triangles, cubes, octahedrons etc.) were determined numerically as weighted \( J_1 \) distributions. Considering of the two highest values of the depolarization factor in a cube, it may be realized that charge arrangements imply the uniform distributed \( \frac{J_1}{3} \) configuration and the one whose charges are arranged at the very opposite vertices along a cube space diagonal \( J_1(d_{si},d_{il}) \rightarrow J_1(d_{si}d_{si}\sqrt{3}) \).

A similar arrangement is exploited for the AuNRs; however, depolarization factors are adopted for the prolation factors, \( \phi_i \), and are transformed into:

\[
\phi_i(d_{si},d_{il}) \rightarrow \phi_i(d_{il} - d_{si}\sqrt{(d_{li} - d_{si})^2 + (d_{si})^2})
\]

\[
\phi_i(d_{si},d_{il}) \rightarrow \phi_i(d_{si}\sqrt{(d_{il} - d_{si})^2 + (d_{si})^2})
\]

for \( y \)- and \( x \)-, \( z \)- axes respectively. Figure SI 2 demonstrates these four assumed charge arrangements that have been adjusted to the \( x \)-oriented AuNRs.

Nonetheless, the platform-deposited particles are also governed by the particle-surface interaction. This situation is assumed differently from the other configurations due to the outer electrical field distribution from the interaction between two different compounds – AuNR and the PE layer. So far, many papers have been published about the issue where the AuNPs are dispersed in a solution, and only a few explain precisely how the interaction may be treated \([2][7][8][9] \) once immobilized on a surface. Moreover, none of them deal with elongated shapes due to the high complexity of the problem. This work introduces the surface effect as the interaction between AuNRs and the PE layer that is considered a flat disk.

Basing on Royer’s and Yamaguchi’s approaches: \([2][10] \):

\[
(a_{i,x})_{sur} = \frac{-\left( d_{si} \right)^3}{3\cdot q_{11} \left( \frac{1 - \phi_i^2}{\phi_i^2} \right)^{1/2}} \frac{\varepsilon_1 - \varepsilon_h}{\varepsilon_1 - \varepsilon_{11} \left( \frac{1 - \phi_i^2}{\phi_i^2} \right)^{1/2}}
\]

\[
(\varepsilon_{i,x})_{sur} = \frac{-\left( d_{si} \right)^3}{3\cdot q_{11} \left( \frac{1 - \phi_i^2}{\phi_i^2} \right)^{1/2}} \frac{\varepsilon_1 - \varepsilon_h}{\varepsilon_1 - \varepsilon_{11} \left( \frac{1 - \phi_i^2}{\phi_i^2} \right)^{1/2}}
\]
\( (a_{\alpha\beta})_{\text{sur}} = \left( \frac{2 \cdot \left( \frac{d_{si}}{2} \right)^3 \cdot \left( \frac{1}{\phi_i} \right) \cdot \varepsilon_1 - \varepsilon_h}{3 \cdot q_{10} \left( i \cdot \left( 1 - \phi_i \frac{1}{2} \right) \right) \cdot \varepsilon_1 - \varepsilon_{10} \left( i \cdot \left( 1 - \phi_i \frac{1}{2} \right) \right) } \right) \) (11)

\( (a_{\alpha x})_{\text{sur}} = \left( \frac{2 \cdot \left( \frac{d_{si}}{2} \right)^3 \cdot \left( \frac{1}{\phi_i} \right) \cdot \varepsilon_1 - \varepsilon_h}{3 \cdot q_{11} \left( i \cdot \left( 1 - \phi_i \frac{1}{2} \right) \right) \cdot \varepsilon_1 - \varepsilon_{11} \left( i \cdot \left( 1 - \phi_i \frac{1}{2} \right) \right) } \right) \) (12)

\[
p_{\Lambda M} \left( i \cdot \left( 1 - \phi_i \frac{1}{2} \right) \right) \left( \frac{d q_{\Lambda M}(i \cdot \psi)}{d \psi} \right) \psi = \left( 1 - \frac{\phi_i}{\phi_i^2} \right)^{\frac{1}{2}}
\]

\[
e_{\Lambda M} = \left( q_{\Lambda M} \left( i \cdot \left( 1 - \phi_i \frac{1}{2} \right) \right) \left( \frac{dp_{\Lambda M}(i \cdot \psi)}{d \psi} \right) \psi = \left( 1 - \frac{\phi_i}{\phi_i^2} \right)^{\frac{1}{2}}
\]

