Multi-layer partial least squares modelling as a method to master model stiffness— applied to moisture measurement in timber

J. Dahlbacka* and T. Lillhonga

Novia University of Applied Sciences, Vasa 65201 Finland.
E-mail: John.Dahlbacka@novia.fi

Introduction

This study originated from a pre-study for an application aiming to characterise wooden bio fuels using NIR spectroscopy. One of the objectives in the pre-study was to evaluate what accuracy could be achieved with the equipment used, when measuring the moisture content in a board piece. It was assumed that the accuracy achieved with the measurements on the board piece would give an indication of the highest obtainable accuracy for wood chips. However, it was concluded that, after proper pre-processing, the main limiting factor for obtaining a high measurement accuracy was the relative inflexibility of the PLS model structure. Although the influence of the background matrix could be described as significant, in particular at lower moisture content values, it was noticed that the predictions of the validation data set improved when the calibration interval was decreased in terms of moisture content span. It was determined if the measurement accuracy could be increased by utilising a concept of multi-layer PLS modelling. In this concept, the prediction of the global PLS model on the first layer decides which of the local model on the second layer should be used, and the prediction of the local model on the second layer decides which of the local model on the third layer that should be used, and so forth. For each layer the concentration span for the local models is decreased, and according to calculations in which the optimal model always was selected, the accuracy increased all the way down to three-point regressions of local models.

Materials and methods

The spectral measurements were carried out with a getSpec spectrometer, model #: NIR-256-L-1.7T1, equipped with a SentroHead measurement head. The spectra were collected as absorbance spectra from 905 to 1683 nm, at a step size of 3 nm. However, in the model regressions only the first 188 data points were used. Each spectrum consisted of 32 co-added scans. The models were computed with the Matlab PLS toolbox, and mean centering and a 13 point second order

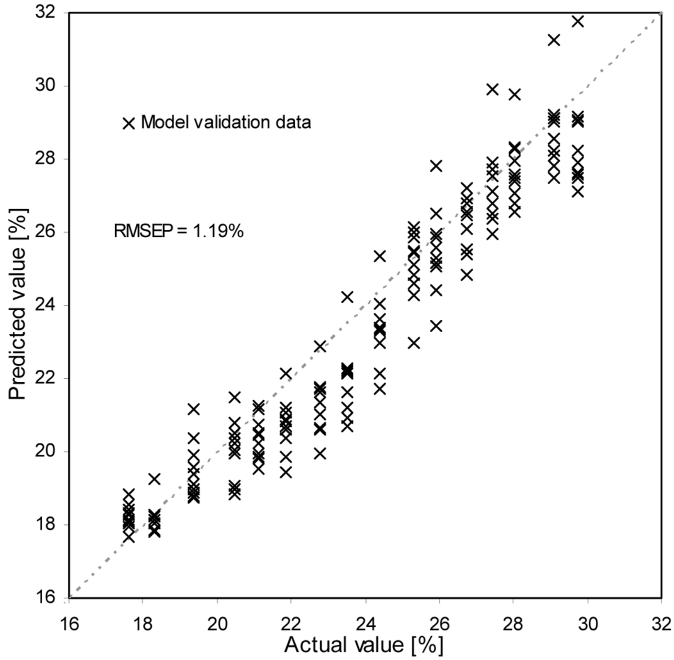

Figure 1. Predictions of the validation data set on the first PLS layer, i.e. the global model.

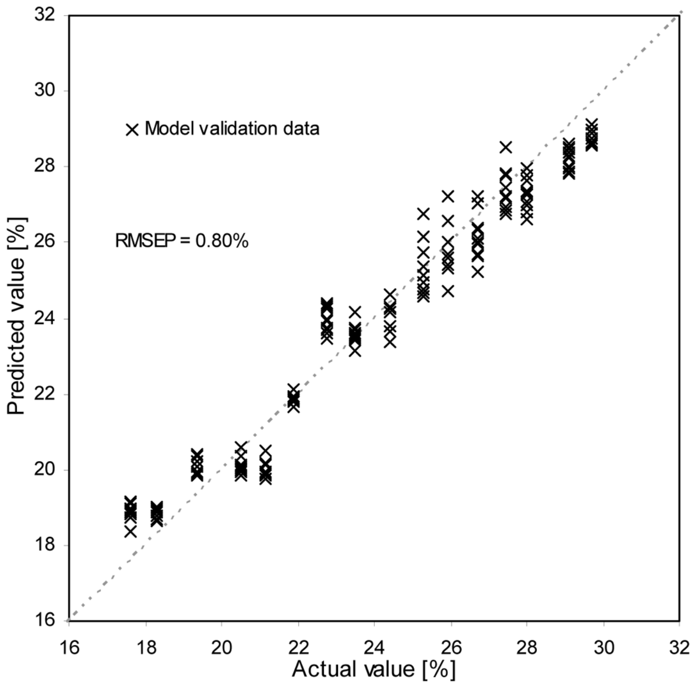

Figure 2. Predictions of the validation data set on the fourth layer, i.e. by the local models.

polynomial and a Savitzky-Golay derivative was used as pre-treatment. All models consisted of 4 PLS components. The sample was a board piece of Norwegian spruce that was soaked in water overnight. As the board piece was drying spectra were collected for the training data set. For each level of moisture content, 10 spectra were collected at different locations on the board piece. This procedure was repeated in order to obtain a validation data set. A total of 150 spectra were collected for the training data set, and 160 for the validation data set.

Results and discussion

The models predictions of the validation data set on the first and the fourth layer are shown in figures 1 and 2.

The *RMSEP* decreased by approximately 30 % from the first to the fourth layer. The spread in predictions of a given moisture content value also decreased significantly. However, one major issue was that a faulty prediction on a previous layer leads to the selection of the wrong local model on the next layer, and this error is inherited to any following layer with an escalating effect. In this study this issue was addressed by allowing only a certain change in predictions between layers, but a more thorough investigation is needed before this problem can be said to be solved. Furthermore, the suggested procedure should be implemented as a software code in order to reduce time spent on model regression. Thus, it can be said that the results from this initial study were promising, but there is still work to be done before this is a fully functional method.

Acknowledgement

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