COMSOL CONFERENCE 2016 BOSTON

Modeling of the Singlet Oxygen Distribution in Photofrin-Photodynamic Therapy of the Plural Cavity

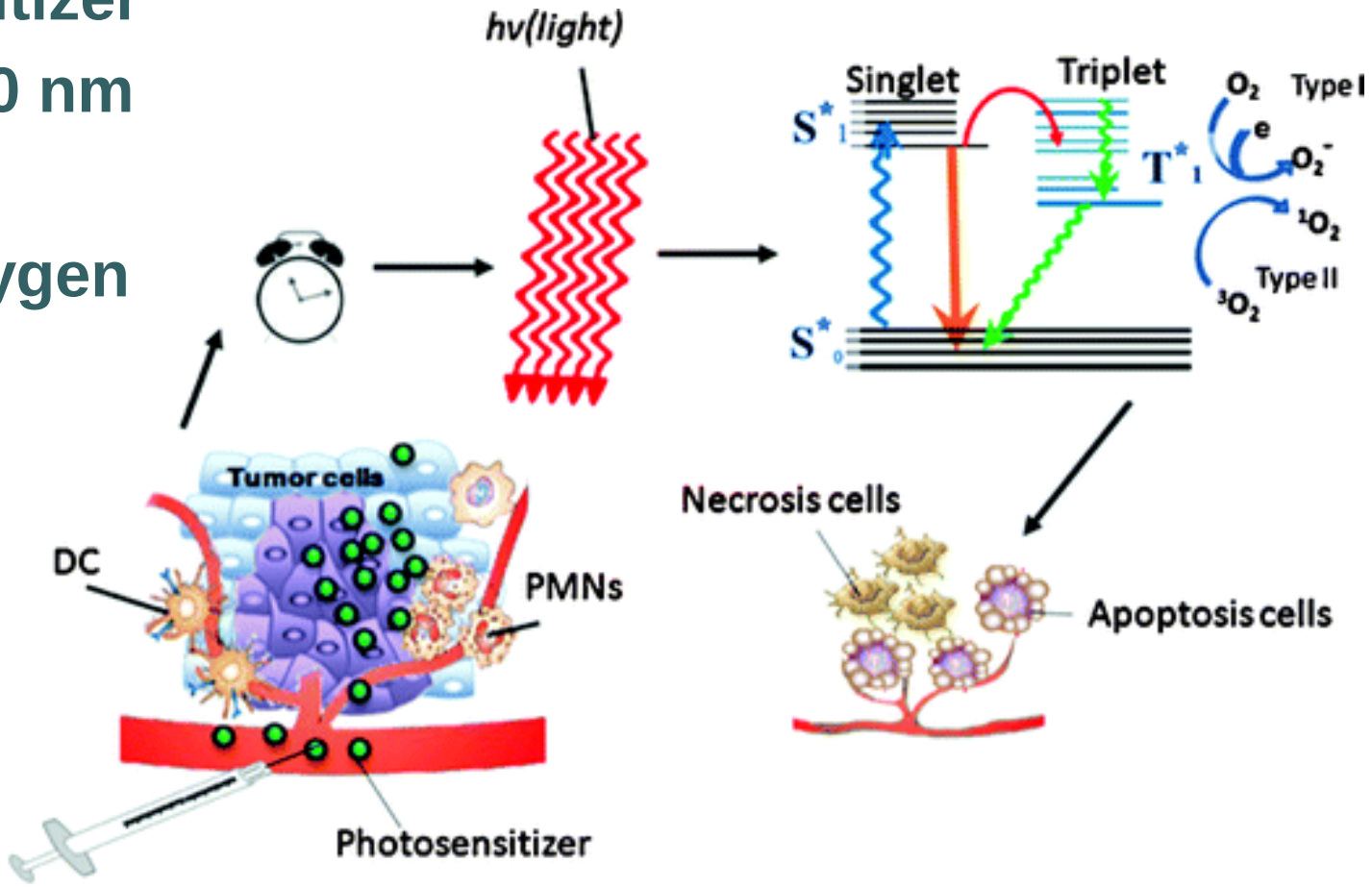
Rozhin Penjweini, Michele M Kim, Timothy C Zhu

Department of Radiation Oncology, School of Medicine, University of Pennsylvania, Philadelphia, PA 19104, USA

