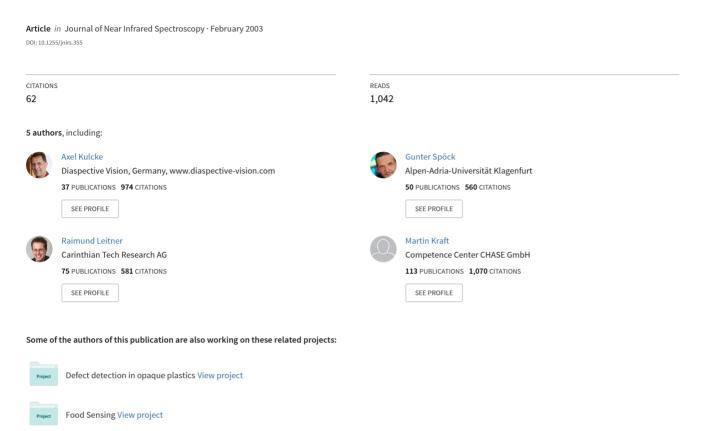
# On-Line Classification of Synthetic Polymers Using near Infrared Spectral Imaging



# On-line classification of synthetic polymers using near infrared spectral imaging

A. Kulcke, C. Gurschler, G. Spöck, R. Leitner and M. Kraft\*

CTR - Carinthian Tech Research AG, Europastraße 4/1, 9524 Villach / St Magdalen, Austria

The lack of industrially-applicable, fast polymer classification systems is currently a major stumbling block in establishing both economically- and ecologically-useful waste recycling systems. With the advent of near infrared (NIR) spectral imaging for online classification, a method capable of distinguishing between different materials while simultaneously providing reliable size and shape information became available. In particular, polymer materials can be identified by their characteristic reflection spectra in the NIR without critical interferences from varying sample sizes and colours. A dedicated laboratory-scale prototype spectral imaging system has been developed and a number of classification algorithms have been evaluated for their applicability for polymer classification. Of the investigated algorithms, the Spectral Angle Mapper algorithm, supplemented by a threshold value and applied to the first derivatives of the normalised spectra, proved to be best suited for a rapid and reliable classification of polymers. Based on these achievements, an on-line system capable of classifying polymer parts delivered on a conveyor belt in real-time has been set up, which can be used, for example, as a sensor for fully-automated industrial polymer waste sorters.

*Keywords:* imaging spectrometry, spectral imaging, near infrared, real-time classification, material identification, polymer waste sorting

### Introduction

Many products used in daily life consist of synthetic polymers and their abundance is still increasing, as they replace other materials. Concurrently with growing production and use, the amount of waste increases. Although efforts are being made to find other ways of disposal than landfill deposition and thermal treatment, currently only about 30% of the total consumer plastic waste can be recycled and even then mostly low-quality products are being produced. <sup>1-3</sup> The reason for this is partly the degradation of the material during processing and use, but more often the fact that the synthetic polymers in municipal and industrial waste are highly diverse and incompatible with each other in direct material recycling. This necessitates introducing a separation

step giving possibly pure fractions prior to the material recycling process. Currently, as the standard methods for the separation of polymers in waste involve a lot of manual work, the recycled material is frequently more expensive than fresh polymers, thus rendering this way of disposal pointless from the economical point of view.4 To overcome this obstacle, rapid automated sorting systems could be used.<sup>5</sup> The key problem is to find a contact-free method capable of identifying the different polymers in realtime at a high throughput, e.g. over a conveyor belt, with high reliability, a robustness suitable for industrial application and low investment and operation costs. For sorting, the system has not only to distinguish between the different items on the belt to control the sorter correctly, but also to differentiate between pure materials and composites.

Following these requirements, the application of an optical method is clearly indicated. The visible region (400-780 nm) of the electromagnetic spectrum delivers no useful information, first, because the natural colours of polymers are too alike to warrant a reliable identification and, second, because many products are heavily dyed. Obviously, a spectral region giving more detailed chemical information has to be evaluated. The mid-infrared range (2.5–25 µm) provides this information in form of characteristic fundamental vibration absorption bands, thus proving a highly reliable possibility for material identification. However, for an application in an industrial environment the optics and sensors required for this spectral range are too expensive and too fragile. Therefore, the near infrared (NIR) region, in particular the range from 1.0 to 1.7 µm, was chosen as the most suitable. This spectral range provides sufficient material-specific information, due to overtone and combination vibration absorption bands, to facilitate a reliable identification while still being accessible with standard optics.

