SPECIES DIFFERENTIATION OF TWO COMMON LUMBER MIXES BY DIFFUSE REFLECTANCE FOURIER TRANSFORM INFRARED (DRIFT) SPECTROSCOPY

Jason R. Nault Chemist

and

John F. Manville

Research Scientist

Pacific Forestry Centre 506 West Burnside Road Victoria, British Columbia, V8Z 1M5 Canada

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ABSTRACT

Diffuse reflectance Fourier transform infrared (DRIFT) spectroscopy was used to differentiate coniferous woods by species. Species mixtures studied were SPF (composed of white spruce [*Picea* glauca Voss], Engelmann spruce [*Picea engelmannii* Parry], lodgepole pine [*Pinus contorta* Dougl.] and subalpine fir [*Abies lasiocarpa* Nutt.]) and HEM/FIR (composed of western hemlock [*Tsuga* heterophylla Sarg.], amabilis fir [*Abies amabilis* Dougl.] and Sitka spruce [*Picea sitchensis* Carr.]). DRIFT spectra of the green wood samples were used in SIMCA (simple modeling of class analogy) pattern recognition to differentiate species. This approach was able to classify SPF with 90% accuracy when all samples were identified, and 94% accuracy when poorly classified samples were eliminated. For the HEM/FIR group, the method was able to classify all samples with 81% accuracy, and up to 99% accuracy when poorly classified samples were eliminated.

Keywords: DRIFT, SIMCA, infrared, SPF, HEM/FIR, species, identification.

INTRODUCTION

Current lumber manufacturing practices in British Columbia (B.C.), Canada, produce species mixtures of lumber according to each mill's furnish, such as spruce/pine/fir (SPF) and HEM/FIR. SPF contains white spruce (*Picea glauca* Voss), Engelmann spruce (*Picea engelmannii* Parry), lodgepole pine (*Pinus contorta* Dougl.) and subalpine fir (*Abies lasiocarpa* Nutt.), while HEM/FIR contains western hemlock (*Tsuga heterophylla* Sarg.), amabilis fir (*Abies amabilis* Dougl.), and sometimes Sitka spruce (*Picea sitchensis* Carr.).

Rapid identification to separate these mixtures would help to create new marketing opportunities. Species separation would en-

Wood and Fiber Science, 29(1), 1997, pp. 2-9 © 1997 by the Society of Wood Science and Technology hance added value opportunities in secondary manufacturing of wood products. The ability to provide single-species dimension lumber to foreign markets may help resolve trade problems where certain species are associated with specific pathogens.

The most reliable method for species identification is by examination of anatomical features on macroscopic and microscopic scales (Strelis and Kennedy 1967). This method is reliable but requires highly skilled personnel and is expensive and tedious.

Another method of differentiating species is by analysis of "extractives" (nonstructural organic chemicals, soluble in neutral solvents) present in the wood. This method has a long history and includes many different chemistry techniques. Examples of this method are reactions of unique extractives with indicator chemicals to form colored complexes (Barton 1973; Miller et al. 1985), gas chromatography either alone or in combination with spectroscopic methods (Manville and Tracey 1989; Swan 1966), and ion mobility spectrometry (Lawrence 1989).

It has been demonstrated (Nault and Manville 1992) that by measuring the reflectance spectrum of wood using diffuse reflectance Fourier transform infrared (DRIFT), the contribution of the extractive compounds can be detected. Differences in the chemical composition of wood extractives between species were detected and formed the basis for species identification. This technique required high resolution spectra (spectral resolution is the size of the smallest feature in a spectrum that can be distinguished) and a sophisticated algorithm for interpreting the spectra. An unexpected result of this classification procedure was its ability to classify both heartwood and sapwood samples.

Both DRIFT and internal reflection infrared spectra of solid wood have also demonstrated differences between the spectra of smooth and rough wood, between earlywood and latewood, and between different grain orientations for the same sample (Zavarin et al. 1990, 1991). Wood weathering has also been studied extensively using DRIFT (Anderson et al. 1991a, b; Horn et al. 1994).

