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ATR-Fourier Transform Mid-Infrared Spectroscopy for Determination of *trans* Fatty Acids in Ground Cereal Products without Oil Extraction

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Fourier transform mid-infrared (FT-IR) spectroscopy was investigated as a method of analysis for *trans* fatty acid content of cereal products without the need for prior oil extraction. Spectra were obtained, with an FT-IR spectrometer equipped with an attenuated total reflectance (ATR) device, of ground samples pressed onto the diamond ATR surface, and *trans* fatty acids were measured by a modification of AOAC Method 996.01. Partial least-squares (PLS) models were developed for the prediction of *trans* fatty acids in ground samples using several wavenumber selections on the basis of bands related to lipids. The models ($n = 79$) predicted *trans* fatty acids in ground samples with standard error of cross-validation (SECV) of 1.10−1.25 (range 0−12.4) % and R^2 of 0.85−0.88 and in validation samples ($n = 26$) with standard error of performance (SEP) of 0.96−1.12 (range 0−12.2) % and r^2 of 0.89−0.92, indicating sufficient accuracy for screening. Sample *trans* fatty acid % was predicted as accurately with the fingerprint region (1500−900 cm^{-1}) as with the entire range (4000−650 cm^{-1}) indicating, in concert with the regression coefficients, the importance of the isolated trans double bonds at 966 cm^{-1} in development of the model. Data is also presented on prediction of *trans* fatty acids using the spectra of residual oil films on the ATR surface after removing the solid portion of the sample.

KEYWORDS: ***trans*** **fats; ATR/FT-IR; cereal products**

INTRODUCTION

Reports that *trans* fats have adverse effects on human health (*1*−*4*) have led to increased consumer interest in the *trans* fatty acid content of foods. The U.S. Food and Drug Administration (FDA) has amended regulations on nutrition labeling to require that *trans* fatty acid content be declared in the nutrition label of conventional foods and dietary supplements if the *trans* fatty acid content of a product is 0.5 g or more per serving (*5*). The regulation became effective on January 1, 2006, along with efforts by manufactures to reduce *trans* fat in foods (*6*).

Most *trans* fat in foods is present because of partially hydrogenated vegetable oils added during food processing although small amounts of *trans* fatty acids can occur naturally as a result of ruminant biohydrogenation in foods such as milk, butter, and tallow (*4*). Commercial hydrogenation or partial hydrogenation of oils can shift double bonds found in unsaturated fatty acids or may transform naturally occurring *cis* configured double bonds to more thermally stable *trans* double bonds. With the formation of *trans* isomers, the boiling point of lipids is raised and stability to oxidation is increased, both desirable traits for food processing.

The quantitation and identification of *trans* fatty acids is difficult because of the wide range of positional monoene, diene, and triene fatty acid isomers present in hydrogenated oils (*7*). Current official methods for determining *trans* fatty acid content are based on chromatographic and spectroscopic techniques. The official gas chromatographic (GC) method of determining total, saturated, polyunsaturated, and monounsaturated fat in cereal products (AOAC method 996.01) can be modified to measure *trans* fatty acids (*8*−*10*). The method involves acid digestion of the sample, extraction of the lipids with organic solvents, addition of an internal standard, and methylation to prepare fatty acid methyl esters (FAME) for GC analysis. The method is modified by use of a 100 m highly polar fused silica capillary column and tailored GC conditions to give optimum separation of *trans* isomers. It is a time-consuming separation technology and is solvent-based.

The most sensitive spectroscopic methods for the quantification of *trans* fatty acids involve Fourier transform infrared (FT-IR) spectroscopy in conjunction with an attenuated total reflectance (ATR) accessory for direct use on fats or oils, for example, AOCS method Cd 14d-99 (*11*, *12*). Fourier transform infrared spectroscopy is a rapid, noninvasive analytical technique that requires minimal labor and does not require chemicals or chemical disposal. However, the method requires extracting the oil from the food sample before spectroscopic evaluation can

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be made. Samples are loaded directly onto the ATR surface and only microliters of the oil sample are required. The IR spectrum is obtained because of a change in the molecular dipole moment after excitation and absorbance of energy from a light source. The resulting vibrational spectrum displays the "fingerprints" of functional groups narrowly and intensely in the IR region (4000−400 cm^{-1}) (*13*). Determination of *trans* fatty acids by FT-IR spectroscopy is based on the C−H out-of-plane deformation band observed at 966 cm^{-1} that is uniquely characteristic of isolated double bonds with trans configuration. These double bonds are found mostly in *trans* monoenes (18:1) and usually at much lower levels in *trans* polyenes (*7*, *14*). For quantitative determination of *trans* fat in edible oils and fat using the FT-IR method, the peak height or the integrated area under 966 cm^{-1} is measured relative to the baseline drawn between 990 and 945 cm^{-1} (*15*, *16*). Most work reported has been performed on fats and oils, and FT-IR determination of *trans* fatty acids in food samples, other than fats and oils, requires initial extraction of the oil.