The lesser specificity of the combination bands in comparison to the mid-IR fundamental absorption bands requires the use of smart chemometric classification algorithms. Suitable data pre-processing and classification algorithms and a careful optimisation of the parameters are crucial for the proposed real-time application. In addition, the system must be easy to use and provide the necessary interfaces to a sorting or separation system.

#### Materials and methods

#### General

The special requirements in plastic sorting call for cost-effective, robust NIR spectrometers capable of macroscopic imaging. The best answer to this problem is the application of a spectral imaging system, which is capable of measuring both the spatial and the spectral information in one step.

Spectral imaging (SI) is a combination of spectroscopy with digital image processing.<sup>6–8</sup> Other than with standard imaging, where only the spatial information plus, if appropriate, the RGB values of the single image pixels are recorded, SI provides full spectral information for each pixel over a selected

wavelength range. In instrumentation there are basically two different approaches. The first approach is the wavelength scanning method, in remote sensing also known as "staring imagers". The sample is kept stationary under the SI camera and single images are recorded for each different wavelength. The spectral information is provided either by (i) a number of discreet filters,9 (ii) tuneable filters5,10 or (iii) by combination with an imaging Fourier-transform spectrometer. 11,12 The images recorded for the different wavelengths are combined in the computer and the spectra calculated. The second method, also known as "push-broom scanning", requires a relative movement between imager and sample to scan over the surface. The spectral imaging system records the spatial information line-wise, and the spectral information for each pixel along the line by projection of the spectral information along the second axis of the two-dimensional camera chip. The spectral encoding is provided either by linearly variable filters,13 by a DMA (digital micro-mirror array) in combination with a grating<sup>14</sup> or by dispersive optics forming an imaging spectrograph.<sup>15</sup> A computer combines the slices, derives the second axis and thus reconstructs the full image. Such an imaging spectrograph based on dispersive optics was chosen as most suitable for the proposed application.

#### Hardware prototype

For the present project, an SI device for macroscopic samples, as depicted in Figure 1, was developed. At the base of the set-up is the sample feed unit. In the first prototype, this was a PC-controlled precision linear slide with variable velocity, covered with a 10 mm thick polytetrafluoroethylene (PTFE) slab. This polymer block acts as (i) a homogeneous background, (ii) increases the contrast and (iii) can be used as a broadband white standard for image correction. In a further development, a conveyor belt equipped with a remote-controlled micro-controller replaced the slide. Positioned perpendicular above the sample feed is the *imaging spectrograph*, with the camera attached to it. Optionally, it is possible to mount a second spectrograph / camera system looking at the same position as the first system at an inclination of  $7^{\circ}$  to the vertical. This option is useful, for instance, when having to evaluate two wavelength regions that cannot be covered with a single instru-

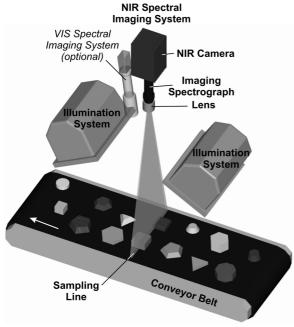


Figure 1. Schematic set-up of the spectral imager laboratory prototype (image to scale).

ment. For the present application, an ImSpector<sup>TM</sup> N17 (SpecIm Ltd, Finland), optimised for the wavelength range from 1000 to 1700 nm, was coupled to a SU320-1.7RT InGaAs NIR camera (Sensors Unlimited, USA) with a sensitive range of 900-1700 nm and a nominal resolution of  $320 \times 240$  pixels. This hyperspectral imaging spectrograph is essentially based on a direct vision dispersing prism-gratingprism (PGP) component, featuring a transmission volume grating cemented, together with a short-pass and a long-pass filter, between two optically matched prisms.<sup>16</sup> To the front of the spectrograph, NIR optimised lenses were attached, governing the spatial resolution perpendicular to the movement axis. In the present layout, the prototype overviews a line of approximately 300 mm length, resulting in an effective resolution of 1.4 mm in the first axis. The frame rate of the camera and the velocity of the sample feed determine the resolution in the second spatial axis. By varying the two parameters, it can be adapted to specific needs. The third essential component, the illumination system, is located in front and behind the spectrograph, looking down on the samples at an angle of 30° to the vertical. The kind of illumination depends on the selected wavelength range. Here, two 1000 W halogen spotlights, equipped with special diffusing glasses to achieve a possibly homogeneous illumination, were used.