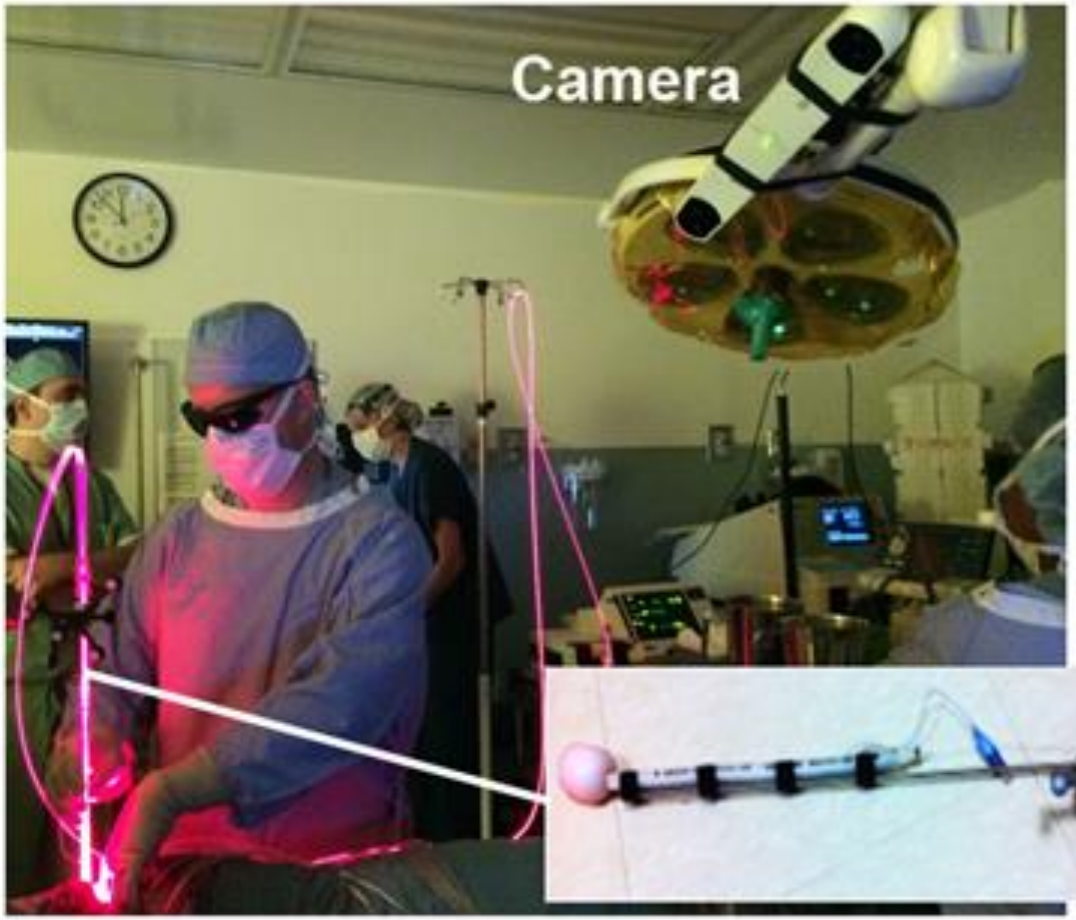
Perelman School of Medicine
University of Pennsylvania

Photodynamic Therapy (PDT)