The objective of this study was to investigate the potential of ATR/FT-IR spectroscopy for the rapid screening of *trans* fatty acids in ground cereal products without the need for prior extraction of oil. Samples included diverse cereal products from snacks to breakfast cereals having a wide range in *trans* fat content (0−12%).

MATERIALS AND METHODS

Samples and Sample Preparation. One hundred and ten products covering a range of cereal foods (crackers, cookies, chips, meal kits, cakes, snacks and breakfast cereal) were purchased from retailers. Products were chosen that are most likely to contain *trans* fats, such as cereal-based snack products and cereal products with partially hydrogenated vegetable oil as a listed ingredient. The types of oil added to the products as ingredients, according to the nutrition label, are soybean oil, cottonseed oil, corn oil, canola oil, palm oil, sunflower oil, butter, and lard. In 90 samples, the vegetable oil occurred as partially hydrogenated oil. The cereal product samples were ground using a household coffee grinder (KitchenAid, St. Joseph, MI). To prevent overgrinding and paste formation in the high-fat samples, small amounts of sample were ground at a time and were combined. Samples with greater than 20% sugar, on the basis of nutrition label values, were ground in liquid nitrogen. After grinding and thorough mixing, the samples were divided into subsamples and were placed in polyethylene bags. Samples were stored at −20 °C, and one subsample was used for reference analysis and another subsample was used to collect FT-IR spectra. All analyses were performed within 5 days of grinding. It was established in duplicate low and high *trans* fat samples that total and *trans* fatty acid content were stable at −20 °C for 7 days.

GC Analysis. Ground sample *trans* fatty acid content was measured by a modification of AOAC Method 996.01 (*8*), a hydrolytic extraction, gas chromatographic method for measurement of total fat and saturated, polyunsaturated, and monounsaturated fatty acids in cereal products. Aliquots of sample were weighed into duplicate Mojonnier tubes and 1 mL of 10 mg/mL tritridecanoin ($C_{13:0}$, T-3882, Sigma, St. Louis, MO) in chloroform was added as internal standard. Sample size was between 0.75 and 2 g and was adjusted depending on the amount of total fat (on the basis of the nutrition label value) in the sample. The sample was digested with hot 8 N HCl for 40 min, and the hydrolyzed fat components were subsequently extracted with diethyl and petroleum ethers. The diethyl and petroleum ethers were evaporated, and the extracts were saponified and esterified. The fatty acid methyl esters (FAME) formed were analyzed in parallel with fatty acid methyl ester standards (Supelco 37 Component FAME Mix, Supelco, Bellefonte, PA) using an Agilent 6890N gas chromatogram (Agilent Technologies Inc., Palo Alto, CA) with an SP-2560 flexible fused silica capillary column (100 m × 0.25 mm internal diameter × 0.2 μm film thickness, Supelco). One injection was made per sample duplicate. The injection port and detector (flame ionization detector) were kept at 200 °C and 250 °C, respectively, with gas flows of 40 mL/min for hydrogen and 450 mL/min for air with a split ratio of 50:1. The oven temperature program was an initial temperature of 120 °C held for 5 min, then increased at 3 °C per min to 240 °C and, finally, held for 20 min. Helium was the carrier gas with a linear velocity of 18 cm/s. Fatty acid methyl esters were quantified according to their percentage areas and FAMEs were converted to corresponding triglycerides or fatty acids by the appropriate conversion factors (*8*). Because of the limited availability of the *trans* fatty acids standard, *trans* fatty acids are assigned according to Ratnayake and Pelletier (*17*) as well as identified by comparison of retention times with four known standard FAMEs including elaidic acid methyl ester (*t*-9-octadecenoic acid), oleic acid methyl ester (*c*-9-octadecenoic acid), linolelaidic acid methyl ester (*t*-9,*t*-12-octadecadienoic acid), and linoleic acid methyl ester (*c*-9,*c*-12-octadecadienoic acid). The *cis*/*trans*- and *trans*/*cis*-18:2 isomers were included as *trans* isomers for the quantitation of *trans* fatty acids. Each fatty acid was converted to its triglyceride equivalent weight, and triglycerides were summed to obtain the total fat measurement. Infant formula (SRM 1846, National Institute of Standards and Technology; 27.1 ± 0.59% total fat) was used as a standard reference material for total fat on a daily basis. Sample dry weight was determined in a forced air oven (105 °C). Total *trans* fatty acids and total fat were expressed as a % of the food product on a dry weight basis. Total *trans* fatty acids were also expressed as a % of total fat (oil) in the product.