(13)

*where:*

\( p_{\Lambda M} \) and \( q_{\Lambda M} \) – associated Legendre polynomials of a first and a second kind, respectively;

\( \Lambda, M \) – orientation modes with respect to a surface

Adopting the formulas to the considered system from Royer et al.\[2\], the oscillation modes, \( \Lambda \) and \( M \), refer to the particle’s orientation. Hence, each electrical dipole perpendicular to the surface (or projected on \( Y \) axis) corresponds to the situation in which \( \Lambda = 1, M = 0 \). On the other hand, for \( x \) and \( z \) axes, charges are not directed towards the surface, thus every mode equals 1.

The surface interaction, however, is also coupled with the distance between particles. From Yamaguchi’s\[44,50\] approach, the nanoparticle distance is governed by the following:

\[
(a_{\alpha x})_{Y\alpha} = \frac{(a_{\alpha x})_{\text{sur}}}{1 + \frac{4 \cdot \left( \frac{d_{si}}{2} \right)^2 \cdot d_{li}}{3 \cdot \pi \cdot a_{si} \cdot d_{li}}} \beta_{|| i} \] (14)

\[
(a_{\alpha y})_{Y\alpha} = \frac{(a_{\alpha y})_{\text{sur}}}{1 + \frac{4 \cdot \left( \frac{d_{si}}{2} \right)^2 \cdot d_{li}}{3 \cdot \pi \cdot a_{si} \cdot d_{li}}} \beta_{\perp i} \] (15)

\[
(a_{\alpha z})_{Y\alpha} = \frac{(a_{\alpha z})_{\text{sur}}}{1 + \frac{4 \cdot \left( \frac{d_{si}}{2} \right)^2 \cdot d_{li}}{3 \cdot \pi \cdot a_{si} \cdot d_{li}}} \beta_{|| i} \] (16)
\[
\beta_{||_i} = \frac{4}{3} \pi d_{s1i}^2 d_{li} \left\{ -\left( \varepsilon_{\text{sur}} - \varepsilon_h \right) \left( d_{s1i} + d_{s2i} \right)^3 + 2 \sum_{l} \left( 1 - 3 \left( \frac{u_l}{u_t}^2 + \left( d_{s1i} + d_{s2i} \right)^2 \right) \right) \right\} \varepsilon_{\text{sur}} \varepsilon_h^{-1}
\]
\[
\beta_{\perp i} = \frac{4}{3} \pi d_{s1i}^2 d_{li} \left\{ -2 \left( \varepsilon_{\text{sur}} - \varepsilon_h \right) \left( d_{s1i} + d_{s2i} \right)^3 + 2 \varepsilon_{\text{sur}} \sum_{l} \left( \frac{1}{u_l^3} \right) \right\} \varepsilon_{\text{sur}} \varepsilon_h^{-1}
\]

where:

\[ p_{\Lambda M} \text{ and } q_{\Lambda M} \] are associated Legendre polynomials of a first and a second kind, respectively;
\[ \Lambda, M \] are oscillation modes;
\[ d_{s1i} \text{ and } d_{s2i} \] are short and long dimension of the internal layer, here: gold, \( m \);
\[ d_{s1i} \] and \[ d_{s2i} \] are thickness of the capping agent (CTAB), \( m \);
\[ u_l \] is NR – NR semidistance from their centers (is identical to the surface disk dimensions): here: \( \sim 98.5 \) for \( x \) - and \( \sim 78.5 \) nm for \( z \)-projected axis;
\[ \beta_{||_i} \] is Yamaguchi’s coefficient for parallel contribution to the surface effect;
\[ \beta_{\perp i} \] is Yamaguchi’s coefficient for perpendicular contribution to the surface effect;

\( l \) refers to the pair of the \( i \) th and \((i + 1)\)th particle, up to the \( \binom{N}{2} \) pairs;
\[ \varepsilon_{\text{sur}} \] is permittivity of surface, here: PE material;
\[ \varepsilon_o \] is vacuum permittivity, \( \text{F}\cdot\text{m} \).

**Figure SI 2.** Electric dipole configurations that have been considered in the calculations for 15-15-55-nm gold nanorods (orange color) coated by a 4-nm CTAB compound (green color).