- Photosensitizer
- Light at 630 nm
- Oxygen
- Singlet Oxygen

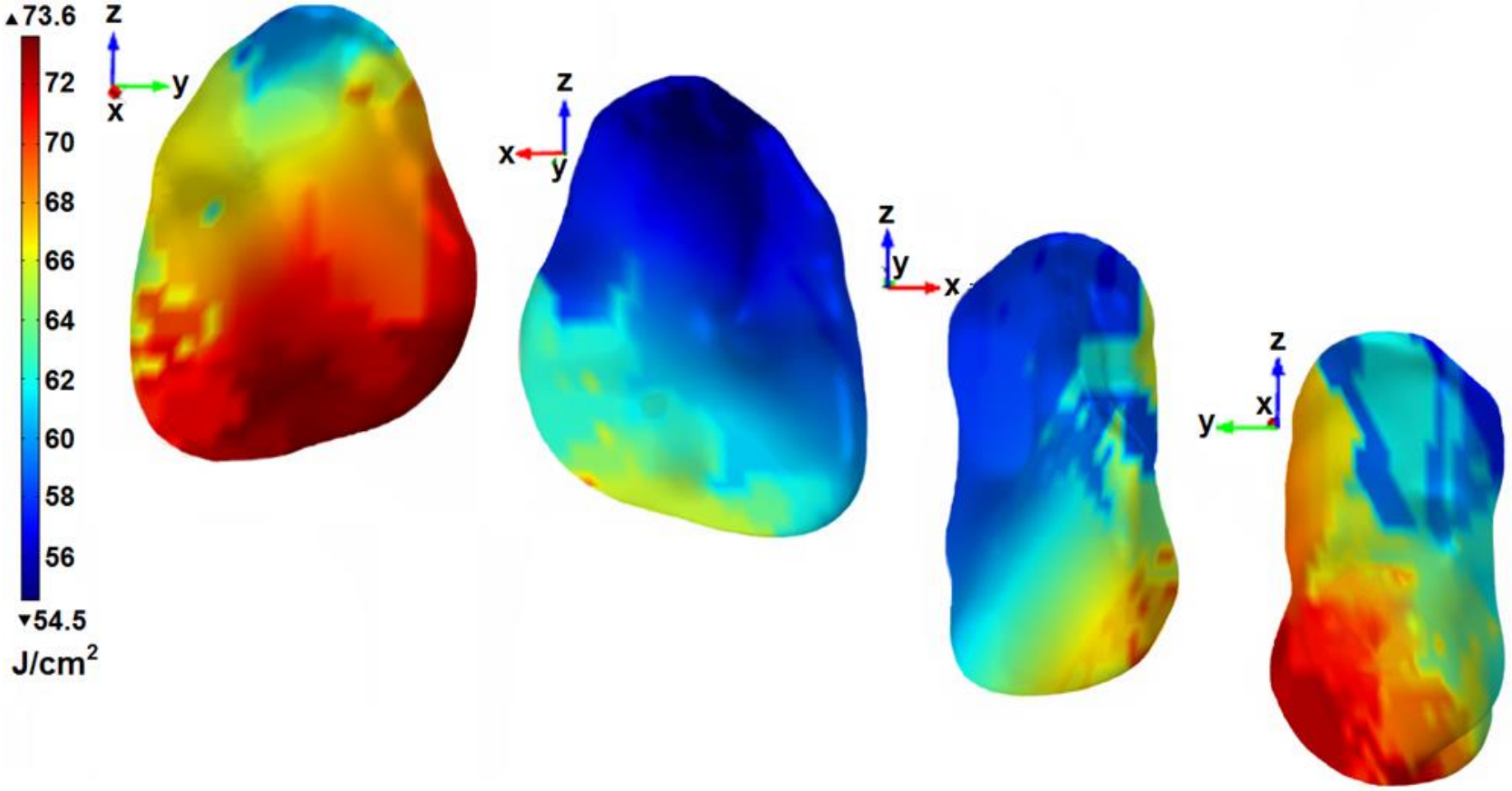


Obtaining Pleural Cavity Geometry

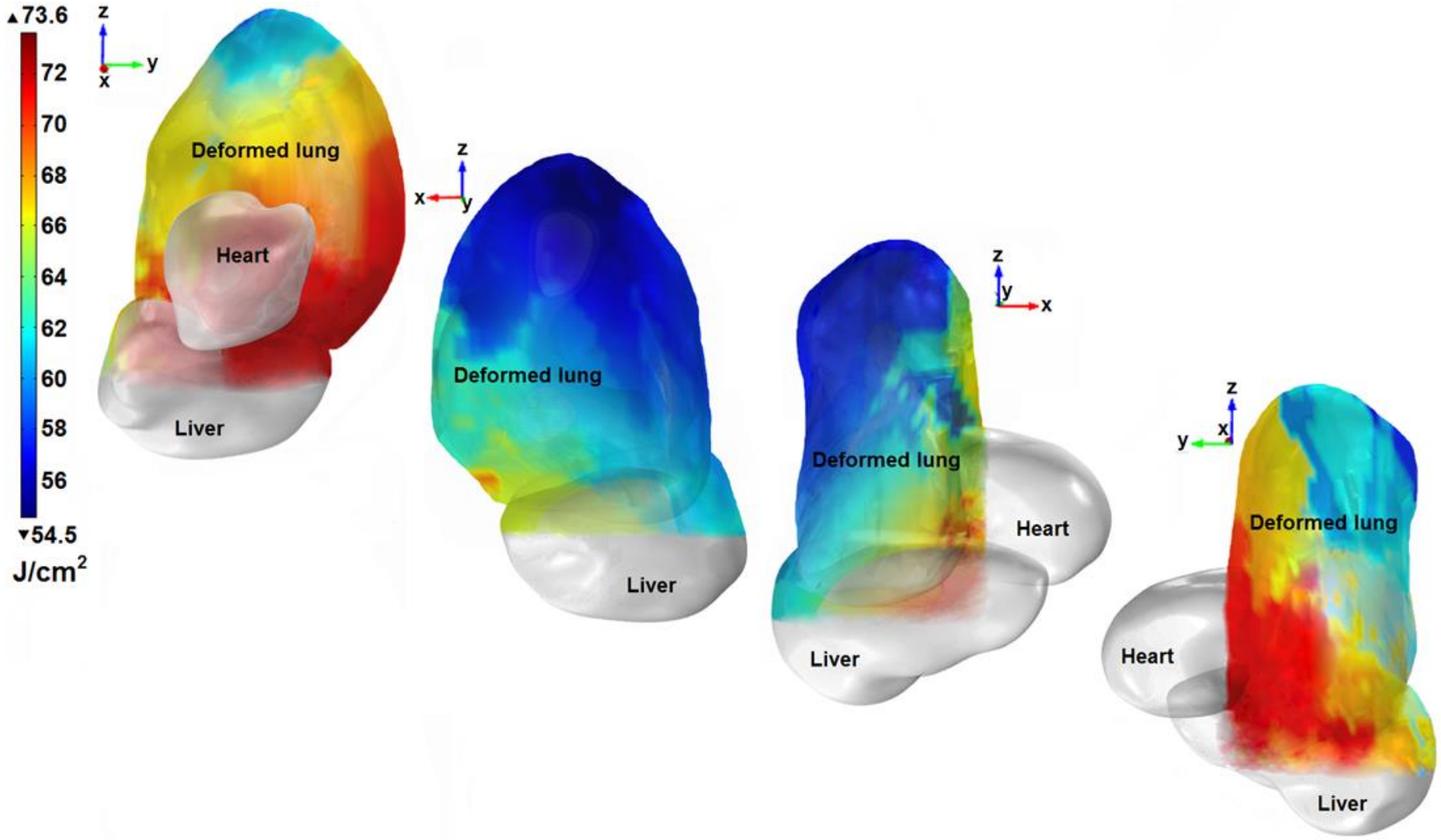


NDI

Delivered Light Fluence



Organs at Risk



Material and Mesh Properties

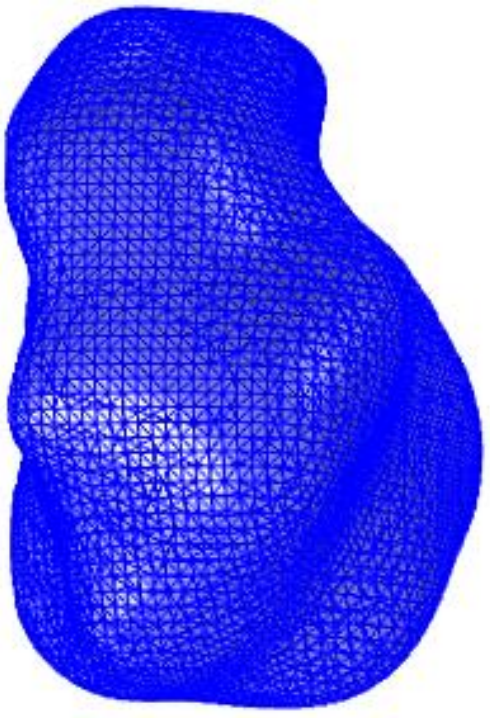


Table 1. Lung stress-strain material properties