ATR/FT-IR Spectroscopic Analysis. FT-IR spectra of individual samples were collected using a Nicolet Magna 850 FT-IR bench (Thermo Fisher Scientific; Madison, WI) employing a DuraScope (Smith's Detection; Danbury, CT) single-contact attenuated total reflectance (ATR) sampling device. The ATR device was equipped with a round (2 mm diameter) diamond crystal, video imaging, and pressure gauge. The IR spectrometer was equipped with a globar source, KBr beamsplitter, and deuterated triglycine sulfate (DTGS) detector. Aliquots of ground sample were placed onto the surface of the diamond ATR crystal and pressure was applied using a metal rod until a rating load of 5.0 (~10 lb) to obtain the first spectrum. Then, the pressure rod was released and the sample was brushed off gently with three or four sweeps of a small soft brush. A second spectrum was then collected of the oil film (called residual film) that remained on the surface of the diamond ATR crystal. The ATR diamond surface and pressure rod were cleaned with hexane followed by ethanol and then with a clean lint-free tissue between sample replicates. Brushes were alternated and thoroughly cleaned with hexane and ethanol before use with another sample. Every 3−4 h, a background scan of the clean diamond crystal was obtained with no sample and no pressure applied. Each spectrum was the result of 128 scans, of the ground sample or residual film, at a resolution of 4 cm^{-1} over the region from 4000 to 650 cm^{-1} and was replicated six times. The OMNIC software (version 6.2; Thermo Fisher Scientific; Madison, WI) was used for data collection. The measurements were performed at room temperature.

Chemometric Analysis. Replicates of the spectral data were averaged and converted into GRAMS format using GRAMS/AI version 7.01 software (Thermo Fisher Scientific: Waltham MA) and were imported into the Unscrambler software 9.0 (CAMO, Trondheim, Norway). On the basis of the Hotelling T2 ellipse on PCA (principal component analysis), five outliers were removed in all from the data sets. Pastelike samples ($n = 7$) were removed from the residual film data set because they were difficult to remove from the ATR surface. Samples ($n = 105$ for ground samples and $n = 98$ for residual films from samples) were divided into calibration and validation sets after sorting by ascending *trans* fatty acid reference values in samples. The first three samples were assigned to the calibration set, and the fourth was assigned to the validation set, and so on. Partial least-squares (PLS) and Marten's uncertainty regression were used to develop the models for ground samples and residual films. Preprocessing methods were selected on the basis of the options that gave optimum performance. The optimum processing methods used and the number of PLS factors selected for calibration were those which gave a minimum error in cross validation. The wavenumber arrangements used to calculate models with the ground product and the residual film data sets were the whole IR range (4000−650 cm^{-1}), three selected functional groups based on the absorption of lipid (3040−2800 cm^{-1}, 1790−1700 cm^{-1},

Table 1. Range, Mean, and Standard Deviation of Percent Total *trans* Fatty Acids and Total Fat in Cereal Products in the Calibration and Validation Data Sets

	calibration				validation			
	n[a]	range	mean	SD	*n*	range	mean	SD
trans fatty acids in products	79	0.02–12.40	4.86	3.22	26	0.05–12.15	4.99	3.29
trans fatty acids in oil	74	0.14–42.03	23.11	12.10	24	0.68–40.63	23.60	11.70
total fat in products	79	4.81–36.46	19.76	7.97	26	6.10–33.63	18.70	8.13

[a] Number of samples (*n*); standard deviation (SD).

