Development of a flexible and fast Monte Carlo radiative transfer code for photon density wave spectroscopy

Christian Peest*, Oliver Reich, and Lena Bressel

University of Potsdam, Institute of Chemistry – Physical Chemistry / innoFSPEC, Am Mühlenberg 3, 14476 Potsdam, Germany

**Presenting author (christian.peest@uni-potsdam.de)*

Photon Density Wave (PDW) spectroscopy [1,2] is a measurement technique for the determination of the absorption coefficient μ_a and the reduced scattering coefficient μ_s' of highly turbid samples [3]. It employs intensity modulated laser light in the MHz to GHz range, coupled into the sample via an optical fiber. The radiation forms a PDW which experiences a phase delay and a dampening in the turbid medium due to scattering and absorption. A receiving fiber feeds a detector attached to a network analyzer which measures the changes in amplitude and phase of the PDW depending on modulation frequency and fiber distance. μ_a and μ_s' can be accurately determined via a nonlinear fit, even for highly turbid samples ($0.1\ \mathrm{mm}^{-1} < \mu_s' < 100\ \mathrm{mm}^{-1}$). This makes the PDW ideally suited for inline process analytics of large-scale industrial processes, e.g., paint, cosmetics or polymer production, without a need for sample dilution [4].

Theoretical considerations of the PDW necessarily make approximations in order to solve the related radiative transfer equations, such as the P1 approximation. Our group is exploring the limits of the PDW with respect to extremely high optical densities ($\mu_s' > 100\mathrm{mm}^{-1}$), both through advancements in theory and through experiments.

In this talk we present the development of a specialized Monte Carlo radiative transfer code for the simulation of PDW measurements. High optical depths ($\tau \gg 1000$) require careful treatment and efficient speed-up procedures. We describe some of the techniques we employ, their adaptations to our specific system, and how they impact the simulations. Our code includes photon splitting, path length biasing, a modified random walk approach, parallelization and the peel-off mechanism.

References

[1] Bressel, L., R. Hass, and O. Reich, 2013: Particle sizing in highly turbid dispersions by Photon Density Wave spectroscopy. *J. Quant. Spectrosc. Radiat. Transfer* **126**, 122–129.

[2] Hass, R., M. Münzberg, L. Bressel, and O. Reich, 2013: Industrial applications of Photon Density Wave spectroscopy for in-line particle sizing. *Appl. Opt*. **52**, 1423–1431.

[3] Münzberg, M., R. Hass, N. D. D. Khanh, and O. Reich, 2017: Limitations of turbidity process probes and formazine as their calibration standard. *Anal. Bioanal. Chem.* **409**, 719–728.

[4] Hass, R., and O. Reich, 2011: Photon density wave spectroscopy for dilution-free sizing of highly concentrated nanoparticles during starved-feed polymerization. *ChemPhysChem* **12**, 2572–2575.

Preferred mode of presentation: Oral