Identification of Plastics among Nonplastics in Mixed Waste by Remote Sensing Near-Infrared Imaging Spectroscopy. 1. Image Improvement and Analysis by Singular Value Decomposition

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A near-IR camera has been installed in an experimental setup for real-time plastic identification. Singular value decomposition (SVD) has been used for qualitative analysis and substantial improvement of the measured multivariate images. The obtained score plots provided spatial correlations between different pixel structures caused by sample material on the one hand and image artifacts on the other. In this way, the score plots have been used as a tool to optimize the experimental setup and image quality. The improved images were offered to a new classification algorithm called multivariate image rank analysis, based on SVD, as described in part 2 of this series of articles, which follows in this issue (Wienke, D.; et al. Anal. Chem. 1995, 67, 3760).

There are several ways for postconsumer plastics to reach their final destiny. In the past, landfiling was a common way to dump plastics waste. Now, product recycling, material recycling, thermal recycling, and chemical recycling are among the methods to reuse plastics. However, for each of these methods, it would be better to sort the plastics before further processing.1-3 Presently, the University of Nijmegen, The Netherlands, and the Institute for Chemical and Biochemical Sensor Research, Münster, Germany, are investigating the possibility for sorting plastics on the basis of their chemical-physical properties.4 One part of the project involves the discrimination of plastics from nonplastics by means of infrared imaging spectroscopy. More about near-IR imaging can be found in refs 12-14. The principle of discrimination lies in the differences of absorption spectra in particular wavelength regions for plastics and nonplastics. Therefore, a set or stack of images that it can determine whether the sample is a plastic or not.5 Because software solutions are very (computation) time consuming, optimization of the hardware was given higher priority. A high-quality image will facilitate the future material identification.

THEORY

Image Correction. Infrared images, obtained with an optical infrared camera, can be described mathematically by two-dimensional light intensity functions, \( F(x, y) \), where \( x \) and \( y \) represent respectively the \( x \) and \( y \) coordinates in a two-dimensional plane, and \( F \) represents the chromatic notion of intensity called brightness or, equivalently, the gray level of the image at a particular point \((x, y)\).6 The intensity is caused by infrared light reflected from the image plane, and it is related to the physical-chemical property of absorption measured from the considered samples and background material. The more a material in the image plane can absorb, the higher its brightness within \( F(x, y) \). Since the images need to be processed and analyzed by a computer, they need to be discretized. A discretized image can be considered as a matrix, expressed as \( I \), with \( n \) image rows and \( m \) image columns. The content of the elements \( i \) (referred to as pixels) of the matrix \( I_{nm} \) represents the gray level. For example, the detector of the camera used in the described experiments has a matrix size of \( 64 \times 64 \) pixels and a 10 bits

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(2) Brandrup, J. Gummi, Fasern, Kunstst. 1993, 46 (6), 732-738.
The whole matrix of 64 x 64 pixels can measure the reflection wavelengths results in a three-dimensional stack of images, enclosed by the image plane. Measuring the images at different wavelengths in a three-dimensional stack of images, these need to be corrected for background and dark current contributions. The raw image, \( I_{raw} \), is the sum of the reflected light from the sample or background and the dark current, \( I_{dark} \). The latter is a contribution of the background signal, reflected light from the sample or background and the dark current contributions. The raw image, \( I_{raw} \), is the sum of the reflected light from the sample or background and the dark current contributions.

In order to compare the images measured at different wavelengths, these need to be corrected for background and dark current contributions. The raw image, \( I_{raw} \), is the sum of the reflected light from the sample or background and the dark current contributions.

\[
I_{raw} = I_{ref} - I_{dark}
\]

When there is no absorption of the sample, \( I_{raw} \) is about equal to \( I_{ref} \), and thus \( I_{raw} \) will be equal to \( \approx 1 \). If one desires to measure the sample absorption, the following correction needs to be made:

\[
I_{corr} = 1 - \frac{I_{raw} - I_{dark}}{I_{ref} - I_{dark}} = \frac{I_{ref} - I_{raw}}{I_{ref} - I_{dark}}
\]