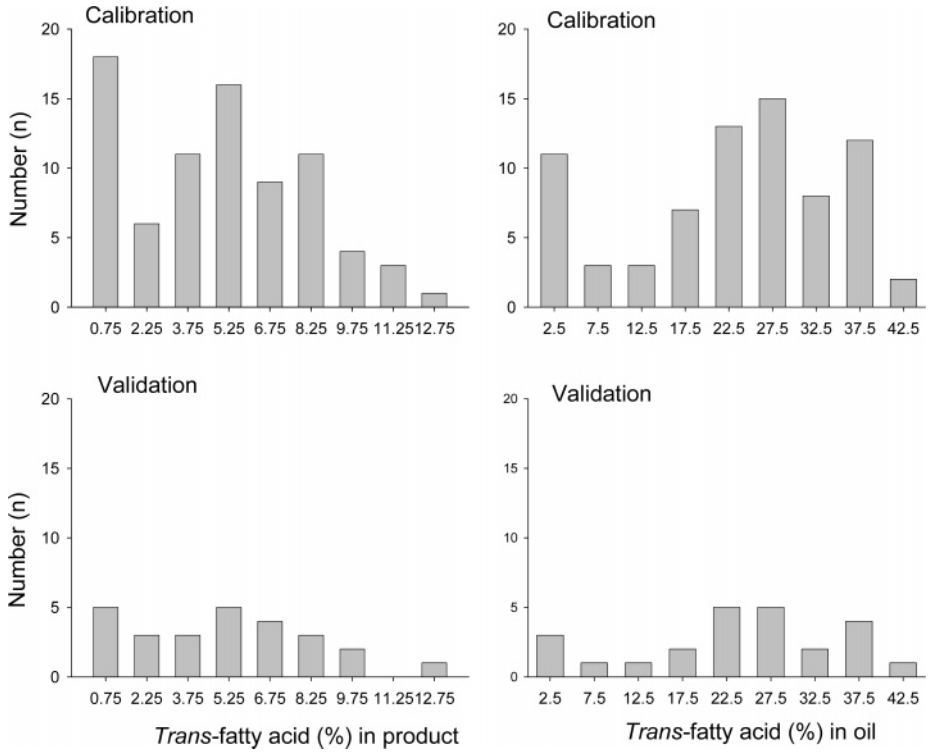

Figure 1. Distribution of *trans* fatty acids as % in product (**A**, **C**) and in oil (**B**, **D**) in the calibration (**A**, **B**) and validation (**C**, **D**) data sets.

and 1500−900 cm^{-1}), and the fingerprint range (1500−900 cm^{-1}) containing the C−H out-of-plane deformation band (966 cm^{-1}) that is uniquely characteristic of isolated double bonds with *trans* configuration. The spectra of ground products were preprocessed with the Savitzky−Golay second-derivative treatment (seven-point, second-order polynomial). The spectra of the residual films were preprocessed with the Savitzky−Golay second-derivative treatment (seven-point, second-order polynomial) followed by range normalization.

Calibration performance (n = 79 or 74) was first calculated as the multiple coefficient of determination (R^2) and standard error of cross-validation (SECV) (*18*, *19*). The models were then tested by predicting independent validation samples (n = 26 or 24), and performance was reported as the coefficient of determination (r^2), standard error of performance (SEP), and RPD (*18*−*20*). The RPD is the standard deviation of the reference values divided by the SEP and provides a standardization of the SEP (*20*). In general, an RPD value of 3.1−4.9 indicates a model is suitable for screening purposes and of 5.0−6.4 indicates the model is adequate for quality control; an RPD of 2.4−3.0 signifies the model is suitable for very rough screening (*20*).

RESULTS AND DISCUSSION

Reference Method Determination of *trans* Fatty Acids in Cereal Products. The range, mean, and standard deviation of *trans* fatty acids as a percent of the cereal product samples and as a percent of the fat in cereal products are given in **Table 1**. The overall range for *trans* fatty acids in 105 cereal products, using AOAC method 990.01, was 0−12.4%. The number of samples with high *trans* fatty acid content was limited by the small number of products commercially available with more than approximately 10% *trans* fatty acid content. The % *trans* fatty acids in the oil portion of the products had a wider range (0.1−42.0%) (**Figure 1**) because of differences in the total fat content of the cereal products. The range, mean, and standard deviation of total fat in the cereal products are also given in **Table 1**.

FT-IR Spectra of Cereal Products. Typical FT-IR spectra of fats in cereal products contain structural or functional group information on lipids present. **Figure 2** shows the spectra (4000−650 cm^{-1} range) of four typical cereal products selected from the data set. The products were corn chips, cheese curls, a cookie product, and a cracker product. The spectra all had three dominant regions related to fat: first is the 3025−2800 cm^{-1} region for C−H stretching absorptions of methylene and methyl groups; second is the 1740 cm^{-1} region for C═O stretching absorption of the fatty acid glycerol ester linkage; and third is the 1500−900 cm^{-1} or fingerprint region which includes a *trans* band at 966 cm^{-1} (*21*). Other bands observed in the fingerprint region are related to CH_3 and CH_2 symmetric and antisymmetric deformations in the 1450−1350 cm^{-1} range and C−O or C−C stretch in the 1200−1000 cm^{-1} range. Some samples (e.g., the cookie product and cracker product) showed a broad band around 3500 cm^{-1} related to absorption by hydroxyl groups (H_2O, ROH, or ROOH).