OBJECTIVES

The aim of this study was to examine the performance of various classification techniques and DRIFT scanning conditions for species classification of lumber. The effects of grain orientation of the samples, different spectral resolutions, and various scanning times were of particular interest.

MATERIALS AND METHODS

At conception, it was decided to make preparation and scanning of samples approximate conditions as they may be found in a mill situation. All fresh green samples were thus scanned at room temperature in an open sample compartment. It was also decided to concentrate upon classification only among the species that would commonly occur within a single mill. Two species groups were selected representing interior and coastal regions of British Columbia (SPF and HEM/FIR, respectively).

Samples as received were green trim ends from various sizes of lumber. Identification of each sample was confirmed by anatomical features (at Forintek Canada Corp.). Samples were sawn on a band saw to yield a 5-mmthick slice from one face (face grain), and for some samples a separate 5-mm slice from one end (end grain). Cut samples were stored in a cold room at 0°C until ready for scanning. Immediately prior to infrared scanning, samples were allowed to warm to room temperature; then a disk of appropriate size for the reflectance accessory was cut using a 9-mm circular punch. Each sample was numbered and identified as heartwood or sapwood.

Samples were received, processed, and scanned in three batches: 1—SPF and HEM/ FIR (received and scanned 1988), 2—SPF (received and scanned 1989), and 3—SPF and HEM/FIR (received and scanned 1991).

A Nicolet model 20SXB FTIR spectrometer equipped with a Spectra-Tech "Collector" DRIFT cell and a deuterated triglycine sulfate (DTGS) detector were used for collection of all spectra. The DRIFT cell has a "blocker" attachment designed to eliminate the specular reflectance portion of the reflectance spectrum. This attachment was not used because the throughput of the spectrometer was too small with it in place, and also because it would probably be impractical to collect purely diffuse reflectance spectra in an industrial application. The spectra collected were thus a combination of spectral information from both specular and diffuse reflectance. Each sample was placed in the sample holder in a random orientation. Sample height was adjusted for maximum throughput, and the sample was scanned from 4,850 to 400 cm⁻¹ (λ = 2.06 to

TABLE 1. Samples used.

Species	Boards	End grain	Face grain	Total
Spruce ¹	15		15	15
Spruce ²	47		47	47
Spruce ³	170	171*	169*	340
Pine ¹	138		138	138
Pine ²	9		9	9
Pine ³	159	159	159	318
Fir ¹	14		14	14
Fir ²	87		87	87
Fir ³	153	151	150	301
Hemlock ¹	92		92	92
Hemlock ³	167	158	159	317
Fir ¹	16		16	16
Fir ³	152	149	152	301
Spruce (Sitka) ¹	59		59	59

Collected and scanned in 1988. ² Collected and scanned in 1989.

^a Collected and scanned in 1989. ³ Collected and scanned in 1991, boards sampled on face and end grain

where possible.

* One board was sampled twice on end grain and not on face grain.

25 μ m) at a varying spectral resolution and number of scans.

As an instrument check, a spectrum of a reference mirror provided with the DRIFT cell was collected daily. These reference spectra were checked over the course of this study to identify any misalignment problems with the cell and to check throughput and the spectrum of the source.

Numbers of samples are included as Table 1. The spectra for 1988 and 1989 were also used in an earlier study (Nault and Manville 1992).

For the purposes of this study, each spectrum consists of a series of intensity measurements at evenly spaced wavelengths. Each of these wavelengths is treated as a variable in the statistical procedures used. The statistical techniques utilized included:

- normalizing (Nault and Manville 1992) of spectra to give spectra a mean of 0.0 and a standard deviation of 1.0.
- selection of wavelengths (variables) for classification based on Fisher weighting (Sharaf et al. 1986). The basis of this routine is "The highest (Fisher) weighted feature (wavelength) is selected as the first feature. The remaining features are then de-

correlated from the chosen feature. The decorrelated features are reweighted and the feature whose new weight is highest becomes the second selected feature. The process continues until either a specified number of features is chosen or a given minimum weight attained" (Arthur User's Manual 1986). This procedure is included as the subroutine "SELECT" in ARTHUR[®] by Infometrix, Inc., which is a suite of statistical utilities for data manipulation and pattern recognition.

 classification of samples was done using SIMCA (simple modeling of class analogy) (Massart et al. 1988; Sharaf et al. 1986), which is also included in ARTHUR[®].