It is worth emphasizing that for dense-packed AuNRs, the formulas (1)-(8)-(18) require to be improved with the AuNR-AuNR multipole interactions, e.g., based on the Lorentz-Lorenz or Mie theory. However, the AuNRs are considered...
The total polarizability also requires some special conditions that are due to the particle’s symmetry, and they are specified with the one following equation \[^2\]:

\[
\alpha_i = \frac{2}{3} \left( (\alpha_{i,y}^a + (\alpha_{i,z})^a) + \frac{1}{3} ((\alpha_{i,x},d)^a) + \frac{1}{3} ((\alpha_{i,y,d})^a + (\alpha_{i,x,d})^a + \frac{1}{3} ((\alpha_{i,x})^a) \right) 
\]  

(19)

where:

- surface polarizability of the \( i \)-particle along the rod space diagonal projected on the \( x \) axis, \( m^3 \);
- surface polarizability of the \( i \)-particle along the rod space diagonal projected on the \( y \) axis, \( m^3 \);
- surface polarizability of the \( i \)-particle along the rod space diagonal projected on the \( z \) axis, \( m^3 \).

For other shapes, like cubes or triangles, the fractions vary considerably, and frequently, numerical methods need to be used.

### 1.2. Temperature distributions

The temperature increase is generally calculated thanks to the standard mass, momenta, and energy balance equations \[^{13}\]–\[^{14}\]:

\[
\frac{\partial}{\partial t} \left\{ \rho \frac{\rho \vec{v}}{\rho} \right\} + \text{div} \left\{ \rho \vec{v} \right\} + \text{div} \left\{ \frac{0}{p} \right\} = \text{div} \left\{ \frac{0}{\vec{v} + \vec{a}} \right\} + \left\{ \frac{0}{\vec{S} \vec{T} \text{TOT}} \right\}
\]

\[
\vec{T} = \text{grad}(X^t) - \frac{2}{3} \mu \vec{q}^T + 2 \mu \vec{d} = \text{grad} \left( \frac{d\sigma}{dT} \text{grad}(T) \right) - \frac{2}{3} \mu \vec{q}^T + 2 \mu \vec{d}
\]

(21)

where:

- \( t \) – time, s;
- \( \rho \) – density (here: water), \( kg \cdot m^{-3} \);
- \( e \) – specific energy, \( J \cdot kg^{-1} \);
- \( c_p \) – specific heat capacity, \( J \cdot kg^{-1} \cdot K^{-1} \);
- \( \vec{v} \) – velocity of the fluid, \( m \cdot s^{-1} \);
- \( \vec{q} \) – Fourier heat flux;
- \( \vec{T} \) – total momentum flux, \( Pa \);
- \( \vec{S} \) – unit tensor;
- \( p \) – pressure, \( Pa \);
- \( X^t \) – diffusive momentum flux; \( Pa \)
- \( d\sigma \)
- \( dT \) – surface tension gradient, \( N \cdot m^{-1} \cdot K^{-1} \), here: \( 0.05263 \ mN \cdot m^{-1} \cdot K^{-1} \);
- \( T \) – temperature, \( K \);
- \( S^\sigma \) – momentum source term, here: gravity;
- \( S^T \text{TOT} = S^\sigma M + S^\sigma NP \) – total source of energy, \( W \cdot m^{-3} \);
- \( S^\sigma \) – source of energy for continuous materials, \( W \cdot m^{-3} \);
- \( S^\sigma NP \) – source of energy for nanoparticles, \( W \cdot m^{-3} \).

Curved geometries, however, also require including the radiative transport equation that is generally calculated using the DOM model. Due to the high-simulation time, however, this work assumes another model that has been proposed in \[^{11}\]–\[^{12}\]–\[^{15}\]. The presence of AuNRs is here treated as a boundary condition, and the whole absorbed part of the irradiation is directly responsible for the heat conversion rate, following the formulas:
\[ S_{NP}^e = \sum_{i=1}^{N} I_{absi} = \xi \sum_{i=1}^{N} (w_i \cdot C_{absi}) I_{absi} = \]

\[ = \xi \sum_{i=1}^{N} (w_i \cdot C_{absi}) \cdot I_{o} \cdot (1 - R_{CTAB}) \cdot (1 - R_{g}) \cdot \left( 1 - \exp \left( - \xi \sum_{i=1}^{N} (w_i \cdot C_{absi}) \cdot l_{p-h} \right) \right) \]  