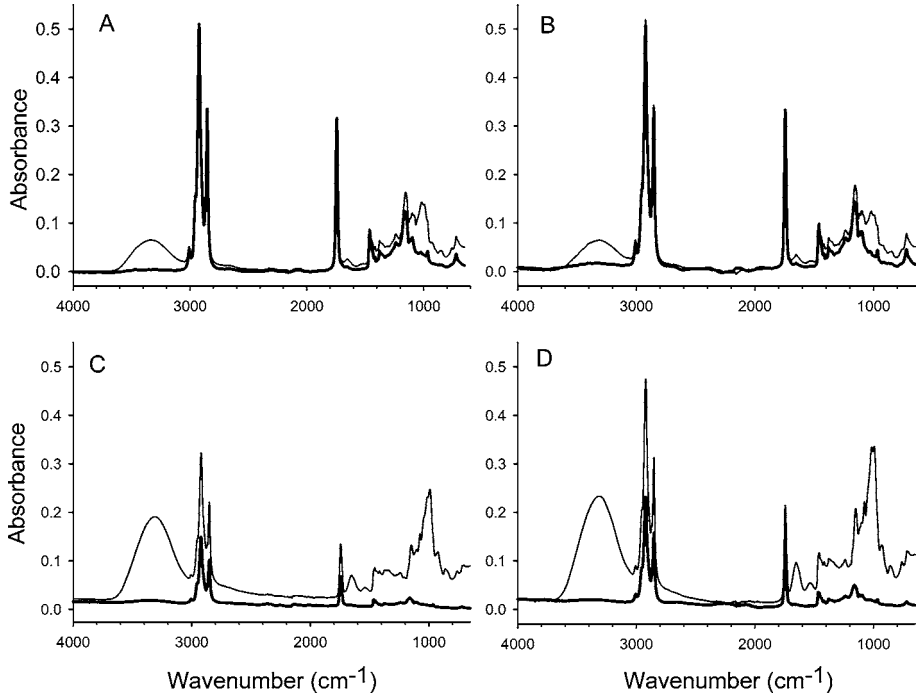

Figure 2. IR spectra (4000–650 cm^{-1}) of typical cereal samples in the ground sample form (fine line) and in the residual film (bold line) for four products: corn chips (**A**), cheese curls (**B**), a cookie product (**C**), and a cracker product (**D**).

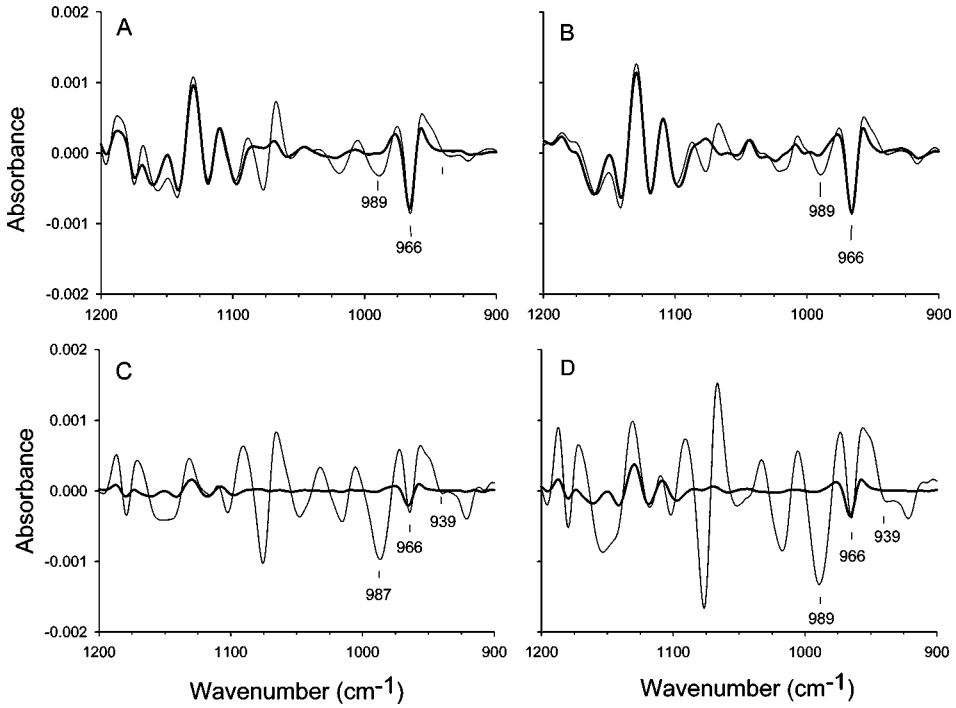

Figure 3. Second-derivative spectra (1200–900 cm^{-1}) of cereal samples in the ground sample form (fine line) and in the residual film (bold line) for four products (as in **Figure 2**): corn chips (**A**), cheese curls (**B**), a cookie product (**C**), and a cracker product (**D**).