	Poisson's value	Young's modulus (kPa)	Density (kg/m^3)
Pleural Cavity	0.36	3	242

Table 2. Element statistics of the tetrahedral mesh generated for the geometry

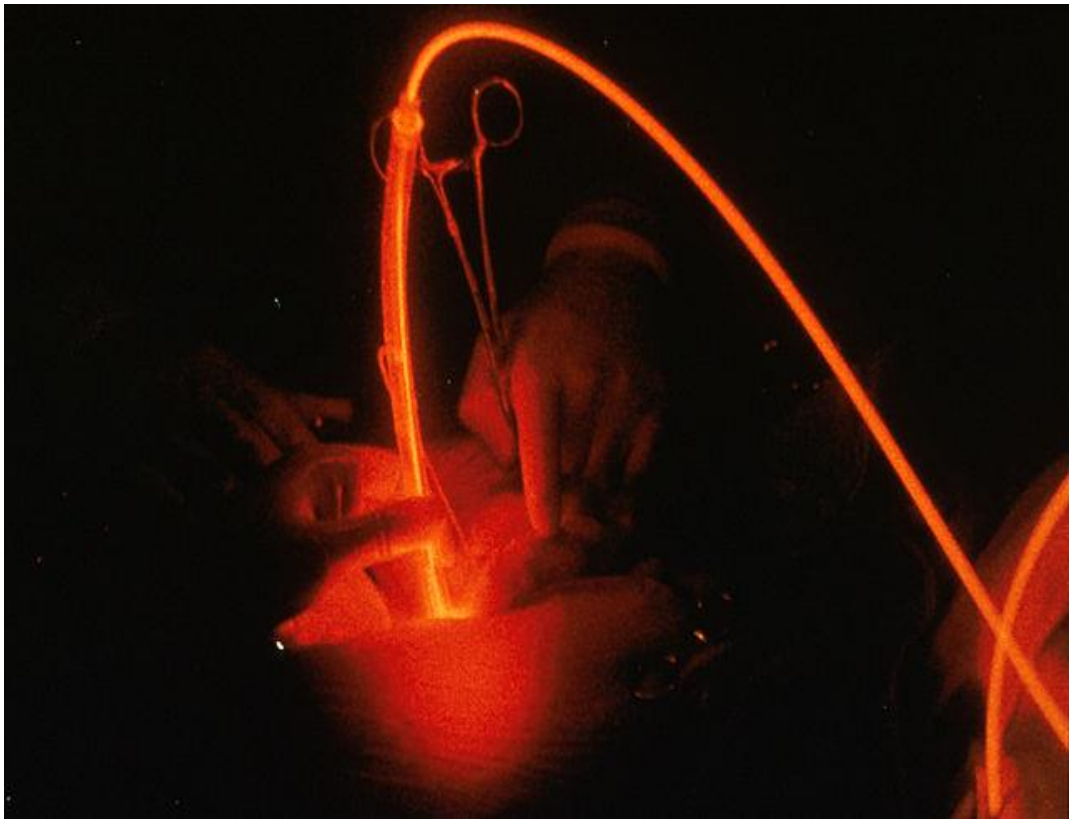
	Element Number	Min element quality	Average element quality	Element volume ratio	Mesh volume (cm^3)	Max growth rate	Mean growth rate
Patient	56052	0.09	0.69	2.93×10^{-7}	2631	4.45	1.85