(22)

\[ I_o = \left( J_o(\lambda) \cdot \max(I_o) \right) \cdot \exp \left( -2 \left( \frac{r}{d_B} \right)^2 \right) \]  

(23)

\[ R_{CTAB} = \left( \frac{n_{CTAB} - n_h(\lambda)}{n_{CTAB} + n_h(\lambda)} \right)^2 \]  

(24)

\[ R_g = \left( \frac{\left| \varepsilon_g + \text{im} (\varepsilon_g) \right|}{2} - n_{CTAB} \right)^2 + \left( \frac{\left| \varepsilon_g - \text{im} (\varepsilon_g) \right|}{2} + n_{CTAB} \right)^2 \]  

(25)

where:

- \( \sigma_{absi} \) – absorbed part of irradiation, \( W \cdot m^{-2} \);
- \( I_{o} \) – incident irradiation, \( W \cdot m^{-2} \);
- \( J_o(\lambda) \) – incident irradiation function in reduced-to-one units, \( W \cdot m^{-2} \);
- \( R_{CTAB} \) – reflected coefficient of the CTAB compound, \( \cdot \);
- \( R_g \) – reflected coefficient of the gold material, \( \cdot \);
- \( l_{p-h} \) – penetration depth, here: 26.0 nm;
- \( P \) – output power of laser, W;
- \( d_B \) – beam size, m;
- \( r \) – radial distance, m;
- \( n_{CTAB} \) – refractive index of the CTAB compound, \( \cdot \);
- \( n_h(\lambda) \) – wavelength function of either the 15%-humid-air or NOA-61 refractive index, \( \cdot \);
- \( \varepsilon_g \equiv \varepsilon_1 \) – complex function of the electrical permittivity of gold, \( \cdot \);
- \( |\varepsilon_g| \) – absolute value of the electrical permittivity of gold, \( \cdot \).

This is the situation when the AuNRs are irradiated with a monochromatic light source. The problem appears if the incident irradiation characterizes an asymmetrical spectra distribution (e.g. solar light). In this paper, the authors suggest that the heat generation rate would be transformed into \( S_{NP}^P \rightarrow S_{P}^P \) and \( S_{NP}^M \rightarrow S_{M}^M \) which are described as:

\[ S_{NP}^e = \frac{\int_{\lambda_o}^{\lambda} S_{NP} d\lambda}{\int_{\lambda_o}^{\lambda} d\lambda} \]  

(26)
\[ S_e^M = \frac{\int_{\lambda_o}^{\lambda_k} S_e^M d\lambda}{\int_{\lambda_o}^{\lambda_k} d\lambda} \]  \hspace{1cm} (27)

where:

\( \lambda_o \) – lower limit of the wavelength interval, here: 250 nm;

\( \lambda_k \) – upper limit of the wavelength interval, here: 1100 nm.

Using discrete numbers, the integral from the formulas (26) and (27) become a sum from \( \lambda_o \) to \( \lambda_k \).

As long as the \( l_p - h \) is treated as a thin surface with the AuNRs as inclusions, the situation is significantly different for the continuous materials where the beam is diminished as the depth increases. Therefore, the \( l_p - h \) is then transformed into the function of the light ray line, yielding the considered system \[^{12}\] \[^{15}\]:

\[ S_e^M = \sigma_{abs} M \cdot l_{abs} M = \sigma_{abs} M (\lambda) \cdot l_o (\lambda) \cdot (1 - R_M (\lambda)) \cdot (1 - \exp (- \sigma_{abs} M (\lambda) \cdot d_M)) \]  \hspace{1cm} (28)

\[ \sigma_{abs} M (\lambda) = \frac{4\pi \cdot \text{im} (n_M (\lambda))}{\lambda} \]  \hspace{1cm} (29)

\[ R_M (\lambda) = \frac{(\text{re} (n_M (\lambda)) - n_{air} (\lambda))^2 + (\text{im} (n_M (\lambda)))^2}{(\text{re} (n_M (\lambda)) + n_{air} (\lambda))^2 + (\text{im} (n_M (\lambda)))^2} \]  \hspace{1cm} (30)

where:

\( \sigma_{abs} M (\lambda) \) – wavelength function of the absorption coefficient of a material, \( m^{-1} \);

\( l_{abs} M \) – the part of the irradiation that has been absorbed by a material, \( W \cdot m^{-2} \);

\( l_o (\lambda) \) – spectral distribution of the light source’s power density, \( W \cdot m^{-2} \);

\( R_M (\lambda) \) – wavelength function of the reflection coefficient of a material, \( - \);

\( d_M \) – optical thickness in the considered material, \( m \);

\( n_M (\lambda) \) – wavelength function of the refractive index of a material, \( - \);

\( \text{re} \) – real part of a parameter

All the abovementioned equations have been investigated and adjusted to the working system. Moreover, the appropriate boundary conditions have to be specified, which is deliberated in Section 2.
2. Calculation methods and boundary conditions

Both optical cross-sections and temperature distributions are determined using two different techniques. Nevertheless, the absorption coefficient and the properties of the surrounding medium do the lion’s share in heat and mass transfer. The absorption cross sections are calculated analytically based on the Rayleigh-Drude approximation following the formulas (1) – (19) and (21) – (30). All calculations have been examined in the Wolfram.Mathematica software (version 11.3.0). The nanoparticle size and shape distributions are included for dimension groups based on the Gaussian curves where the maximum value has been located at the 15 x 15 x 55 nm size. The material parameters are specified in table 2.1 in the range from 250 to 1100 nm.

Table 2.1. Assumed parameters for absorption spectra calculations

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Assumed value</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>NPs size, $d_{x1} \times d_{y1} \times d_{z1}$</td>
<td>15 x 15 x 55 nm</td>
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<tr>
<td>Thickness of the capping agent (CTAB), $d_{s2}$</td>
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<td>Average NR – NR distance</td>
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<td>Nanoparticles density, $\xi$</td>
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<td>Fluid refractive index, $n_R$</td>
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<tr>
<td></td>
<td>NOA-61</td>
<td>[16]</td>
</tr>
<tr>
<td></td>
<td>water</td>
<td>[17]</td>
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<td>Refractive index of PE platform, $n_{surf}$</td>
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<td></td>
<td>NOA-61</td>
<td>[17]</td>
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<td>Refractive index of borosilicate glass, $n_{glass}$</td>
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<td>Refractive index of CTAB compound, $n_{CTAB}$</td>
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<td>[18]</td>
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<td>$\varepsilon_\text{im}$</td>
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<td>$1.33190^1$</td>
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</table>

On the other hand, the temperature distributions are determined using CFD methods and algorithms following the formulas (20) – (21). The calculations have been performed via Ansys.Fluent software (version 22.1) using the Tryton supercomputer of the TASK resources of 72 cores (Intel®Xeon®Processor E5 v3 @ 2.3 GHz).

Figure SI 3 demonstrates the geometry reproduced based on the experiments, whereas meshes and their specifications are revealed in Appendix A. The simulations are run using the SIMPLE algorithm and the second-order scheme for the general (20) equations. The control parameters are established at 0.5, except pressure and density, whose values equal 0.3. Before the simulations start, materials properties and boundary conditions have been specified for the considered system, which is highlighted in Tables 2.2 and 2.3. Due to the lack of some parameters about the NOA-61 glue, epoxy resin has been adjusted.

Figure SI 3. Scheme of the reproduced geometry applied in the simulations (scale has not been saved)

---

2 At standard conditions: $\lambda=600$ nm, $p=1$ atm, $T=24^\circ$C
Table 2.2. Material properties in the considered simulations

<table>
<thead>
<tr>
<th>Material</th>
<th>Density ((kg \cdot m^{-3}))</th>
<th>Specific heat capacity ((J \cdot kg^{-1} \cdot K^{-1}))</th>
<th>Thermal conductivity coefficient ((W \cdot m^{-1} \cdot K^{-1}))</th>
<th>Dynamic viscosity ((Pa \cdot s))</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Borosilicate glass</td>
<td>2124.9</td>
<td>779.74</td>
<td>0.9245251</td>
<td>+ 0.0004777689 (T) + 9.178795 (10^{-7} \cdot T^2)</td>
<td>[21][23]</td>
</tr>
<tr>
<td>Gold</td>
<td>19320</td>
<td>129.81</td>
<td>317</td>
<td></td>
<td>[24][25]</td>
</tr>
<tr>
<td>Air</td>
<td>352.965 (T^{-1})</td>
<td>1006.43</td>
<td>0.004204762</td>
<td>+ 7.242857 (10^{-5} \cdot T)</td>
<td>[26][27][28]</td>
</tr>
<tr>
<td>NOA61</td>
<td>1231</td>
<td>1100</td>
<td>0.50</td>
<td>0.30</td>
<td>[17][29]</td>
</tr>
</tbody>
</table>