The *trans* band at 966 cm^{-1} was not always apparent in the raw spectra of ground products (**Figure 2**). Visibility depended on the amount of *trans* fatty acid present and whether the band was masked partially or completely by the shoulders of other peaks nearby. After removing pressure and brushing away the granular portion of a sample from the ATR surface, the spectrum of the remaining oily film on the ATR surface gave a more obvious *trans* band at 966 cm^{-1} than that of the ground sample. The intensity of bands around 3500 cm^{-1} and the fingerprint region (1500−900 cm^{-1}) of the residual film were reduced compared to the spectrum of the ground sample. The *trans* band at 966 cm^{-1} is more evident in the second-derivative spectra for both ground products and residual films (**Figure 3**). In residual films, spectral peaks adjacent to the *trans* band, especially at 989 and around 939 cm^{-1}, had less intensity or disappeared after removing solid materials.

FT-IR Models for *trans* Fatty Acids. Statistics and plots for the IR prediction of *trans* fatty acids in ground samples using the spectra of the ground products are shown in **Table 2** and **Figure 4**. All models used five PLS factors. The models (n = 79) predicted *trans* fatty acids in ground samples with an SECV of between 1.10 and 1.25 (range 0−12.4) % *trans* fatty acids

Table 2. Statistics for FT-IR Prediction of *trans* Fatty Acids in Cereal Products[c]

	calibration						validation						
model[a]	*n*[b]	IR mean	IR SD	SECV	R^2	factors	*n*	IR mean	IR SD	SEP	r^2	bias	RPD
trans Fatty Acids (%) in Ground Products													
whole range	79	4.86	3.07	1.14	0.88	5	26	4.79	3.40	0.96	0.92	–0.20	3.4
three selected ranges	79	4.88	3.00	1.25	0.85	5	26	4.83	3.34	1.12	0.89	–0.16	2.9
fingerprint range	79	4.89	3.09	1.10	0.88	5	26	4.90	3.35	1.00	0.91	–0.09	3.3
trans Fatty Acids (%) in Total Fat of Products													
whole range	74	23.10	11.69	3.14	0.93	5	24	24.08	11.47	3.39	0.92	0.48	3.5
three selected ranges	74	23.17	11.69	3.24	0.93	5	24	24.04	11.19	3.26	0.92	0.44	3.6
fingerprint range	74	22.99	11.97	3.80	0.90	2	24	23.95	12.19	3.42	0.92	0.35	3.4

[a] Wavenumber treatments: whole range (4000–650 cm^{-1}), three selected functional groups (3040–2800 cm^{-1}, 1790–1700 cm^{-1}, and 1500–900 cm^{-1}), fingerprint region (1500–900 cm^{-1}). [b] Number of samples (*n*), standard deviation (SD), standard error of cross-validation (SECV), multiple coefficient of determination (R^2), standard error of performance (SEP), coefficient of determination (r^2), and ratio of the standard deviation of the AOAC values to the SEP (RPD). [c] On the basis of the spectra of ground products and the reference values for % *trans* fatty acid in the ground products and on the basis of the spectra of residual films and the reference values for % *trans* fatty acids in total fat (oil).