RESULTS AND DISCUSSION

Preliminary work showed that no advantage was gained in performing background correction on the spectra, so single beam spectra were utilized throughout this work. Each single beam spectrum was normalized. Heartwood and sapwood samples were not separated.

SPF (1988 and 1989 samples)

The following procedure was followed:

1) A subset of spectra for each of the three species was randomly chosen to yield a "training set" (3 species \times 20 samples/species = 60 samples), with the remainder of the spectra used as a "test set" (250 samples).

2) Wavelengths that did not contribute to the species separation were removed using the routine "SELECT." This reduced the set from 4,615 to 382 wavelengths. These 382 wavelengths were then used to classify the samples using SIMCA. The results (Table 2) were not as good as the results from linear discriminant analysis (Nault and Manville 1992), where 83% of the same spectra were correctly classified.

When the principal component scores calculated by SIMCA were examined, it was found that the samples collected and scanred in 1988 were easily distinguished from those

	Classified into:			Total	%
True class	Spruce	Pine	Fir	spp	by spp
Spruce	42	11	9	62	67.7
Pine	17	116	14	147	78.9
Fir	20	7	74	101	73.3
Total in assigned					
class	79	134	97		
% assigned					
correctly	53.2	86.6	76.3		74.8

 TABLE 2.
 SIMCA classification of green SPF samples using three classes and 382 wavelengths.
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 TABLE 3.
 Training and test set disposition for green SPF

 samples divided into six classes.

Class	Training set	Test set	Total
Spruce ¹	7	8	15
Spruce ²	23	24	47
Pine ¹	69	69	138
Pine ²	4	5	9
Fir ¹	7	7	14
Fir ²	43	44	87
Total	153	155	310

¹ Collected and scanned in 1988

² Collected and scanned in 1989

collected and scanned in 1989. This suggests that either the samples differed (different sample site, different season?) or that the spectrometer characteristics had changed. A study of background spectra collected at the same time as the sample sets found no discernible differences, suggesting that a difference between sets of samples was responsible. To test this theory, the samples were further subdivided into classes by year and species, yielding 6 classes, which were then evenly divided between training and test sets (Table 3).

After the number of classes had been refined, the SELECT routine was applied to the new training set data (382 wavelengths), resulting in further reduction in the number of wavelengths to 66. Of these 66 wavelengths, 9 were found to be highly correlated (R > 0.990) with the wavelength immediately preceding it and were dropped as redundant, leaving 57 wavelengths. These wavelengths were then used to classify the samples into 6 classes based upon species by year. Predictions were then pooled into the three species groups (Table 4).

No significant differences in classification were observed between the training and test sets. Further modifications to number of wavelengths or sorting criteria yielded no improvement in sorting.

A second approach to classification also used SIMCA, but instead of classifying into six classes, each sample was classified three times as either belonging to a species or not belonging to a species. Thus each sample carried three classifications: spruce or not spruce, pine or not pine, and fir or not fir.

By combining the three classifications, it was possible for a sample to be classified as belonging to 0, 1, 2, or 3 species groups. All samples ambiguous in the combined classification (those belonging to 0, 2, or 3 species groups) were relegated to a fourth class (poorly classified). For convenience, we will henceforth refer to this method of classification as a "binary" sort, and the proportion of samples unambiguously classified as the "recovery." When this routine was applied, the results obtained were improved. Pooling the results by species (Table 5), the recovery was 79.0%, with 92.6% of these being correctly classified.

As an alternative method of classification, the binary technique produced a 6% in provement in overall classification, with a cost of not classifying 21% of the samples.

TABLE 4. SIMCA classification of green SPF samples using 57 wavelengths and six classes (results pooled by species).