**Image Analysis by Singular Value Decomposition (SVD).**

As mentioned in the previous paragraph, the data measured from a single sample are collected as a three-dimensional stack of images \( X_{m,n,p} \) at \( p \) wavelengths. To facilitate the interpretation of this stack, a decomposition of \( X_{m,n,p} \) is proposed. According to Geladi et al., \( S \) it is usually necessary for practical reasons to unfold this three-dimensional stack of images into a two-dimensional matrix before decomposition. All images measured at \( p \) variables are first unfolded into \( p \) vectors having \( n \times m \) elements, called objects. These vectors are arranged in a 2D matrix \( Z_{nm,p} \). One method for doing such a decomposition is by a SVD, as given by eq 3, where \( Z_{nm,p} \) is the unfolded stack of images (as explained below), \( U_{nm,p} \), and \( V_{p} \) are orthogonal matrices containing respectively left and right singular vectors, and \( S_{p} \) is a diagonal matrix with the corresponding singular values. This method does not require a priori knowledge of a statistical distribution of \( Z \). The \( Z \) matrix can be decomposed into eigenvalues and eigenvectors. The maximum number of eigenvectors that can be obtained mathematically is \( p \) provided that \( p \leq \min(p,n,m) \), correspond-

\[
Z_{nm,p} = U_{nm,p} S_{p} V_{p}^T
\]

In imaging, one is mostly interested in the correlation (structure) between the objects or pixels. In the present work, these pixels give information about the material composition of the measured samples. Besides this, information about experimental artifacts can be obtained, too, such as shadow effects, specular reflection, and background inhomogeneity. All these effects form structures in the stack of images. In order to visualize these effects, score plots can be used. A score plot is a graph of two score vectors from the US matrix. It demonstrates the correlation between pixels representing the same material or artifact effects. Here, a score plot is graphically represented by only the vectors in \( U \), since the scaling with \( S \) will not have an effect on the graph. Clusters can be formed only when the information is preserved in the data, which means that the choice of variables is very important for an appropriate cluster discrimination. The inherent power of a score plot is that clusters can be extracted independently and transformed back to the original image space, called reconstructed fractional images (Figure 1). This is done by first selecting the desired cluster with a border line. Only the pixels within the border are used to fill the new score matrix. All other pixel values are set to zero. The new score matrix has to be multiplied with \( S V^T \) to get a fractional reconstructed image matrix, which is built up only by the pixels belonging to the selected cluster. In this way, underlying pixel correlations in the stack of images can be found which were not detected or were difficult to detect in the original data. Score plots can now be used for qualitative investigation of a large amount of image information.

**Criterion for Image Optimization.** In order to check whether an image has been improved by practical adaptation of the experimental setup or by software processing, the images need to be evaluated. Since the main goal of the project is to discriminate plastics from nonplastics, an evaluation criterion must be defined which is able to assess the quality of discrimination. We have chosen to use the gray level ratio of the objects in the images. The ratio is calculated in such a way that the numerator

\[
Z^2 Z = VS^{1/2} V^T
\]

\[
ZZ^T = US^{1/2} U^T
\]
The plot and projected back to the original image space by a reversed clustering of the pixels. An arbitrary cluster can be extracted from the plot comprising only two vectors from the U matrix. Depending on the problem, a certain combination of vectors may give clustering of the pixels. An arbitrary cluster can be extracted from the plot and projected back to the original image space by a reversed SVD (RSVD). The only pixels shown in the so-called fractional reconstructed image belong to the extracted cluster in the score plot. Note that, for these selected pixels, all their p scores vectors from U are used in the RSVD step. The evaluation criterion (A) can be calculated by

$$A = \frac{||\text{filtered image at filter 1}||}{||\text{filtered image at filter 2}||}$$

(7)

When there are artifacts present in the image, these will decrease the ratio due to independency of wavelength. Different filters will not affect the artifact contribution. This results in an increasing norm for both images, which will lower the ratio. This can be illustrated when two filter combinations are compared. Suppose filters 1 and 2 have the following norm contributions: 0.400/0.200 = 2.00 au and 10.4/10.2 = 1.02 au, respectively. The absolute differences are 0.2, but a significant difference will be obtained upon calculating the ratios. Artifacts will cause extra contributions to the norm and lower the ratio. The evaluation criterion can be interpreted as finding the highest ratio for the best image quality.

**EXPERIMENTAL SECTION**

The experimental macro setup for discrimination between plastics and nonplastics is shown schematically in Figure 2. A near-IR camera, provided with a 64 x 64 pixel focal plane array detector, is able to detect spectroscopic information over the wavelength range from 1 to 5.5 μm. Each pixel is a semiconductor device which is able to register incoming photons. Contrary to conventional detector materials, the detector used in this experiment was made of InSb (Cincinnati Electronics Inc., Mason, OH). In front of the detector array, inside the camera, a cold shield filter has been positioned to prevent the detector from sensing background light emitted by the optical components. This cold shield filter has to be cooled with N₂. The wavelength range of the cold shield filter has been extended to 1.1–4.6 μm.