Mathematical Simulations of PDT

$$\frac{d[^3O_2]}{dt} + \left(\xi \frac{\phi[S_0]}{[^3O_2] + \beta} \right) [^3O_2] - g \left(1 - \frac{[^3O_2]}{[^3O_2](t=0)} \right) = 0$$

$$\frac{d[S_0]}{dt} + \left(\xi\sigma \frac{\phi([S_0] + \delta)[^3O_2]}{[^3O_2] + \beta} \right) [S_0] = 0$$

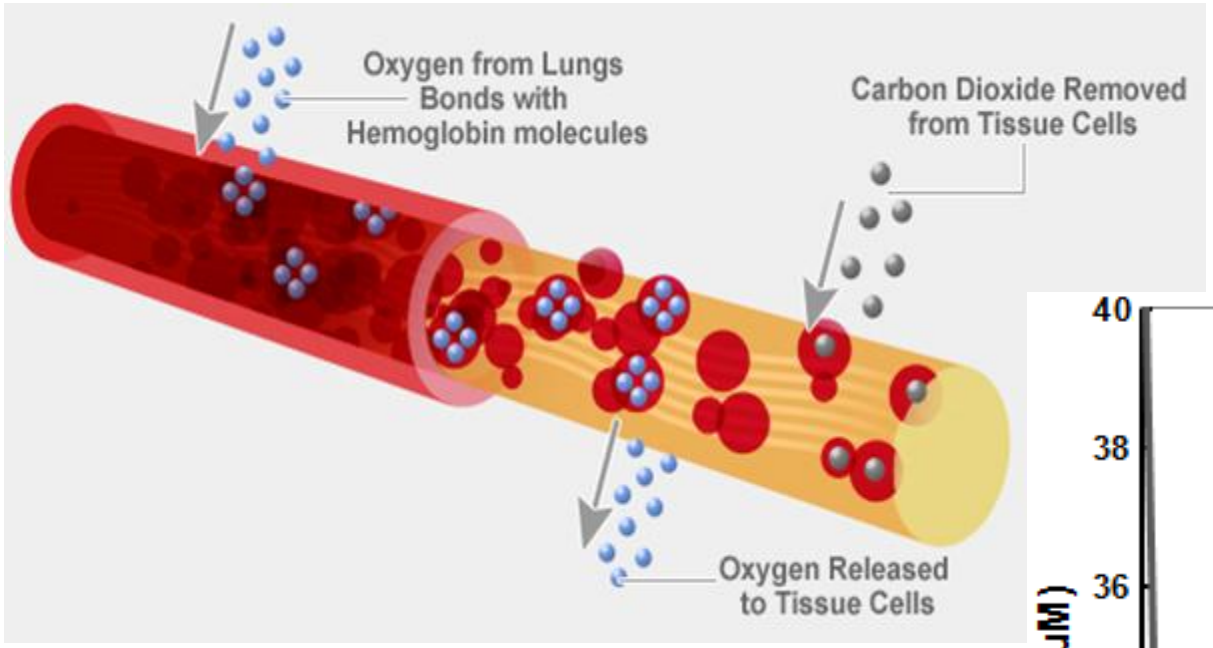
$$\frac{d[^1O_2]_{rx}}{dt} - \left(\xi \frac{\phi[S_0][^3O_2]}{[^3O_2] + \beta} \right) = 0$$