	C	lassified int	o:	Total	%
True class	Spruce	Pine	Fir	spp	by spp
Spruce	48	8	6	62	77.4
Pine	8	130	9	147	88.4
Fir	6	5	90	101	89.1
Total in assigned class % assigned	62	143	105		
correctly	77.4	90.9	85.7		86.4

samples using 57 wavelengths and six classes (results SPF samples using 57 wavelengths. pooled by species).

True class	Classified into:			Total	۰%
	Spruce	Pine	Fir	. by spp	by spp
Soruce	36	5	2	43	83.7
Pine	1	109	3	113	96.5
Fir	3	4	82	89	92.1
Total in assigned class	40	118	87		
% assigned correctly	90.0	92.4	94.2		92.6

TABLE 5. Binary SIMCA classification of green SPF TABLE 7. Binary SIMCA classification of green 1991

True class	Classified into:			Total	%
	Spruce	Pine	Fir	spp	by spp
Spruce	206	16	1	223	92.4
Pine	30	171	6	207	82.6
Fir	5	1	250	256	97.7
Total in assigned	241	100	257		
% assigned	241	100	237		
correctly	85.5	91.0	97.3		91.4
Unambiguously classifie	d as one spe	cies (Reco	very) = 6	86/957 ((71.5%).

71.5% (686 of 959) of the samples being unambiguously classified, and 91.4% of these

being correctly classified. No significant dif-

ferences in classification were observed be-

tine from set to set, the entire wavelength se-

lection was repeated using only the training set

from the 1991 samples. The routine selected

59 wavelengths, which were highly correlated

to the 57 chosen from the 1988/89 samples.

When SIMCA classification was performed

with the new wavelengths (Table 8), perfor-

mance was approximately equal to that of the

previous classification (Table 6). The binary

classification was somewhat better (Table 9),

although recovery was poorer (48.3% vs.

in the binary sort, the 1988/89 and 1991 wave-

lengths (57 + 59) were combined. The result-

ing 116 wavelengths were put through the SE-

LECT routine using the 1991 training set, re-

To try to improve the recovery of samples

To test the consistency of the SELECT rou-

tween the training and test sets.

71.5%).

Unambiguously classified as one species (Recovery) = 245/310 (79.0%).

SPF (1991 samples)

As differences were found between the 1988 and 1989 spectra, the 1991 end and face grain samples were treated as a separate set. The spectra were normalized and divided roughly evenly between training and test sets. The 57 wavelengths selected using the 1988 and 1989 samples were then used to classify both the training and test sets using SIMCA.

The classification results (Table 6) were roughly the same as before, with 82.5% (vs. 86.4%) of samples correctly classified. There were slight changes in each of the species groups, with improvements in spruce and fir, and pine being poorer. Of the misclassified pieces, end grain and face grain were about equally represented (83 vs. 85 pieces), showing that end grain was scanned and classified with the same degree of success as face grain.

Using a binary SIMCA classification, the results (Table 6) were again improved, with

TABLE 6. SIMCA classification of green 1991 SPF samples using three classes and 57 wavelengths.

	Classified into:			Total	%
True class	Spruce	Pine	Fir	spp	by spp
Spruce	292	40	8	340	85.9
Pine	81	227	10	318	71.4
Fir	21	8	272	301	91.4
Total in assigned class	394	275	290		
% assigned correctly	74.1	82.5	93.8		82.5

TABLE 8. SIMCA classification of green 1991 SPF scmples using three classes and 59 wavelengths.

	Classified into:			Total	9,
True class	Spruce	Pine	Fir	spp	by opp
Spruce	292	45	1	338	86.4
Pine	84	230	2	316	72.8
Fir	9	12	282	303	93.1
Total in assigned class	385	287	303		
% assigned correctly	75.8	80.1	98.9		84.0

	Classified into:			Total	%
True class	Spruce	Pine	Fir	- by spp	by spp
Spruce	88	3	1	92	95.7
Pine	20	78	1	99	78.8
Fir	2	4	265	271	97.8
Total in assigned					
class	110	85	383		
% assigned					
correctly	80.0	91.8	99.5		93.3

SPF samples using 59 wavelengths.

