MONTE CARLO RADIATIVE TRANSFER PEEL OFF MECHANISM FOR RESOLVED DETECTORS

Christian Peest^{*}, Oliver Reich, Lena Bressel

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

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 liquid samples (0.1 mm⁻¹ < μ'_s < 100 mm⁻¹). PDW is therefore ideally suited for inline process analytics of large-scale industrial processes, e.g. paint, cosmetics or polymer production, without a need for sample dilution [3].

Our group is exploring the limits of the applicability of PDW to samples with high turbidities, e.g. highly concentrated titania samples, using both experiments and theoretical approaches. Under these conditions, the experiment - employing optical fibers as light source and detector - and the P1-approximation - used for data analysis - might not match each other anymore e.g. due to small necessary fiber distances compared to the fiber diameter. To investigate these and possible additional influences and to further develop theory and experiments, we are creating a flexible Monte Carlo radiative transfer code to simulate the PDW measurements.

A variety of speed up mechanisms are employed to address the high optical depths ($\mu'_s \gg 100 \text{ mm}^{-1}$; $\tau \gg 1000$) we aim for. One mechanism is the peel off method, also called next-event estimator or point detector [4,5]. A drawback of the mechanism is that the contribution of scattering events very close to the detector can become arbitrarily large, leading to physically impossible results. This limitation has been reported before and solutions have been presented for infinitesimal detectors. In PDW experiments, the fibers have a finite size and a new approach needs to be taken.

We present two variations on the standard peel off scheme. One is to calculate the peel off intensity through a subdivision scheme. Alternatively, an integration scheme is applied. We compare the performances in a realistic scenario and derive guidelines for a general treatment. This allows for precise peel off calculations at any distance to the detector surface in our simulations.

References

- [1] L. Bressel, R. Hass, and O. Reich, 2013: JQSRT, 126, 122–129.
- [2] R. Hass, M. Münzberg, L. Bressel, and O. Reich, 2013: Appl. Opt., 52, 7, 1423–1431.
- [3] R. Hass, and O. Reich, 2011: ChemPhysChem 12, 2572–2575.
- [4] H. Kalli and E. Cashwell, 1977: *Evaluation of three Monte Carlo estimation schemes for flux at a point,* tech. rep., Los Alamos Scientific Lab, N. Mex. (USA).
- [5] J. Hendricks and T. Booth, 1985: *MCNP variance reduction overview in Monte-Carlo Methods and Applications in Neutronics, Photonics and Statistical Physics*, pp. 83–92, Springer.

^{*} Corresponding Author: christian.peest@uni-potsdam.de