Computational Modeling Of Nanoparticle Heating For Treatment Planning Of Plasmonic Photothermal Therapy In Pancreatic Cancer

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INTRODUCTION: Pancreatic cancer is one of the deadliest cancers, with a 7% survival rate at five years from diagnosis. Different modalities of thermal therapy have been developed as potential tumor debulking tools; however, the outcome of these tissue treatments in-vivo is difficult to predict, thus causing a reduction in specificity and increasing pancreatitis risk. Gold nanoparticles (GNPs) may improve the efficacy of thermal therapy. Before in-vivo studies are undertaken, we propose a computational model of plasmonic photothermal therapy (PPTT) to study the laser-particle-tissue interactions and determine the optimum parameters for this treatment. This model may also serve as a future treatment planning tool for physicians.

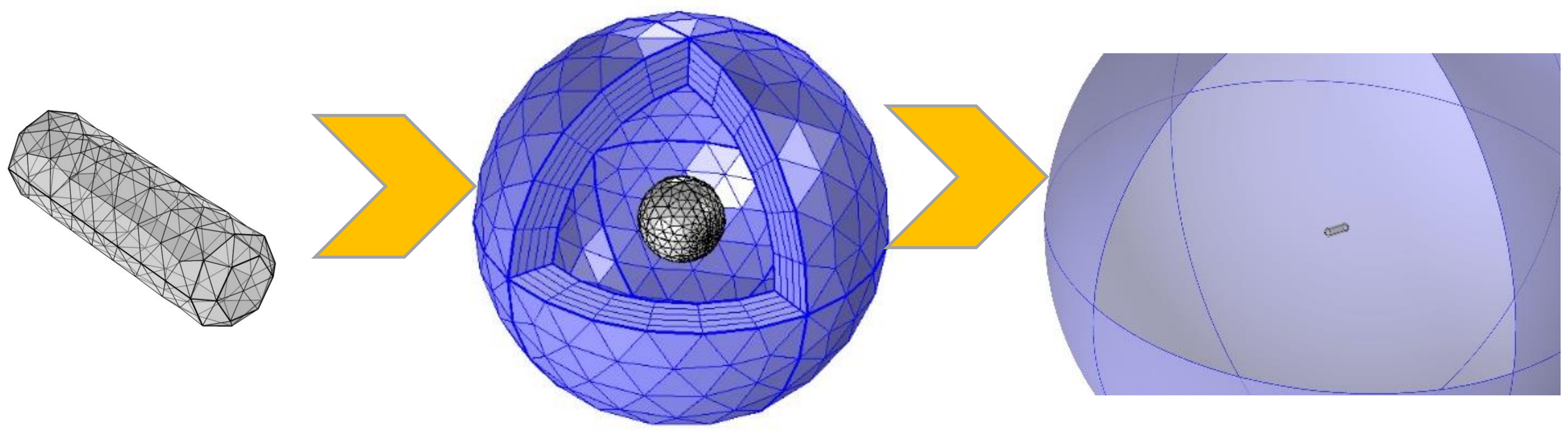

Figure 1. Model pipeline from SOLIDWORKS® to PDE Module

COMPUTATIONAL METHODS: We compared different shapes of nanoparticles and studied the temperature gradient induced in the surrounding media in both water and tissue.
RF Module was used to compute the energy absorbed by the nanoparticles using the following equations

$$\nabla \times \mu_r^{-1}(\nabla \times E) - k_0^2 \varepsilon E = 0$$

$$E_b = E_0 e^{\left(-j\frac{2\pi n}{\lambda}z\right)}\hat{\imath}$$

$$\sigma_{abs} = \frac{W_{abs}}{S_{in}};\ W_{abs} = \iiint_{\Omega} Q_h \, d\Omega$$

Coefficient Form PDE Module was used to compute heat distribution around the particle, the clusters, and point sources. General equation is simplified as

$$\nabla \cdot (-k\nabla T) = f;\ f = W_{abs}$$

RESULTS: Particles with absorption cross section peak (Fig. 2) near the wavelength of the laser (808 nm) absorbed the higher amounts of energy (see Table 1).

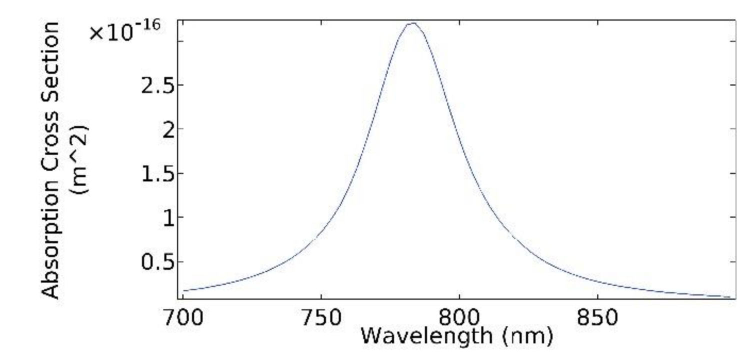

Figure 2. Absorption cross section

Table 1. Energy absorbed by different GNPs

Nanoparticle Type	Dimensions (nm)	Energy Absorbed (W/m^3)
Nanorod	80	1.37E18
Nanorod	60	7.41E17
Nanobipyramid	110	4.90E17
Nanobipyramid	146	4.40E17
Nanosphere	40	5.81E14
Nanosphere	150	8.43E14