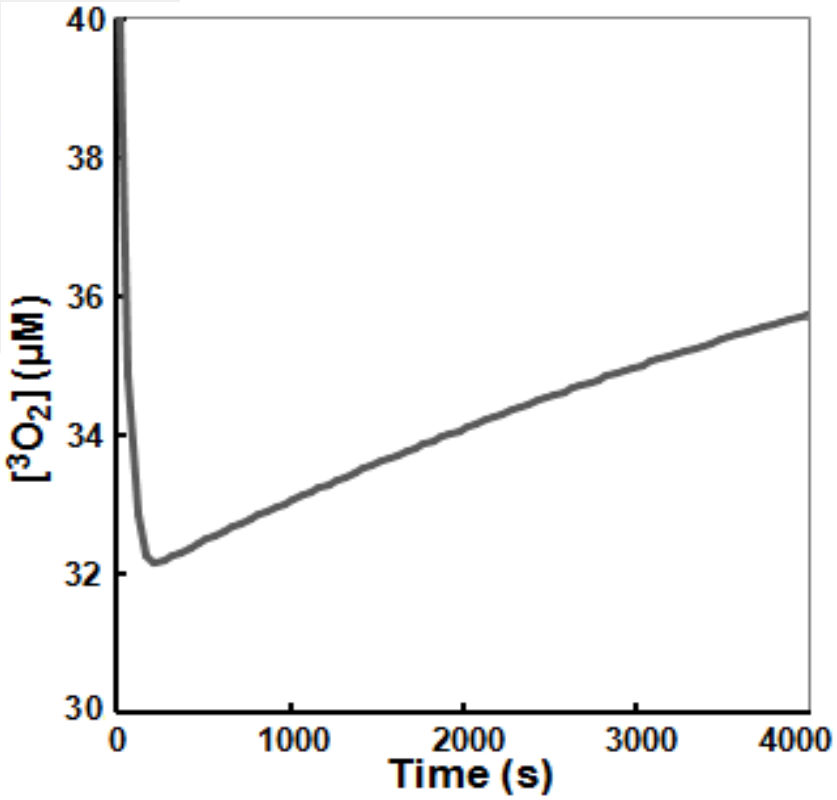


Photochemical Parameters

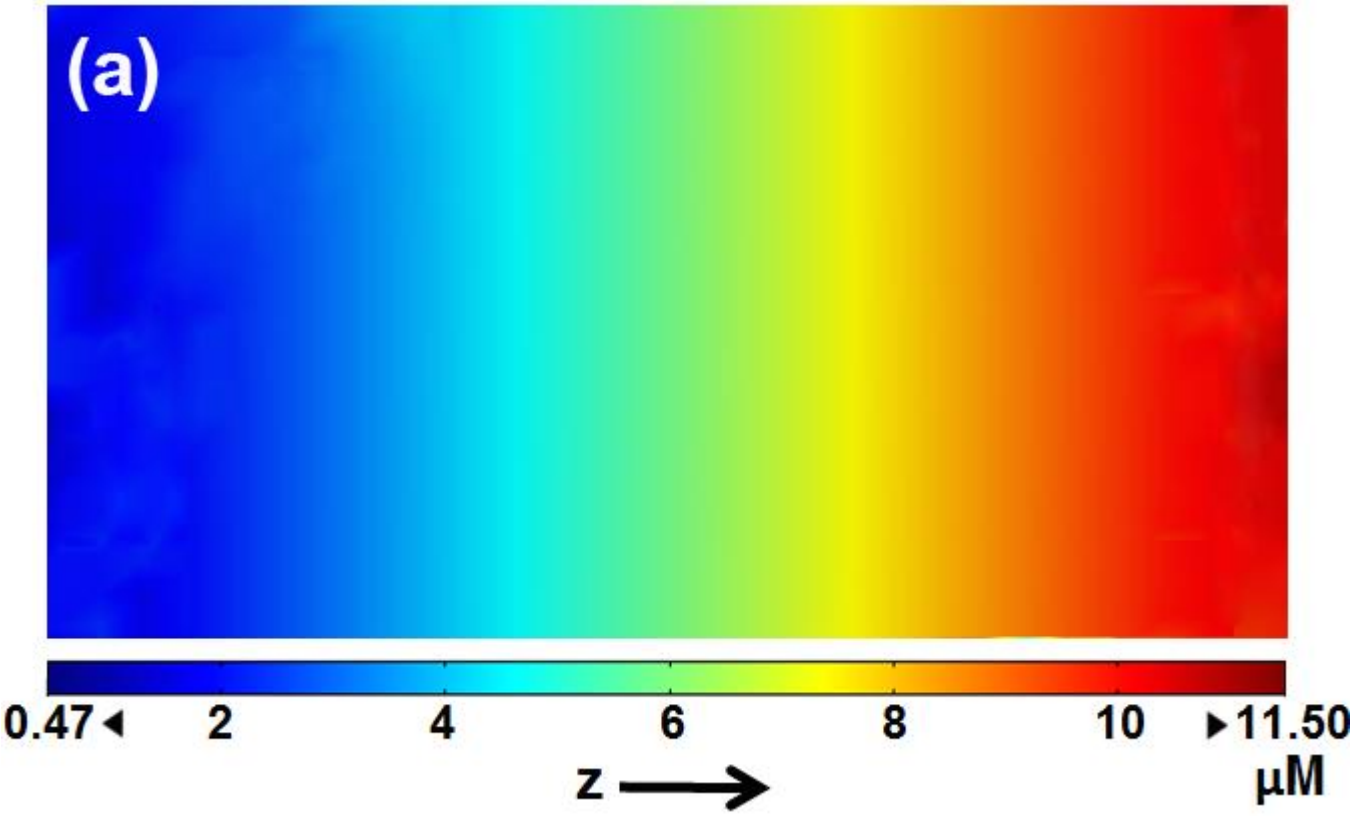
Parameter	Definition	Value
ξ ($cm^2 s^{-1} mW^{-1}$)	Specific oxygen consumption rate	3.7×10^{-3}
σ (μM^{-1})	Specific photobleaching ratio	7.6×10^{-5}
β (μM)	Oxygen quenching threshold concentration	11.9
δ (μM)	Low concentration correction	33
g ($\mu M/s$)	Maximum oxygen supply rate	0.76
$[^3O_2]_0$ (μM)	Initial ground-state oxygen concentration	40

