DIRECT SIMULATIONS AND INVERSE PROBLEMS INVOLVING NON-UNIFORMLY HEATED PALLADIUM NANOFLUIDS

Nilton P. Silva^{1,2}, Cláudia C. R. Cruz³, Henrique M. Fonseca⁴, Leonardo A. B. Varon⁵, José Mir J. da Costa⁶, Claudio L. Cesar⁷, Dilson S. Dos Santos^{3,8} and Helcio R. B. Orlande^{1,3}

¹Mechanical Eng. Program, COPPE - Oncobiology Program, Federal University of Rio de Janeiro, Brazil
²Department of Mechanical Eng., Federal University of Amazonas, Brazil
³Nanotechnology Eng. Program, COPPE, Federal University of Rio de Janeiro, Brazil
⁴Department of Mechanical Engineering, Fluminense Federal University - Volta Redonda, Brazil
⁵Faculty of Engineering, Bioengineering, Universidad Santiago de Cali, Colombia
⁶ Department of Statistics, Federal University of Amazonas, Brazil
⁷Institute of Physics, Federal University of Rio de Janeiro, Brazil
⁸Metallurgical and Materials Eng. Program, COPPE, Federal University of Rio de Janeiro, Brazil

ABSTRACT

Hyperthermia with mild heating of tumors can be used as an adjuvant to conventional cancer treatments, such as chemotherapy or radiotherapy. If heat is used solely for the destruction of cancer cells, the treatment is generally denoted as thermal ablation. Nanoparticles have been developed to improve the selective heating of tumor cells, by improving the localized absorption of external energy sources used in thermal therapies. Nanoparticles can also serve as carriers of drugs that specifically act on the tumor when heated, including hydrogen that can be desorbed to locally promote an antioxidant effect and reduce the viability of cancer cells.

In this work, palladium nanocubes and PdCeO₂ nanoparticles were synthesized and nanofluids produced with these nanomaterials were hydrogenated. Experiments that involved the heating of the nanofluids with a diode-laser revealed a substantial improvement of the absorbed energy as compared to distilled water, particularly for hydrogenated palladium nanocubes. The absorption coefficients of the nanofluids at the diode-laser wavelength were then estimated with the Markov Chain Monte Carlo (MCMC) method, which was implemented by the Metropolis-Hastings algorithm with sampling by blocks. The results obtained with Monte Carlo parameter estimation and direct simulations of an *in vitro* hyperthermia-chemotherapy experiment are also presented in this talk.