TABLE 9. Binary SIMCA classification of green 1991 TABLE 11. Binary SIMCA classification of green 1991 SPF samples using 35 wavelengths.

	C	lassified in	Total	%	
True class Spruce Pine Fir	Spruce	Pine	Fir	spo	by spp
Spruce	239	15	0	254	94.1
Pine	36	194	2	232	83.6
Fir	5	0	279	284	98.2
Total in assigned class	280	209	281		
% assigned correctly	85.4	92.8	99.3		92.5

Unambiguously classified as one species (Recovery) = 464/957 (48.3%)

Unambiguously classified as one species (Recovery) = 770/957 (80.5%).

sulting in 35 selected wavelengths. SIMCA classification using these wavelengths was slightly better (Table 10), and the binary SIM-CA classification was about the same (Table 11) with much better recovery (80.5% vs. 48.3%).

No significant differences in classification were observed between the training and test sets. Further modifications to number of wavelengths or sorting criteria yielded no improvement in sorting.

Analysis speed

One drawback to the technique for possible in the mill use has been the speed of analysis. At 2 cm⁻¹ resolution, 100 scans take about 3 minutes. Several methods of increasing the speed are possible:

1) collect fewer scans

2) collect at lower resolution (lower resolution means faster scanning rates)

3) use faster equipment (spectrometers are

TABLE 10. SIMCA classification of green 1991 SPF samples using three classes and 35 wavelengths.

True class	Classified into:			Total	%
	Spruce	Pine	Fir	spp	by spp
Spruce	293	44	1	338	86.7
Pine	53	257	6	316	81.3
Fir	6	6	291	303	96.0
Total in assigned class	352	307	298		
% assigned correctly	83.2	83.7	97.7		87.9

available with much higher scanning rates than the model used)

4) use a more sensitive detector.

To test whether speed of analysis could be improved, a subset of 297 samples (from the 1991 samples) was chosen to evenly represent each species and grain. This subset was scanned in the DRIFT cell again under three sets of conditions:

1) 32 cm⁻¹ resolution, 100 scans

- 2) 2 cm⁻¹ resolution, 10 scans
- 3) 2 cm⁻¹ resolution, 1 scan

These spectra were normalized, and the samples were evenly divided into training and test sets. The 35 selected wavelengths were then used for SIMCA classification.

Overall there was no change in the percentage of correctly identified samples under any of the scanning regimes. Although there were changes for each species, gains for one species were offset by losses in others (Table 12). These results were repeated for the binary SIMCA sort (Table 13).

TABLE 12. SIMCA classification of a subset of green 1991 SPF samples using three classes and 35 wavelengths and different scanning parameters.

		Percent correctly classified				
Species	100 scans ^a 2 cm ⁻¹	10 scans ^b 2 cm ⁻¹	1 scan ^b 2 cm ⁻¹	1 30 scans ^b 32 cm ⁻¹		
Spruce	86.7	81.0	78.3	66.7		
Pine	81.3	86.3	93.1	96.0		
Fir	96.0	95.4	94.4	98.8		
All	87.9	87.1	88.2	86.2		

^a All samples ^b Subset of 297 spectra

TABLE 13. Binary SIMCA classification of a subset of green 1991 SPF samples using three classes and 35 wavelengths and different scanning parameters.

		Percent corr	ectly classifie	ed
Species	100 scans ^a 2 cm ⁻¹	10 scans ^b 2 cm ⁻¹	1 scan ^b 2 cm ⁻¹	100 scans ^b 32 cm ⁻¹
Spruce	94.1	87.1	93.0	75.4
Pine	83.6	94.9	96.2	97.7
Fir	98.2	98.8	100.	100
All	92.5	94.0	96.6	91.9
% recovery	80.5	78.6	78.4	81.3

TABLE 14. SIMCA classification of green 1991 HEN!/ FIR samples using two classes and 22 wavelengths.