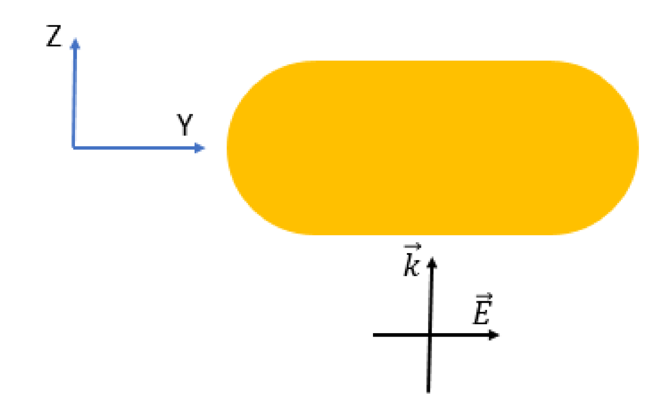

Figure 3. Light propagating along Z and polarized along Y

Orientation of the particle with respect to the light propagation affects the amount of energy absorbed. Table 2 shows the average energy absorbed to account for this effect. The nanorod is the best suited for enhanced photothermal effects. The temperature field of a cubic array of nanorods with the same energy is shown in Figure 4

Table 2. Average energy absorbed and maximum temperature reached

Nanoparticle Type	Average Energy Absorbed (W/m^3)	Max Temperature (°C)
NR (80 nm)	6.81E17	252
NR (60 nm)	3.71E17	93.9
BP (110 nm)	2.45E17	136
BP (146 nm)	2.20E17	203
NS (40 nm)	5.81E14	37.2
NS (150 nm)	8.43E14	40.6

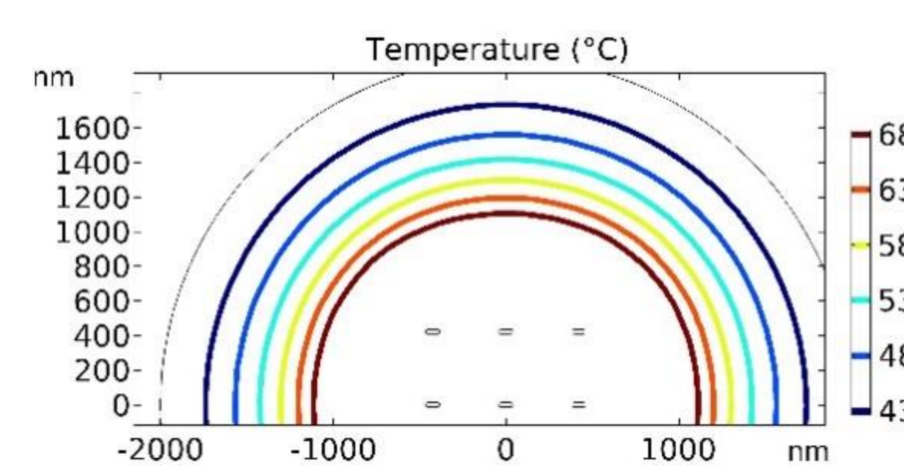

Figure 4. Temperature field by NP cluster

The size of the cluster is small enough that can be represented as a point in the tissue-level simulations (Fig. 5). Tissue properties from literature [1] are not representative of the wavelength used in this work. Laser effects in tissue are larger than anticipated, but NP clusters show localized thermal effects in the mm size scale (Fig. 6)

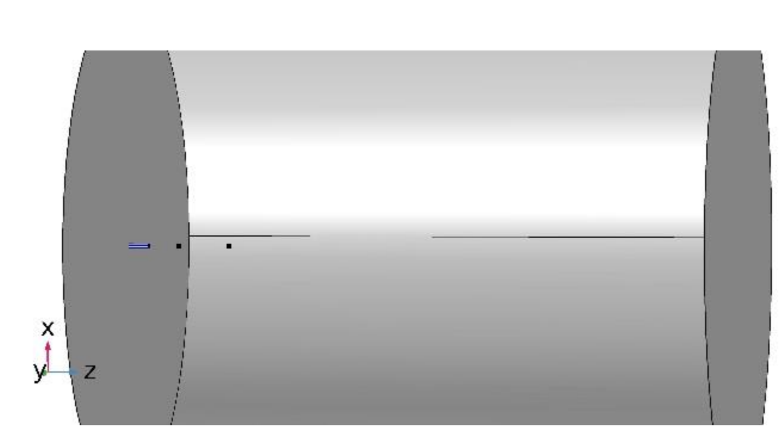

Figure 5. Tissue phantom model

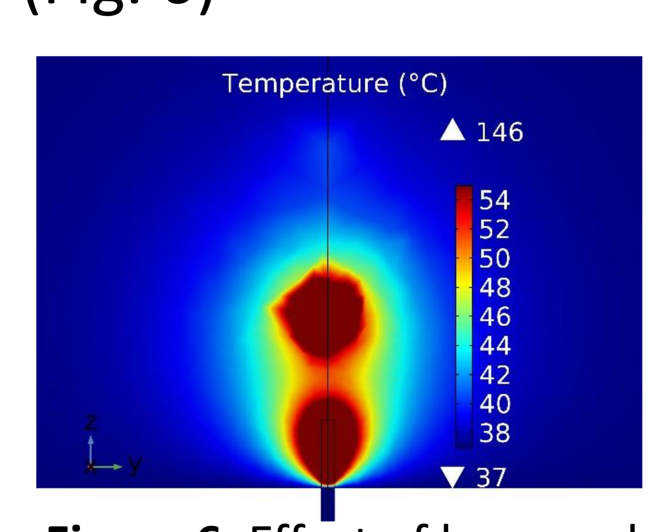

Figure 6. Effect of laser and NP clusters in tissue

CONCLUSIONS: Successfully developed a model to compute photothermal heating following the light absorption mechanisms of gold nanoparticles. Furthermore, effect of NP clusters in tissue were assessed.

REFERENCES:

1. Saccomandi, P., et al., Theoretical analysis and experimental evaluation of laser-induced interstitial thermotherapy in ex vivo porcine pancreas. 2012. 59(10): p. 2958-2964.