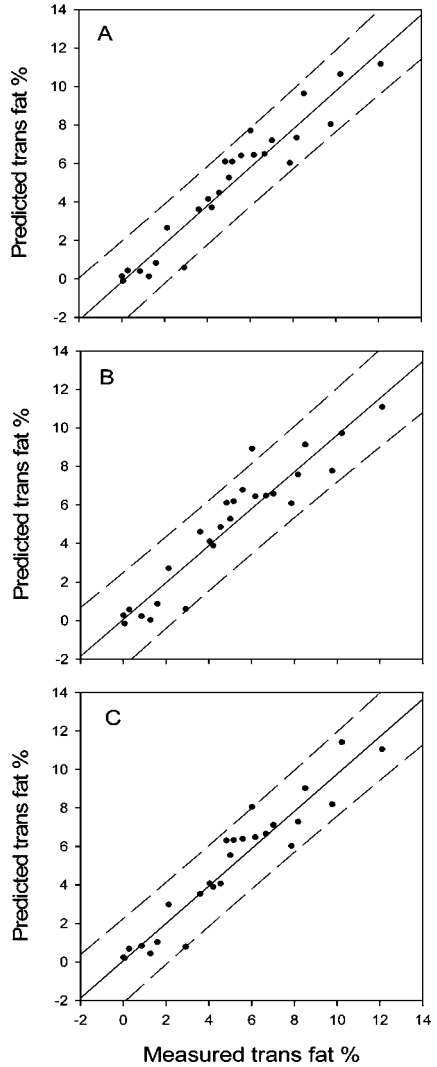

Figure 4. Reference method determined versus ATR/FT-IR predicted *trans* fatty acids (%) in validation samples of ground cereal products plotted with 95% prediction intervals. The wavelength regions used for modeling were the whole range (4000–650 cm^{-1}, **A**), three selected functional groups (3040–2800 cm^{-1}, 1790–1700 cm^{-1}, and 1500–900 cm^{-1}, **B**), and the fingerprint range (1500–900 cm^{-1}, **C**).

and R^2 of 0.85 or 0.88. The different models predicted *trans* fatty acid content in independent validation samples ($n = 26$) with an SEP of between 0.96 and 1.12 (range 0−12.2) % and r^2 between 0.89 and 0.92. *trans* Fatty acid % was predicted with the greatest accuracy in the models developed with the whole range and the fingerprint range with RPD values of 3.4 and 3.3, respectively, indicating suitability of the models for screening purposes. The prediction intervals for the regressions (Sigma Plot, version 9.0, Systat Software, Inc., Point Richmond, CA) denote the range in which the data values will fall 95% of the time for repeated measurements (**Figure 4**). Reference method data and predicted data were converted to grams *trans* fat/serving of the product, on the basis of product nutrition label values for serving sizes (**Table 3**). The reference values ranged from 0.01 to 6.98 with 80% of the samples having more than 0.5 g/serving.

Table 3. *trans* Fatty Acid Content for 26 Cereal Products in the Validation Data Set Expressed as Grams/Serving of Product[a]

sample	reference method	ATR/FT-IR predicted[b]
classic water crackers	0.01	0.01
wheat crackers	0.02	–0.02
melba rounds	0.05	0.06
water crackers	0.28	0.13
baked snacks	0.39	0.03
breakfast cereal	0.53	0.21
pretzel	0.65	0.78
low fat club crackers	0.65	0.66
meat extender	0.83	0.15
cheese crackers	0.95	0.93
chocolate chip cookies	1.24	1.20
cheese snack crackers	1.28	1.10
variety snack mix	1.36	1.70
baked snack mix	1.61	1.88
cheese balls	1.62	1.67
cheddar snack crackers	1.69	1.91
original snack crackers	1.86	1.92
original snack mix	2.02	1.93
barbecue snack crackers	2.37	1.80
oatmeal cookies	2.39	2.68
sandwich chocolate cookies	2.40	2.43
sandwich cream cookies	2.55	2.26
cheese curls	2.75	2.24
fudge brownies	3.70	4.67
vegetable snack crackers	3.77	3.45
short cakes	6.98	7.21

[a] Grams/serving calculated from serving size information on the product's nutrition label. [b] Model developed with the whole range (4000–650 cm^{-1}).

The fingerprint region appears to be the area of the spectrum that contributes most to the prediction of *trans* fatty acid content as the addition of wavenumbers representing other functional groups for lipids did not improve the models appreciably (**Table 2**); in addition, the model developed with the fingerprint range had the least bias. The second-derivative PLS regression