Two objective lenses are needed for operation in the whole wavelength range. The first is the original objective lens made from CaF₂, and it has a standard 50 mm EFL f/2.3 multiple element lens (Cincinnati Electronics Inc.), which is transparent from 1.8 to 4.6 μm. The second objective lens is made of boron crown glass (BK-7), with a standard 50 mm EFL f/1.8 multiple element lens (Pentacon). This objective lens is transparent from 0.3 to 2.7 μm.

The output of the camera is a 12 bit digital data port which is able to send 51.44 frames (complete images) per second. Each pixel exhibits a sensitivity range of 10 bits, resulting in 1024 gray levels. No framegrabber is used since the digital output of the camera is sent indirectly, via an external interface SC-01 (electronic buffer) and a high-speed 16 bit S16D I/O interface (Engineering Design Team, Inc., Beaverton, OR), to the memory of the computer. The computer is a SUN SPARC 10 workstation containing 32 MB RAM. By avoiding a time delaying device such as a framegrabber, the high frame speed of the camera can almost be conserved. This is an important step in real-time measurements. A heat source is used to illuminate the sample with infrared light. The total distance between sample and detector is about 2 m (remote sensing mode), and therefore a powerful light source is required (600–1800 W) to get sufficient photons on the detector for a safe identification of the samples. Because of this, the turning filter wheel has to be positioned between the camera and sample. If placed between sample and light source, the filters would become damaged due to the emitted heat of the light source. However, our implementation involves the problem of refocusing the BK-7 objective lens for each filter because the refraction index of this lens material is wavelength dependent. The filter wheel is prepared for eight filters maximum. At present, six filters can be used which are transparent in the following wavelength regions: 1548–1578, 1545–1655, 1655–1745, 1700–2150, 2207–2321, and 2115–2530 nm, respectively. Several materials have been investigated for background material in the experimental setup. Sanded aluminum gave the highest contrast for macroscopic plastic samples.

The images can be recorded and processed using the Khoros 1.0 software environment (The Khoros Group, University of New Mexico, Albuquerque, NM), with its accompanying graphical user interface CANTATA. Khoros can be used as a visual programming tool for software development in scientific image visualization. This package entails a library of over 260 routines to facilitate research in image processing, pattern recognition, remote sensing, and machine vision.

Also, a way exists for direct data access using the S16D interface combined with a library of C procedures. The library enables real-time image acquisition by self-written software. The necessary acquisition software and external interface SC-01 were developed and installed by Starling Consultancy (Hengelo, The Netherlands).

The score plot program software was in-house developed using C for a SUN SPARC 10 workstation. Additional XITE software procedures (Torr Lonnestad and Otto Milvang, Image Processing Laboratory, Department of Informatics, University of Oslo, Norway) were included for graphical display of the images. Matlab (The MathWorks, Inc., Natick, MA) was used for further calculations and image representations.

RESULTS AND DISCUSSIONS

First, it was found that the dark current image, $I_{dark}$, of the camera is about 25% of the total signal, which is too large to ignore. Second, the reference image, $I_{ref}$, needs to be measured because for three reasons: First, the optical width of the filters are different, so different amounts of light per filter (flux) are falling on the detector. In order to compare samples in different images, there has to be correction for this effect. Second, the light source has a wavelength-dependent emission spectrum in the optical near-IR region. Third, the transmission spectrum of the camera lens is wavelength dependent, too. Therefore, both correction images, $I_{dark}$ and $I_{ref}$, need to be used in eqs 1 and 2.

The assumption we make in the corrected images is that both the background and the sample material have similar surface scattering properties. Although this will not be the case in all measurements, we found that it did not influence our evaluation criterion, since this entailed the calculation of gray level ratios of the object.

The appropriate choice for the background material can help to maximize the background-to-sample contrast in the image. Geladi et al. have chosen black velvet because of the low specular reflection. We found that this was not the only variable of influence in our measurements. Also, the gray level contrast needs to be taken into account. Therefore, we have chosen aluminum as background material because it has low absorption coefficients for near-IR radiation. For both filters, the sanded aluminum gave the highest brightness (contrast) after image correction (Table 1). To avoid specular reflection, the aluminum was sanded to give a smooth diffuse reflected near-IR background. After this successful treatment, the only specular reflection found was caused by the samples. Furthermore, we have tried to reduce this disturbing effect by optimizing the light source position, as will be demonstrated in the following section.

