Evaluation of household drainage from food materials by near infrared spectroscopy

M. Omasa,[a] H. Takamura[b,c] and T. Matoba[a,b]

[a]*Graduate School of Human Culture, Nara Women's University, Nara 630-8506, Japan*

[b]*Department of Food Science and Nutrition, Nara Women's University, Nara 630-8506, Japan*

[c]*KYOUSEI Science Center for Life and Nature, Nara Women's University, Nara 630-8506, Japan*

Introduction

Near infrared (NIR) absorptions derived from overtones and combinations of the fundamental vibrations of molecules found in mid-IR region. Especially, the absorptions by C–H, O–H, and N–H groups are major. Therefore, NIR technique is suitable for the determination of organic compounds. In addition, the determination in aqueous system is possible since NIR absorption by water is much lower than that in mid-IR region. NIR technique has been widely used for food, agriculture, medicine, *etc*. In our laboratory, spectral analysis for protein determination,[1–5] lipid oxidation[6] and moisture content[7] by NIR has been studied for years.

The main source of water pollution is home drainage. The indices of water pollution are biochemical oxygen demand (BOD), chemical oxygen demand (COD) and total organic carbon (TOC). BOD and COD are the amounts of oxygen which are consumed to oxidise the organic compounds by microbe and chemicals, respectively. These need a long time and skill to determine. TOC is usually determined by TOC analyser, which determines carbon dioxide formed by combustion of organic carbon. Therefore, the development of simple and easy methods for the determination of water pollution is required. However, only a few studies on the application of NIR technique for environmental pollutions has been reported.[8–10] Hence, we have developed the method for evaluation of water pollution from food components[11] and a sewage plant.[12]

In this work, we analysed the relationship between the water pollution indices and NIR spectra in a model system of home drainage in order to develop a method for determination of the water pollution indices by NIR spectroscopy.

Materials and methods

Sample preparation

A model system of home drainage was prepared by using some food components and liquid foods. As food components, 0–5000 ppm solution of ovalbumin, glycine, sucrose, soluble starch, and monosodium glutamate were used. As liquid foods, 0–500 ppm solution of *miso* soup, tea with milk, coffee with milk, milk, juice (prune/vegetable), soy sauce, and rice-washed water (water in which rice has been washed containing rice bran) were used.

Determination of NIR spectra

NIR transmittance spectra (680–1235 nm) of the drainage were determined in 10 mm cuvette cell by using the NIRSystems (Pacific Science) Model 6250 Research Composition Analyzer at 10–40°C. Statistical analysis was performed with NSAS Ver. 3.27 (NIRSystems).

Near Infrared Spectroscopy: Proceedings of the 11th International Conference.

Determination of TOC and COD

TOC was using a Shimadzu TOC-5000A TOC Analyser. COD was determined by using the potassium permanganate titration method.

Regression analysis

A partial least squares (PLS) regression analysis was used for calibration and prediction. All spectra at different temperatures were used for calibration in order to obtain a robust calibration.

Results and discussion

Near infrared (NIR) absorptions derived from overtones and combinations of the fundamental

NIR spectra of water and home drainage model

Figure 1 shows the NIR raw spectra of water (TOC = 0) and rice-washed water (TOC = 140) in the region of 680–1235 nm. Other samples showed similar NIR spectra.

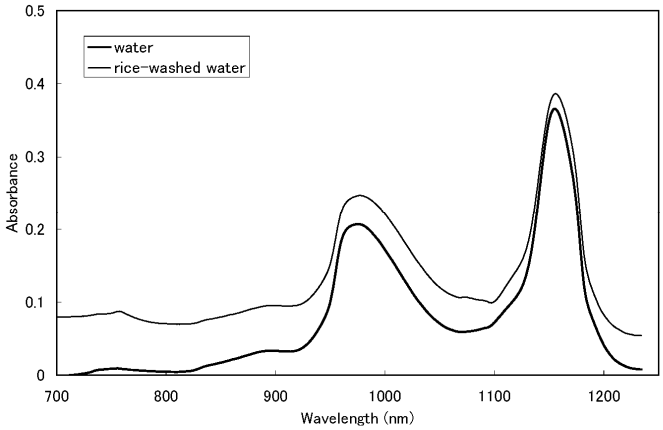

Figure 1. NIR raw spectra of water and rice-washed water.

Correlation between NIR raw and derivative spectra and COD/TOC

Table 1 shows the correlation between the NIR raw spectra and TOC/COD in the wavelength range of 680–1235 nm. The samples of water and home drainage model were first determined by NIR spectrometer at 10–40°C and then TOC and COD were determined. Calibration was calculated by PLS using all determinations at different temperatures to get a robust calibration against the change of temperature. As shown in Table 1, fairly good correlations between the NIR spectra and TOC/COD were obtained, which suggests that the NIR raw spectra determined at different temperatures were correlated with TOC and COD.

Table 2 shows the correction between the NIR raw and derivative spectra and COD/TOC at factor = 15. The best correlation statistics were obtained in the first derivative spectra. However, the raw spectra were used for prediction since the difference between raw and first derivative was small.

Table 1. Correlation between NIR raw spectra and COD/TOC.