Table 2.3. Specified boundary conditions in the considered simulations

<table>
<thead>
<tr>
<th>No.</th>
<th>Material</th>
<th>Type of boundary conditions</th>
<th>Details</th>
<th>Formulas &amp; equations</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)</td>
<td>Bottom borosilicate glass</td>
<td>Mixed</td>
<td>(T_o = 297.15 K \left(75.20^oF\right))</td>
<td>(15) ((21) \rightarrow (25))</td>
<td>[11][13]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(k_{glass-air} = 13.6 W \cdot m^{-2} \cdot K^{-1})</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(d_M = 0.001 m)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(\max(I_o) = 286000 W \cdot m^{-2})</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(\max(S^M_e) = 347.75 W \cdot m^{-3})</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(d_B = 0.004 m)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(2)</td>
<td>Air</td>
<td>Outlet (Neumann)</td>
<td>(T_o = 297.15 K \left(75.20^oF\right))</td>
<td>(15)</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(v_o = 0)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(3)</td>
<td>NOA61</td>
<td>Neumann</td>
<td>(T_o = 297.15 K \left(75.20^oF\right))</td>
<td>(15)</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(\dot{q} = 0 W \cdot m^{-2})</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(4)</td>
<td>Top borosilicate glass</td>
<td>Mixed</td>
<td>(T_o = 297.15 K \left(75.20^oF\right))</td>
<td>(15) ((21) \rightarrow (24))</td>
<td>[11][13]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(k_{glass-air} = 13.6 W \cdot m^{-2} \cdot K^{-1})</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(d_M = 0.001 m)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(\max(I_o) = 286000 W \cdot m^{-2})</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(\max(S^M_e) = 1.2057 \cdot 10^6 W \cdot m^{-3})</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(d_B = 0.004 m)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(5)</td>
<td>Gold surface</td>
<td>Neumann</td>
<td>(T_o = 297.15 K \left(75.20^oF\right))</td>
<td>(1) ((2) \rightarrow (20))</td>
<td>[2][11][12][24]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Figure SI 4. Intensity spectrum distribution \(J_o(\lambda)\) of the applied lamp.
3. References

[20] T. A. A. Laboratory.
[27] Engineering ToolBox 2009.
Appendix A: Mesh and time independent tests

This part demonstrates the mesh and time independence procedure based on Richardson’s and Roache’s extrapolations. The first one allows the determination of the continuum values of a selected quantity $f_{ext}$ and highlights the relative and fractional error between the different mesh or timestep results. Moreover, this approach is dedicated to lower-order discrete values. The methodology is bases on the formula:\(\text{(A1)}\):

$$f_{ext} = f_{h=0} + g_1 h + g_2 h^2 + ...$$

where:
- $\epsilon$ – relative error between two sets/values of data, - ;
- $f_{1,2,3...}$ – value for the 1st, 2nd, 3rd set of data,
- $f_{h=0}$ – continuum value as if the mesh or time size equals zero
- $g_{1,2,3...}$ – constant or a function of the selected parameter that is other than $h$

For the second-order scheme that has been utilized in this work the continuum value $f_{h=0}$ yields:

$$f_{h=0} = f_1 + \frac{f_2 - f_1}{\left(\frac{h_2}{h_1}\right)^\delta - 1}$$

where:
- $h_{1,2,3...}$ – 1st, 2nd, 3rd... grid or time size;
- $\delta$ – rank of accuracy, here: $\delta = 2$

Accordingly, the equation (A2) is transformed for three meshes into:

$$f_{ext} = \frac{2^n f_1 - f_2}{2^n - 1}$$

(A3)

$$n = \log_2 \left(\frac{f_2 - f_3}{f_1 - f_2}\right)$$

(A4)

which allows the investigated value to be extrapolated with a specified error, e.g., the relative $\epsilon$ and fractional error $E_1$ between two sets of data that follow:

$$\epsilon = \frac{f_2 - f_1}{f_1}$$

(A5)

$$E_1 = \frac{\epsilon}{\left(\frac{h_2}{h_1}\right)^\delta - 1}$$

(A6)