Another problem that arises in reflection mode measurements is due to shadows caused by the sample in the image plane. Due to a large variety in height, size, and shape of these samples and due to illumination, different shadow patterns may occur. For flat samples, shadow effects are negligible, but for higher samples this effect cannot be ignored. In theory, there are two kinds of shadows (Figure 3). The first is called cast shadow (umbrail), caused in an area which cannot be illuminated by the light source. The second is called self-shadow (penumbra), caused in an area which can only be partly illuminated. The aim of the following

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Table 1. Results for Optimal Selection of Background Material, Given by Numbers That Represent the Mean Pixel Gray Level Values for the Corrected Reflection Intensities of the Measured Tile Sample

<table>
<thead>
<tr>
<th>background material</th>
<th>filter 1 - 1545-1655 nm mean intensity</th>
<th>filter 2 - 1655-1745 nm mean intensity</th>
</tr>
</thead>
<tbody>
<tr>
<td>sanded aluminum</td>
<td>0.77</td>
<td>0.79</td>
</tr>
<tr>
<td>wood</td>
<td>0.60</td>
<td>0.61</td>
</tr>
<tr>
<td>black cloth</td>
<td>0.57</td>
<td>0.59</td>
</tr>
<tr>
<td>green velvet</td>
<td>0.49</td>
<td>0.49</td>
</tr>
<tr>
<td>green velvet on aluminum</td>
<td>0.47</td>
<td>0.44</td>
</tr>
<tr>
<td>smooth iron</td>
<td>0.57</td>
<td>0.56</td>
</tr>
<tr>
<td>black carbon</td>
<td>-0.25</td>
<td>-0.39</td>
</tr>
</tbody>
</table>

* A high positive value corresponds to a good diffuse reflecting background material. The negative values found for black carbon are due to a better reflection of the background compared to the sample.

Table 2. Results of the Experimental Design for Optimization of the Light Source Position

<table>
<thead>
<tr>
<th>variable number</th>
<th>variable name or interaction term</th>
<th>calculated regression coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>a0</td>
<td>intercept</td>
<td>4.2100</td>
</tr>
<tr>
<td>a1</td>
<td>horizontal (H)</td>
<td>-0.8544</td>
</tr>
<tr>
<td>a2</td>
<td>vertical (V)</td>
<td>-0.6056</td>
</tr>
<tr>
<td>a3</td>
<td>intensity (I)</td>
<td>-0.8869</td>
</tr>
<tr>
<td>a4</td>
<td>HH</td>
<td>0.0050</td>
</tr>
<tr>
<td>a5</td>
<td>V</td>
<td>-0.0300</td>
</tr>
<tr>
<td>a6</td>
<td>H</td>
<td>-0.0100</td>
</tr>
<tr>
<td>a7</td>
<td>V</td>
<td>0.1375</td>
</tr>
<tr>
<td>a8</td>
<td>I</td>
<td>0.2825</td>
</tr>
<tr>
<td>a9</td>
<td>HI</td>
<td>0.1800</td>
</tr>
<tr>
<td>a10</td>
<td>VHI</td>
<td>-0.0513</td>
</tr>
</tbody>
</table>

* Three factors have been investigated: horizontal (H) and vertical (V) position of the light source and its intensity (I). A second-order model including all interactions has been chosen. Low values for H and V mean the light source is farthest away from the sample. A low value for the intensity means a low radiation.

Table 3. Mean Gray Level Values and Their Corresponding Variances, Calculated from the Five Fractional Reconstructed Images

<table>
<thead>
<tr>
<th>cluster</th>
<th>image 1 mean (au)</th>
<th>variance</th>
<th>image 2 mean (au)</th>
<th>variance</th>
</tr>
</thead>
<tbody>
<tr>
<td>background</td>
<td>-0.0424</td>
<td>0.0011</td>
<td>-0.0214</td>
<td>0.0021</td>
</tr>
<tr>
<td>umbra</td>
<td>0.6069</td>
<td>0.0014</td>
<td>0.5282</td>
<td>0.0039</td>
</tr>
<tr>
<td>penumbra</td>
<td>0.2582</td>
<td>0.0223</td>
<td>0.2359</td>
<td>0.0176</td>
</tr>
<tr>
<td>specular refln</td>
<td>-0.1718</td>
<td>0.0078</td>
<td>-0.6380</td>
<td>0.0300</td>
</tr>
<tr>
<td>sample</td>
<td>0.5216</td>
<td>0.0025</td>
<td>0.1090</td>
<td>0.0121</td>
</tr>
</tbody>
</table>

* It can be seen that the variances for the background are very low, which means that the image quality is very good. The variances of the penumbra are much higher because these are decreasing in the opposite direction from the light source (Figure 3). Specular reflection can cause oversaturation of the pixels, leading to large negative values after image correction.

Figure 3. Schematic representation of two kinds of shadow, cast shadows and self-shadow, respectively. The cast shadow is caused in an area which cannot be reached by radiation from the light source. The self-shadow is caused in an area which can be only partly reached by light from the light source.