Species	Percent correctly classified			
	100 scans ^a 2 cm ⁻¹	10 scans ^b 2 cm ⁻¹	1 scan ^h 2 cm ⁻¹	
Hemlock	80.3	68.2	71.4	
Fir	90.4	84.1	77.6	
All	85.6	76.0	74.6	

^a All samples. ^b Subset of 334 spectra.

^a All samples. ^b Subset of 297 spectra

HEM/FIR (1988 samples)

The procedures noted above were then applied to the HEM/FIR samples. From these samples, 167 spectra were available representing 92 hemlock, 16 fir, and 59 Sitka spruce. The spectra were normalized, and each species was randomly divided into training and test sets. The SELECT routine reduced the number of wavelengths from 4,615 to 21. Classification was done using SIMCA. No significant differences were found between training and test sets. Results were fair, with 78.4% of samples (83.7% for hemlock, 56.3% for fir, and 76.3% for Sitka spruce) correctly classified. This was an improvement over previous work (Nault and Manville 1992) where only 68% (67% for hemlock, 63% for fir, and 69% for spruce) were correctly classified.

HEM/FIR (1991 samples)

The spectra from the 1991 samples of HEM/FIR (containing no Sitka spruce) were normalized, and each species split evenly between a training and test set. SIMCA classification was performed based on the 21 wavelengths chosen from the 1988 spectra. Results were disappointing, with only 65.0% of samples correctly identified (58.5% of hemlock and 70.7% of fir).

Applying the SELECT routine to the 1991 training set, 29 wavelengths were selected as most useful for classification, with some of these being different from the wavelengths selected using the 1988 samples. This was ex-

pected as the 1991 samples contained no Sitka spruce, while the 1988 samples did.

The 29 wavelengths selected were used by SIMCA to classify the samples. Results were improved, with 73.4% of samples correctly identified (84.7% of hemlock and 60.8% of fir).

Wavelengths selected for 1988 samples and 1991 samples were pooled, yielding 50 wavelengths (21 + 29). Application of the SELECT routine to these wavelengths reduced these to 22 wavelengths, which were then used by SIMCA. Results were improved, with 85.6%of samples correctly identified (90.3% of hemlock and 80.3% of fir).

To test whether speed of analysis could be improved, a subset of 334 samples was chosen to evenly represent each species. This subset was scanned in the DRIFT cell again under two sets of conditions:

1) 2 cm⁻¹ resolution, 10 scans

2) 2 cm⁻¹ resolution, 1 scan

These spectra were normalized, and the samples evenly divided into training and test sets. The 22 selected wavelengths were then used for species classification (Table 14).

In the case of HEM/FIR, reducing the number of scans reduced the number of correctly identified samples.

CONCLUSIONS

We have demonstrated that DRIFT coupled with SIMCA is a reliable method for classifying green-wood samples from the SPF and HEM/FIR groups as to species. No differences were observed in sorting between heartwood vs. sapwood or end-grain vs. face-grain samples. As well, given the size of the infrared beam (2 mm^2) , we can assume that sample spectra represented all possible weightings of earlywood and latewood; thus these are ruled out as a confounding influence.

No attempt was made to equilibrate the moisture content of the samples. This indicates that moisture content variation should not significantly affect the classification. However, given the small size of the samples, some surface drying was inevitable during sample handling and scanning.

Provided that the source spectrum does not change, no correction for background is necessary when spectra are normalized, making single beam spectra useful for classification.

The most effective overall classification technique found utilized SIMCA analysis, and allowed samples to be assigned to a separate group for samples that are poorly or weakly associated with one of the assigned species groups. This also creates a flexible classification technique that can be adjusted for parameters of greater accuracy by rejecting marginally classified samples, or slightly lower accuracy by forcing classification of all samples. This should enable the technique to be adapted to varying mill and market conditions to maximize profit.

The method has shown the ability to distinguish between sets of spectra collected on different dates using the same equipment, scanning parameters, and species. More research is needed to determine the causes for this.

The sorting routine has been shown to be effective for lower resolution spectra (32 cm⁻¹) and using as few as 1 scan/sample. This makes very rapid scanning and identification possible.

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