Furthermore, Roache’s approach[31] has introduced the grid convergence index (GCI) methodology that indicates how far the error may change as the mesh is finer, which for Richardson extrapolation is defined by the GCI parameter:
\[ GCI_{(\text{fine})} = F_s |E_1| = F_s \frac{|e|}{\langle h_2 \rangle_s} - 1 \]  

where:

- \( F_s \) – factor of safety, here: 1.25

In this work, three meshes are consumed so as to provide the mesh and timestep to be independent. Figure A01 reveals the discretization used, whereas Table TA01 highlights the details of these grids. As the quantity value, two parameters have been selected – the maximum temperature in the whole system (\( \text{max} \)) and top glass (4) mean temperature (\( \text{mean} \)) have been utilized for the Richardson extrapolation and GCI methodology, both in spatial and time regimes. The obtained comparison are reported in Figure A01, whereas the error data are included in Table TA02.
Figure A01. Three meshes that have been utilized in the simulations from the top view

Table TA01. Details of the applied meshes

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Mesh 1</th>
<th>Mesh 2</th>
<th>Mesh 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mesh size</td>
<td>0.166667 mm</td>
<td>0.083333 mm</td>
<td>0.055556 mm</td>
</tr>
<tr>
<td>Maximum aspect ratio</td>
<td>40.0695 \textsuperscript{2}</td>
<td>28.0307 \textsuperscript{2}</td>
<td>28.7873 \textsuperscript{2}</td>
</tr>
<tr>
<td>Mean volume cell</td>
<td>$1.717776 \times 10^{-11}$ m$^3$</td>
<td>$1.717163 \times 10^{-11}$ m$^3$</td>
<td>$1.717050 \times 10^{-11}$ m$^3$</td>
</tr>
</tbody>
</table>

\textsuperscript{2} Cells with maximum aspect ratio are located in the bottom glass (1) or in the NOA-61 zone (3)
<table>
<thead>
<tr>
<th>Extrapolate error</th>
<th>Mesh 1 – Mesh 2</th>
<th>Mesh 2 – Mesh 3</th>
<th>( t_{s1} - t_{s2} )</th>
<th>( t_{s2} - t_{s3} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>(</td>
<td>\epsilon</td>
<td>\max )</td>
<td>0.050368645 %</td>
<td>0.009325662 %</td>
</tr>
<tr>
<td>(</td>
<td>\epsilon</td>
<td>\mean )</td>
<td>0.069894595 %</td>
<td>0.020863796 %</td>
</tr>
<tr>
<td>( f_{h = 0} \max )</td>
<td>322.43526114 K</td>
<td>322.43161627 K</td>
<td>322.43212863 K</td>
<td>322.43291446 K</td>
</tr>
<tr>
<td>( f_{h = 0} \mean )</td>
<td>315.49611408 K</td>
<td>315.48450273 K</td>
<td>315.48696179 K</td>
<td>315.48766655 K</td>
</tr>
<tr>
<td>( GCI_{(fine)} \max )</td>
<td>0.020986936 %</td>
<td>0.009325662 %</td>
<td>0.036675509 %</td>
<td>0.017593777 %</td>
</tr>
<tr>
<td>( GCI_{(fine)} \mean )</td>
<td>0.029122748 %</td>
<td>0.020863796 %</td>
<td>0.007315010 %</td>
<td>0.002567504 %</td>
</tr>
<tr>
<td>( f_{ext} \max )</td>
<td>322.4303321 K</td>
<td>322.44180391 K</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( f_{ext} \mean )</td>
<td>315.4821112 K</td>
<td>315.48891530 K</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Since the spatial errors decrease below 1% significantly, the second mesh is consumed to repeat the procedure for three timesteps – \( t_{s1} = 1.0 \), \( t_{s2} = 0.5 \), and \( t_{s3} = 0.2 \) ms. Likewise, the obtained comparison implies the time errors at the maximum 0.1% level. Under the abovementioned results from the figures and the tables A01 and TA01,TA02, the 0.5-ms-second-mesh case has been declared to be spatial and time independent and is shifted to the experimental confrontations.