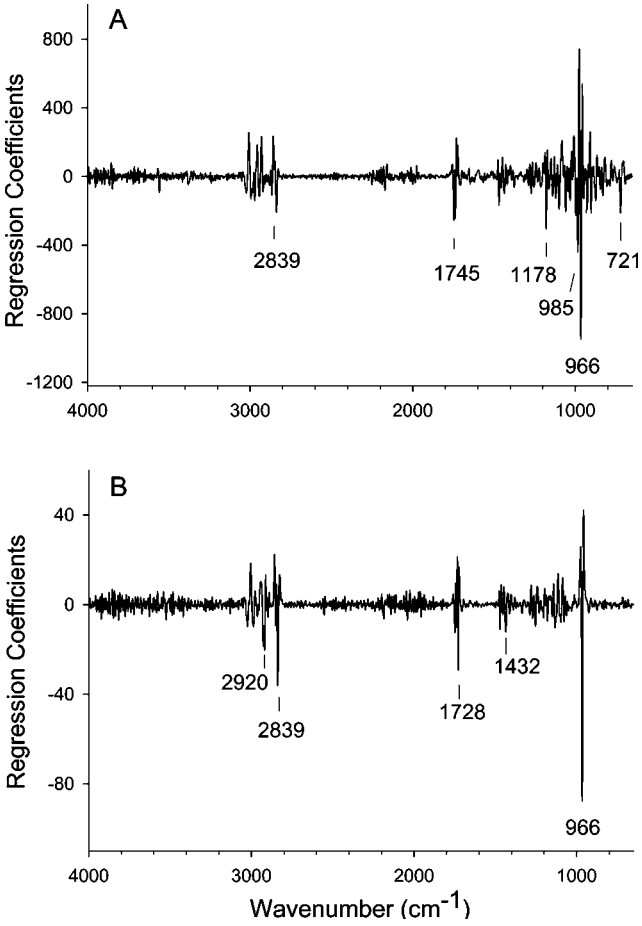

Figure 5. Second-derivative regression coefficients for PLS models (range 4000–650 cm^{-1}) developed to predict *trans* fatty acid in ground cereal products using the spectra of ground products and % *trans* fatty acids in total fat (**A**) using the residual film (**B**).

coefficients support this conclusion in that the model developed with the whole range (4000−650 cm^{-1}) showed that the band at 966 cm^{-1}, uniquely characteristic of the *trans* configuration, made the predominant contribution to the model (**Figure 5A**).

Normalization was required during preprocessing of the data to give optimum performance of FT-IR models developed with the spectra of residual films and reference values for *trans* fatty acids as a % of the products and as a % of total fat (oil) in the products. This is probably because of lower intensity of the *trans* band after the brushing away of the ground sample. Without normalization, the model utilized peaks around 3000 cm^{-1} rather than 966 cm^{-1} as indicated by the regression coefficients of models (not shown). The bands around 3000 cm^{-1} are related to total fat.

The residual film spectra and ground product *trans* fatty acid content were not well correlated and models developed with the whole range, fingerprint region, and three selected groups did not appear to be adequate for screening or any application with SEPs of between 1.91 and 1.93 (range 0−12.4) % *trans* fatty acid, r^2 of 0.68, and RPDs of 1.8 (not shown). Better correlations occurred between residual film spectra and *trans* fatty acids as a % of total fat or oil in the products for all three wavenumber treatments (**Table 2**). The models ($n = 74$) predicted % *trans* fatty acids in the oil of cereal products with an SECV of between 3.14 and 3.80 (range 0.1−42.0) % and R^2 of between 0.90 and 0.93. All models had similar performance when used to predict *trans* fatty acids in the validation samples ($n = 24$) with an SEP of between 3.26 and 3.42 (range 0.7−40.6) % *trans* fatty acid, r^2 of 0.92, and RPD of 3.4−3.6%. Thus, wavenumbers outside the fingerprint region did not contribute appreciable additional information to the model. Fewer factors were required to predict *trans* fatty acids in the residual film using the fingerprint region than using other wavenumber regions. As with the model developed with the spectra of ground cereal products, the isolated *trans* double bond at 966 cm^{-1} made the predominant contribution to the model developed with the whole IR region, as shown by the second-derivative PLS regression coefficients (**Figure 5B**). The relative contributions of groups at 2920, 2839, and 1728 cm^{-1} in the whole region model were greater than for the ground products model, probably because much of the oil remained when other materials were brushed away. In contrast, the contribution of the band at 985 cm^{-1} was considerably diminished in the residual film model compared to the ground sample model. This is consistent with brushing away carbohydrates with the solid materials.

When the purpose of analysis is to obtain information on the *trans* fat as a % of total fat, FT-IR analysis of the residual film provides a suitable method for screening for this information. However, when the purpose is to express *trans* fatty acids as a percent of the product, the utility of the residual film model is limited because of the need to measure total fat content before this can be calculated. The laboratory measurement of total fat involves the extraction of lipids from the sample followed by gravimetric or GC analysis, and existing ATR/FT-IR methods are available for use on extracted oils (*12*).

In summary, an ATR/FT-IR model has been developed to predict the amount of *trans* fatty acids in processed cereal foods without the need for lipid extraction. The method is rapid and can be used for screening of ground samples for *trans* fatty acid content. It involves pressing the ground sample onto the ATR surface of an IR spectrometer and collecting the IR spectrum, repeating the process with additional portions of the sample, averaging the spectra, and predicting the *trans* fatty acid content with the ATR/FT-IR model. The time required for analysis can be reduced from approximately 8 h with the conventional AOAC method to 30 min when six replicate IR spectra are obtained for each sample. The fingerprint region containing the spectrally unique isolated *trans* double bond configuration at 966 cm^{-1} appears to be the most important part of the IR spectrum for development of the model.

ACKNOWLEDGMENT

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