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A particle string model for the optical properties of needle-shaped leaves

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The optical properties of needle-shaped leaves are difficult to model due to their complicated morphologies. The Harron's method measures the partial directional-hemispherical reflectance (DHR) and transmittance of needles by holding them in the slots of a carrier. Using the measured reflectance and transmittance may lead to an overestimation the leaf biochemical constituents since the laterally transmitted radiation has been counted into the absorptance. This research represents a particle string model that is able to model not only the measured reflectance and transmittance but also the lateral transmittance which denotes the fraction of radiation scattered by needles and absorbed by slot walls. To evaluate the performance of this particle string model, we compared it with (1) the PROSPECT5 model in forward mode; and (b) PROSPECT5 and the boundary constrained PROSPECT model (PROSPECT_zh) in backward mode. The dataset used in the study was collected near Sudbury, Ontario, Canada. It covers the optical, biophysical and biochemical properties of 87 black spruce needles. However, only chlorophyll and carotenoid were measured. Due to the absence of other biochemical constituents, the spectral region of interest was restricted in 400 nm to 690 nm where the absorption was assumed to be dominated by chlorophyll and carotenoid only. The particle string model needs additional calibrations for the particle scattering ratios, therefore a 10-fold cross validation scheme was applied 100 times for it when run in the forward simulation. The calibrations were achieved by an iterative algorithm. Finally, the wavelength-specific coefficient of determination (R2), root mean square error of prediction (RMSEP), bias (BIAS) and standard error of prediction corrected from the bias (SEPC) between measured and simulated reflectance and transmittance were calculated. In order to facilitate model comparisons, the chlorophyll and carotenoid concentrations estimated by PROSPECT_zh and PROSPECT5 were converted from area to volume basis according to the measured widths and thicknesses of needles. The backward estimations of three models were achieved by a constrained Powell's line-search method. The results of forward simulation showed that the reflectance and transmittance of black spruce needles were simulated more accurately by the particle string model than by PROSPECT5 with respect to R2, RMSEP, BIAS and SEPC. When run in backward mode, the particle string model estimated chlorophyll and carotenoid with a smaller RSME (162.05 μg/cm3 and 62.40 μg/cm3, respectively) than PROSPECT_zh did (227.21 μg/cm3 and 93.93 μg/cm3, respectively). The PROSPECT5 model had an overestimation of both chlorophyll and carotenoid (RMSE is 365.58 μg/cm3 and 131.61μg/cm3, respectively). These results demonstrate the capability of the particle string model to simulate the optical properties of needle-shaped leaves accurately.