Temporal Changes of Tissue Oxygenation

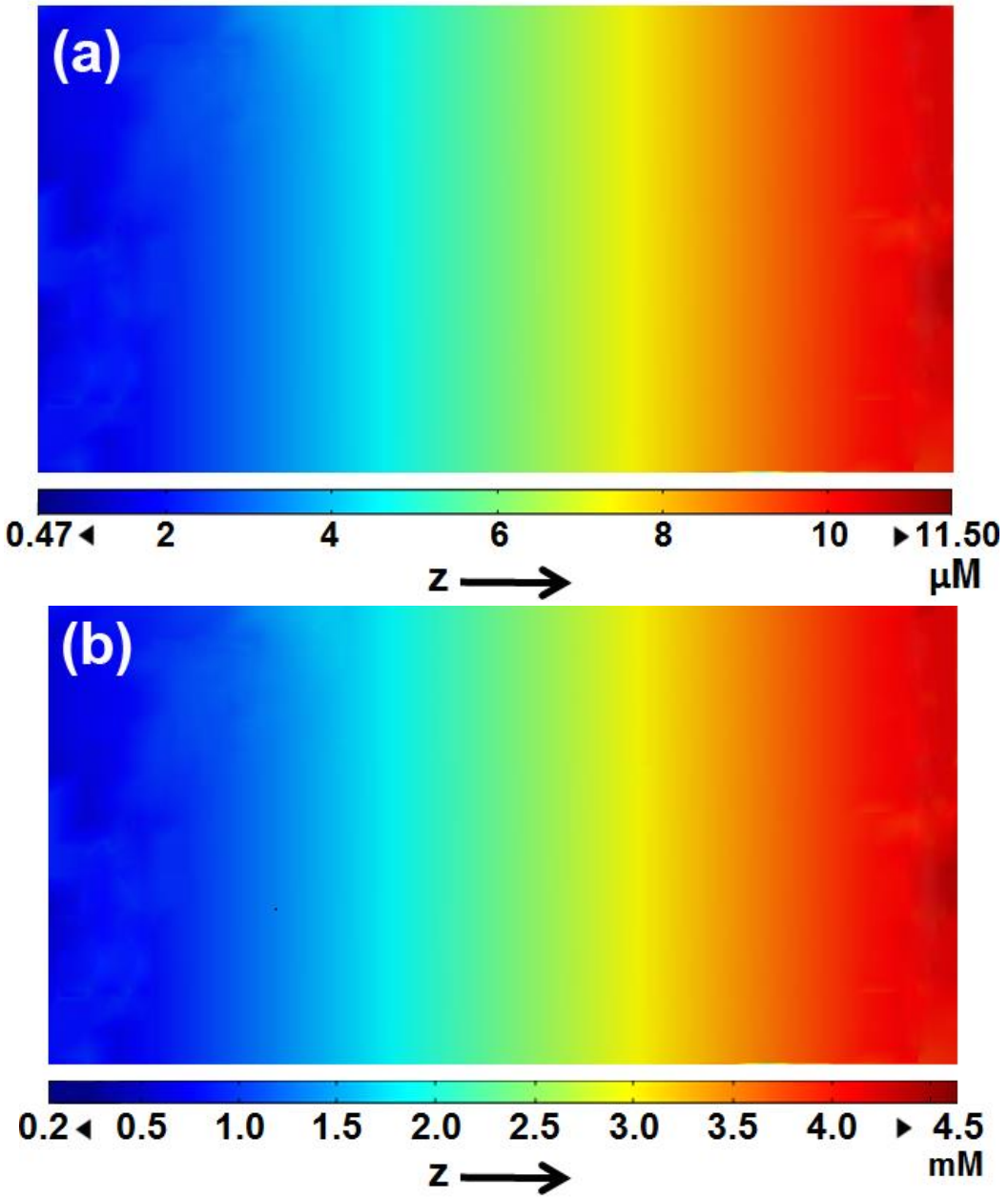




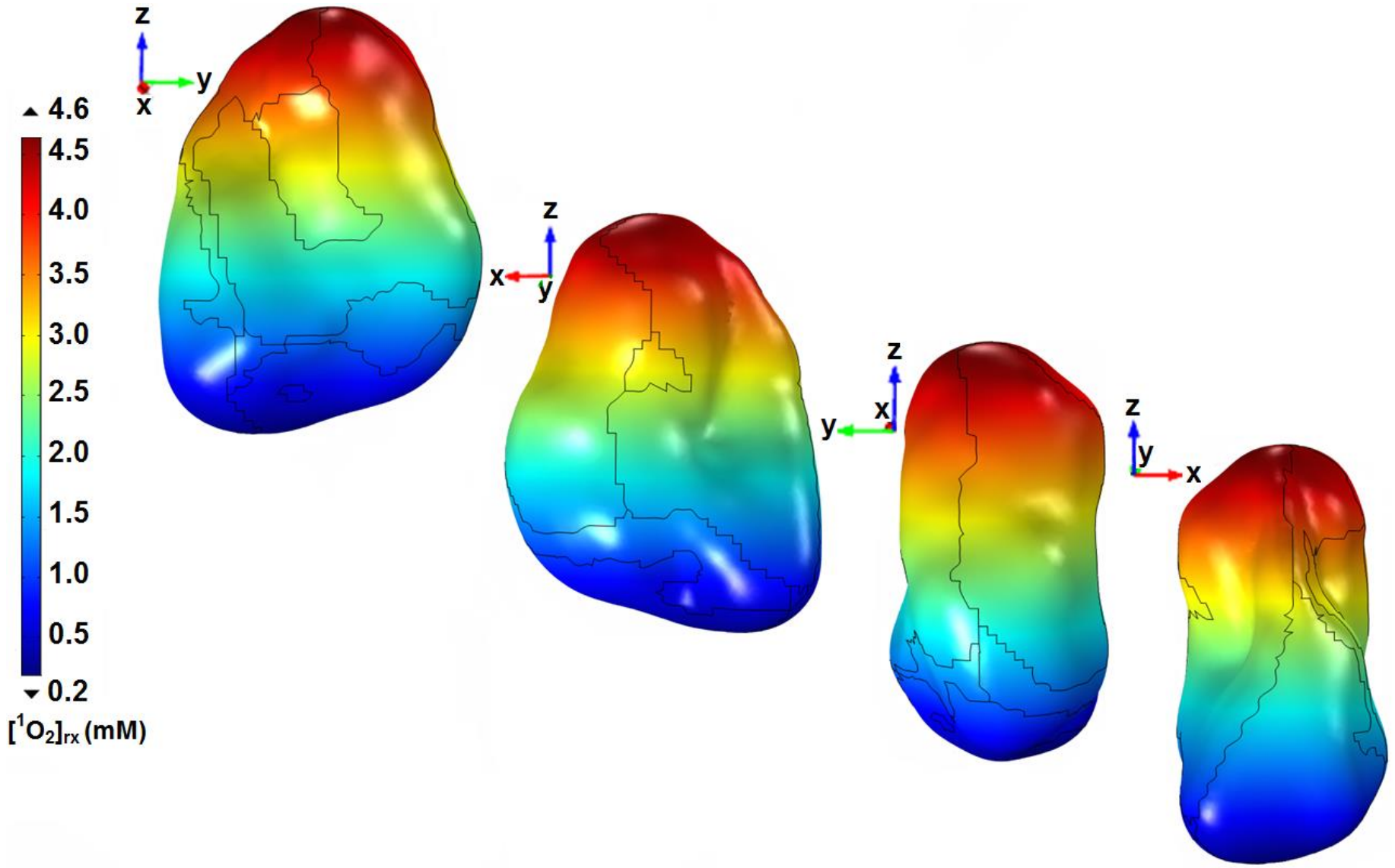
Photosensitizer Distribution



Singlet Oxygen Simulation



Singlet Oxygen Distribution



Conclusion

- In the ongoing clinical trial, the prescribed light fluence dose for Photofrin-PDT for mesothelioma is 60 J/cm^2. The magnitude of the delivered fluence changes from 54.5 to 73.6 J/cm^2 on the surface of the pleural cavity.
- The distribution of $[^1O_2]_{rx}$ during PDT was simulated and mapped on the treated plural cavity by using COMSOL.
- We believe that *in situ monitoring of the under-* and *over-exposed* regions to $[^1O_2]_{rx}$ can significantly improve the treatment.

PDT Group at UPenn

Physics

- Timothy Zhu
- Jarod Finlay
- Arjun G. Yodh
- Sophie Chung
- Carmen Rodriguez
- Andrea Dimofte
- Michele Kim
- Rozhin Penjweini
- Arash Darafsheh

Biology, Medicine, Chemistry

- Theresa M. Busch
- Keith Cengel
- Charles B Simone
- Jess Appleton
- Sally McNulty
- Joann Miller
- Min Yuan
- Sunil Singhal

Thank you

Perelman
School of Medicine
University of Pennsylvania

COMSOL
CONFERENCE
2016 BOSTON