# Parameter Optimization for Finite-Element Method (FEM) based modeling of singlet oxygen during PDT

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**Introduction** *(Mandatory)*

Singlet oxygen ($^1O_2$) is believed to be the major cytotoxic agent during photodynamic therapy (PDT), and the reaction between $^1O_2$ and tumor cells define the treatment efficacy at the most fundamental level. Incorporating the diffusion equation governing the light transport in turbid medium, the spatially and temporally-resolved concentrations of $^1O_2$, oxygen, sensitizer and biological targets described by the macroscopic kinetic equations can be modeled with finite-element method, and the distance-dependent reacted $^1O_2$ can be numerically calculated. The formula of reacted $^1O_2$ concentration involves a number of photophysical parameters which need to be determined explicitly. We first performed a comparison between the macroscopic model with the average result from a microscopic model to determine the corresponding model parameters. In addition, we observed a sudden drop of the calculated reacted $^1O_2$ along with the distance following the decrease of light fluence rate that can be correlated with the edge of necrosis depth. Based on this observation, we have performed a series of FEM calculation to determine the model parameters for CW treatments with different fluence rates and fractionation treatments with different on/off time interval, respectively. The sensitivity of each model parameters to the necrosis depths and treatment conditions are examined.