

Prediction of SOC concentration for shelterbelts and agricultural fields in Saskatchewan using ATR-FTIR

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INTRODUCTION

Attenuated total reflectance Fourier transform infrared (ATR-FTIR) spectroscopy is a rapid, non-destructive technique for the determination of soil organic carbon (SOC) and other elements within soil. While a few studies have investigated the potential of spectroscopic techniques for the determination of carbon in soils, most of these studies are limited to a few sites with little diversity in soil type and land use. This study investigates the potential of using ATR-FTIR spectroscopy and partial least squares regression (PLSR) for the determination of SOC on a diverse set of soil samples collected from 40 sites distributed across the province of Saskatchewan.

SAMPLING AND METHODOLOGY

Soil Sampling - A total of 897 sample were collected from 40 shelterbelt sites which consisted of five major shelterbelt species viz. green ash (*Fraxinus pennsylvanica*), hybrid poplar (*Populus* spp.), white spruce (*Picea glauca*), Scots pine (*Pinus sylvestris*) and caragana (*Caragana arborescens*) and the adjoining agricultural fields across Saskatchewan using Randomized Branch Sampling technique. The soil samples were collected at the depths of 0-5 cm, 5-10 cm, 10-30 cm and 30-50 cm from the shelterbelts and the agricultural fields.

Laboratory analysis – Soil samples were analyzed on the LECO C632 analyzer for measuring soil organic carbon concentration.

Spectral analysis – A Perkin-Elmer spectrometer equipped with a DTGS or MCT detector was used for FTIR-ATR spectra acquisition. The spectra were collected by averaging 128 scans at 4 cm⁻¹ resolution over a spectral range of 400-4000 cm⁻¹.

Chemometric analysis – Partial least squares regression (PLSR) was used to build a calibration model of SOC as a function of ATR-FTIR spectra using a calibration dataset (n = 577) and validated against an independent dataset (n = 320).

RESULTS

Absorption Spectra

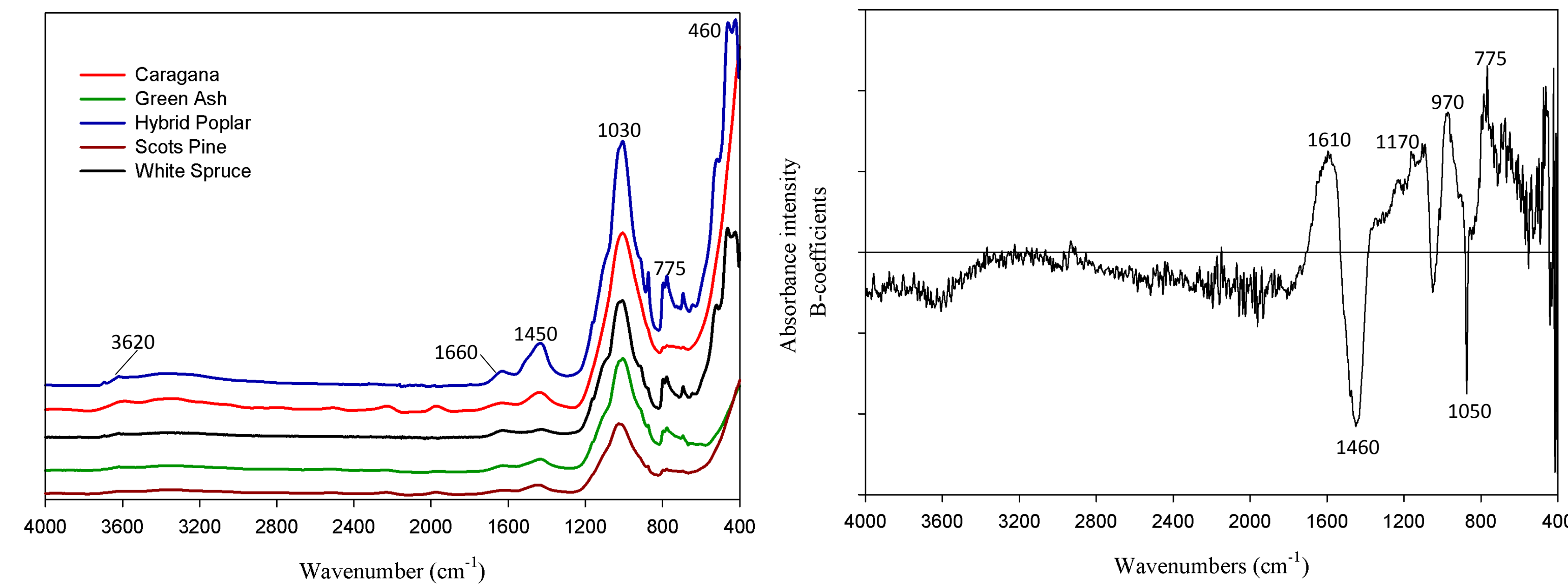


Figure 1: a) ATR-FTIR spectra for each of the six shelterbelt species and b) B-coefficient curve obtained from the PLSR analysis of transformed spectra

Spectral pre-processing and analysis

□ Prior to modeling, FTIR spectra were subjected to spectral pre-processing techniques in order to remove the offset and noise from spectra. Normalization of spectra followed by standard normal variate (SNV) transformation was found to be the most effective.