The experiment is to investigate whether it is possible to separate shadow patterns mathematically from the sample absorption pattern within the image. If this would be possible with a multivariate technique, it will not be necessary to spend much effort on homogeneous image illumination or mathematical shadow removal, e.g., using an erosion filter, as mentioned by Geladi et al.. Multivariate image rank analysis (MIRA), as, e.g., a classifier tolerates these shadow artifacts. To demonstrate that both shadow types are additive effects that can be separated from the sample pattern in the image, score plots from singular value decomposition eqs 3 and 4, were used. Even without preprocessing (mean centering and variable scaling) of the original data (Figure 4), five different clusters were formed in the score plot in Figure 5: two significant distant shadow clusters, two significant distinguishable clusters for background and sample, and one distant cluster for specular reflection. Specular reflection is caused by direct projection of the illuminated light onto the camera detector by the smoothness of the sample surface for certain angles of incidence. The umbra and penumbra clusters can be clearly distinguished from the remaining clusters, although penumbra shows some overlap with the background pixels. This score plot shows that shadow effects can be separated from other pixel structures by using decorrelated eigenvectors (eqs 3 and 4). Figure 6 shows the reconstructed fractional images, calculated from the score matrix U, in one single combination image. The five clusters were given arbitrary gray levels in order to visualize them. With this in mind, it can be understood why multivariate classifiers are able to extract a desired sample pattern out of a shadowed image. Table 3 shows the mean gray level values and their variances for the five fractional reconstructed images.

For the optimization of the light source position, a statistical central composite design was carried out on a representative sample, providing a second-order model including all interaction terms for three factors. These factors were the horizontal (H) and vertical (V) positions and the intensity (I) of the light source:

\[ g(V,H,I) = a_0 + a_1H + a_2V + a_3I + a_4H^2 + a_5V^2 + a_6I^2 + a_7HV + a_8HI + a_9VI + a_{10}HIV \]  (8)

As response, g, the absorption ratio of the sample at two distinct wavelengths (1545–1655 and 1655–1745 nm, respectively), was chosen. The higher the ratio, the better the image quality. A high value for the horizontal and vertical position means that the...
Figure 4. Two typical images measured from a high round plastic cap showing clearly the original disturbances, such as specular reflection on the left edge and shadow effects on the right side of the sample. The filters used were transparent in the wavelength regions (left) 1545-1655 and (right) 1655-1745 nm. Only one light source was used, which was positioned on the left side of the sample.

Figure 5. Score plot from score vectors 1 and 2, calculated from the stack of images shown in Figure 4. Five clusters can be extracted: two for shadow effects, one for specular reflection, and two respectively for background and sample correlations.

Figure 6. Five reconstructed fractional images superimposed on a single image. The gray level values were chosen arbitrarily to visualize the different clusters. These clearly represent the mentioned effects in the original images (see also Figure 5). A few intermediate pixels (not belonging to any cluster) were filtered out.

light source is farthest away from the sample or image plane. The terms in the model were able to describe 94% of the factor residuals, and it turned out that there was no lack of fit. The calculated model is given in Table 2. The model optimum was found at maximum values for $V$ and $H$ and a minimum value for $I$. This means that it is more favorable to position the light source farther away from the image plane (a larger angle between the triangle of light source, sample, and camera) for both the horizontal and vertical positions. Although the first introduces a larger shadow effect, it will be compensated by a much better brightness of the image in the pixels. The optimal position of the light source found for the macro setup in the present work is different to that for the micro setup (e.g., microscopy). In the latter, an illumination ring of glass fiber is commonly used for homogeneous image plane illumination. This ring is attached close to the objective, which gives a small angle of incidence. The opposite is true for an optimal position in the macro setup, where a large angle gives significantly better results. Although a large angle generates more shadow contributions, these can easily be separated by multivariate techniques from sample patterns, as has already been successfully proven using SVD.

CONCLUSIONS

Two ways to remove or reduce experimental artifacts in a multivariate stack of remote sensing near-infrared images have been presented. Inhomogeneity of the background illumination, lamp source intensity, and fluctuating optical transmission characteristics can be reduced by correcting the raw images via reference and dark current images. Shadow artifacts and specular reflection can be separated from the important sample structures in the images using singular value decomposition. This is a powerful tool for analyzing and improving multivariate images and optimizing the experimental setup with respect to undesired
artifacts. In the optimization of the experimental setup, we showed that the position of the light source differs fundamentally from that of a micro setup. After this optimization, the background material showed no further specular reflection and provided the desired high contrast for the measured samples within the stack of images.

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