Factor	Food Components				Liquid Foods			
	COD		TOC		COD		TOC	
	R	*SEC*	*R*	*SEC*	*R*	*SEC*	*R*	*SEC*
4	0.426	520	0.453	260	0.475	2023	0.590	911
5	0.446	516	0.488	257	0.490	2014	0.615	895
6	0.566	477	0.569	243	0.506	2004	0.634	882
7	0.618	457	0.619	233	0.550	1951	0.650	871
8	0.700	461	0.676	219	0.587	1902	0.669	857
9	0.712	410	0.695	214	0.611	1870	0.690	839
10	0.740	394	0.707	211	0.681	1739	0.733	793
11	0.757	384	0.727	206	0.715	1671	0.753	772
12	0.774	374	0.744	201	0.738	1498	0.844	636
13	0.812	346	0.778	190	0.784	1498	0.844	636
14	0.850	314	0.821	173	0.822	1383	0.896	531
15	0.863	302	0.833	168	0.852	1280	0.922	466

Table 2. Correlation between NIR raw and derivative spectra and COD/TOC

Factor	Derivative	Food Components				Liquid Foods			
		COD		TOC		COD		TOC	
		R	*SEC*	*R*	*SEC*	*R*	*SEC*	*R*	*SEC*
15	Raw	0.863	302	0.833	168	0.852	1280	0.922	466
	First Derivative	0.898	263	0.869	151	0.880	1163	0.929	445
	Second Derivative	0.839	325	0.828	171	0.869	1211	0.917	478

Prediction of NIR spectra for COD and TOC

Figure 2 shows the relationship between NIR predicted and laboratory values for COD and TOC. On this prediction, the prediction statistics were shown in Table 3. Correlation coefficients (*R*) were higher than 0.8. Though correlation coefficients are not so high, these results suggest the possibility that NIR spectroscopy can be used to evaluate the water pollution derived from the household drainage.

Table 3. Prediction statistics of NIR raw spectra for COD and TOC

Index	R	SEP	Bias
COD	0.863	288	0.0129
TOC	0.833	160	0.0231

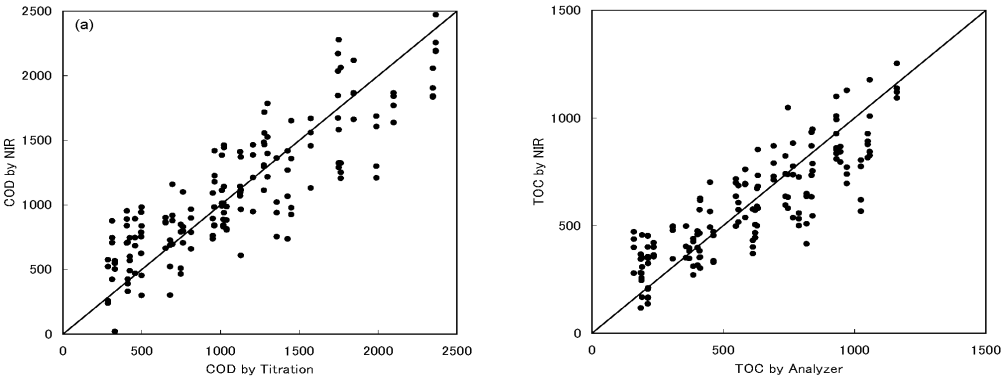

Figure 2. Relationship between NIR predicted and laboratory values for (a) COD and (b) TOC.

Conclusion

A good correlation between the raw NIR spectra and COD/TOC was obtained. Correlation coefficients (R) were higher than 0.8 in the wavelength range of 680–1235 nm with 10 mm light path. These results suggest the possibility that NIR spectroscopy can be used to evaluate the water pollution derived from the household drainage.

References

1. H. Kamishikiryo, K. Hasegawa and T. Matoba, *J. Jpn. Soc. Food Sci. Technol.* **38,** 850 (1991).
2. H. Kamishikiryo, K. Hasegawa, H. Takamura and T. Matoba, *J. Food Sci.* **57,** 1239 (1992).
3. H. Kamishikiryo-Yamashita, M. Tatara, H. Takamura and T. Matoba, *J. Jpn. Soc. Food Sci. Technol.* **41,** 65 (1994).
4. H. Kamishikiryo-Yamashita, Y. Oritani, H. Takamura and T. Matoba, *J. Food Sci.* **59,** 313 (1994).
5. H. Yamashita, H. Takamura and T. Matoba, *J. Near Infrared Spectrosc.* **2,** 145 (1995).
6. H. Takamura, N. Hyakumoto, N. Endo, T. Nishiike and T. Matoba, *J. Near Infrared Spectrosc.* **3,** 219 (1997).
7. H. Takamura, N. Endo and T. Matoba, *J. Near Infrared Spectrosc.* **6,** 235 (1998).
8. T. Korsman, M. Nilsson, J. Ohman and I. Renberg, *Environ. Sci. Technol.* **26,** 2122 (1992).
9. M.B. Nilsson, E. Dabakk, T. Korsman and I. Renberg, *Environ. Sci. Technol.* **30,** 2586 (1996).
10. D.F. Malley, P.C. Williams and M.P. Stainton, *Water Res.* **30,** 1325 (1996).
11. H. Takamura, H. Miyamoto, M. Imatani and T. Matoba, in *Near Infrared Spectroscopy: Proceedings of the 9th International Conference*, Ed by A.M.C. Davies and R. Giangiacomo. NIR Publications, Chichester, UK, p. 503 (2000).
12. H. Takamura, H. Miyamoto, Y. Mori and T. Matoba, in *Near Infrared Spectroscopy: Proceedings of the 10th International Conference*, Ed by A.M.C. Davies and R.K. Cho. NIR Publications, Chichester, UK, p. 405 (2002)