□ Based on the standardized regression coefficient values, spectral range of 400-1700 cm⁻¹ was determined to be most important predictor for SOC. However, the removal of parts of spectra lead to decrease in accuracy of the model. Hence, complete spectra was used in the development of calibration model.

ATR-FTIR calibration model

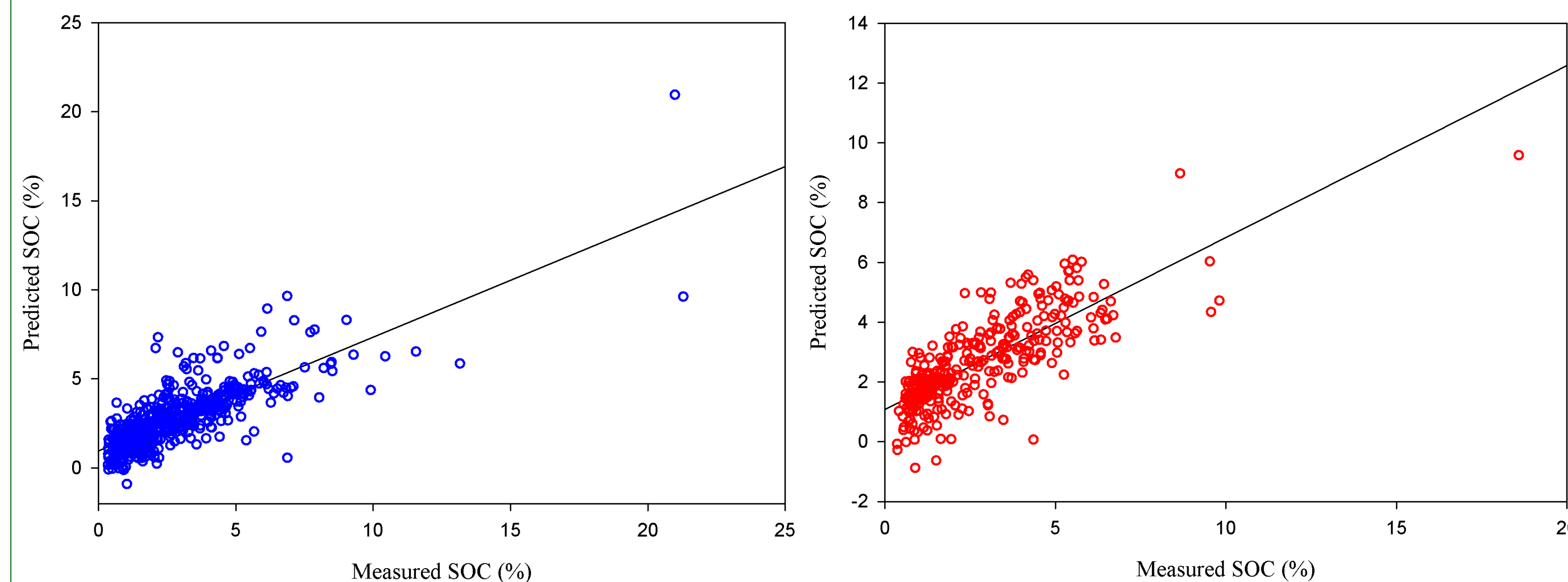


Figure 2: Measured vs. predicted values of SOC based on the a) ATR-FTIR calibration model ($R^2_{CV} = 0.85$; n = 577) and b) independent validation ($R^2_{IV} = 0.86$; n = 320)

CONCLUSIONS

- The ATR-FTIR calibration model has $R^2 = 0.85$ for training and $R^2 = 0.86$ for independent validation. This is comparable to other studies that performed independent validation of MIR-based PLSR models for SOC such as Randhawa (2008) ($R^2 = 0.67-0.94$) and Viscarra Rossel et al. 2006 ($R^2 = 0.73$). The RPD (residual predictive deviation) of 1.99 for the calibration model also indicates an acceptable prediction accuracy (Chang et al. 2001)

- The B-coefficient curve exhibits several distinctive peaks between the spectral range of 400-1700 cm⁻¹ (Figure 1). These peaks correspond to specific C bands such as aromatic C=C stretching (1610 cm⁻¹), aliphatic C-H stretching (1460 cm⁻¹) and C-O stretching of carbohydrates (1050 cm⁻¹) and polysaccharides (1170 cm⁻¹). These spectral signatures may be used for qualitative analysis of SOC in soil samples.

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ACKNOWLEDGEMENT

The financial support from the Agricultural Greenhouse Gases Program (AGGP) of Agriculture and Agri-food Canada is gratefully acknowledged. We are also thankful to Beyhan Amichev, Doug Jackson and the crew for helping with the sampling.