#### Samples

Two sample sets were used during the experiments. The first set ("training set") was used for the model training and consisted of 16 samples of commonly used polymers (Table 1). The training set samples had a uniform rectangular parallelepiped shape (40 × 40 mm), but varied in thickness between 3 and 20 mm. The spectra obtained from these measurements were verified against diffuse reflectance data measured for the identical samples with a Nexus 870 FT-IR spectrometer (ThermoNicolet, USA) equipped with a NIR UpDrift accessory. The results of this comparison are thoroughly satisfying, examples are shown in Figure 2, thus proving both the suitability of the method and the correctness of the wavelength calibration of the spectral imager.

A second set of about 150 polymer samples ("evaluation set"), covering a wide range of differently sized, shaped and coloured items, was used for testing the suitability and stability of different classification algorithms. Also, polymers with different additives, e.g. plasticisers or fillers and modified polymers were investigated at this stage. In a final step, real polymer waste fractions were investigated.

#### Data acquisition

The images were acquired at a frame rate of 50 frames per second (fps) and 12-bit resolution and fed into the data evaluation PC via a high-performance frame-grabber card. An example spectral image, both in 2D and 3D representation, is shown in Figure 3. From the 3D contour plot, single spectra can be extracted for each spatial point.

Prior to the experimental series, dark current spectra were acquired and stored for use in spectral pre-processing. Additionally, PTFE white standards were measured at regular intervals. Besides functioning as reference reflectance standard in spectral pre-processing, the spectra obtained for these chemically and thermally highly stable samples could be used to monitor long-time system drifts in the system.

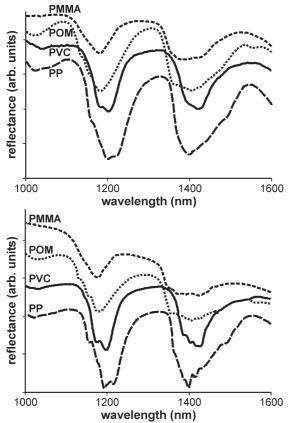


Figure 2. Comparison of example spectra obtained from the spectral imager (upper image) to reference spectra recorded for the identical samples using a commercial FT-IR spectrometer with diffuse reflectance measurement accessory (lower image).

# Data analysis and classification

Most technical polymers can be distinguished by their characteristic absorption bands in the NIR, in the investigated range between 1000 and 1700 nm in particular the second overtone C-H stretching and the C-H combination bands. The spectral differences between the plastics should enable a robust classification for the majority of the more abundant technical polymers. To test this assumption, the first derivatives of the normalised spectra measured for the training set of 16 different polymer samples were analysed using the principal component analysis (PCA) method (Figure 4). This investigation shows up the most significant differences of the spectra, which in the present investigation are the slope(s) and fine structure(s) of the band sides. The first three principal components represent 93.9% of the variance, the first five components 97.7%, whereas the original spectral data contain over 100 chemometric bands. Hence, the transformation produced by the PCA can be used to reduce the typically high dimensionality of spectral data which otherwise may complicate training classifiers (curse of dimensionality).

The results of the PCA in combination with manual inspection of the diffuse reflection spectra show that most of the polymers can be clearly separated and hence classified. This is illustrated in Figure 5, presenting feature space plots of the first four princi-

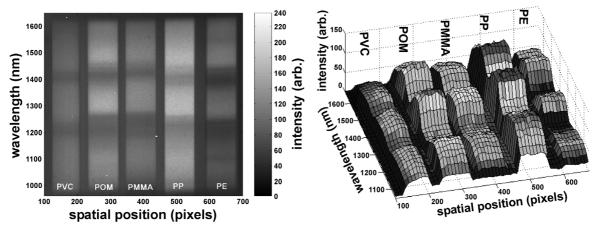


Figure 3. Spectral images of five example polymer samples. The left-side image shows the 2D grey-scale image as delivered from the spectral imaging system, the right-hand image shows it as a three-dimensional profile plot to illustrate the spectral content.

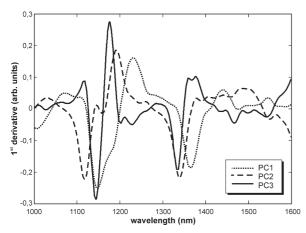


Figure 4. First three principal components of the polymer spectra, derived via standard PCA from first derivative normalised diffuse reflection spectra.

pal component scores, where each point represents the first derivative of a normalised spectrum. The class labels correspond to the classes assigned in Table 1. Most of the areas of the different classes (polymers) are clearly separated in clusters and are sufficiently distinct from each other to warrant a reasonably stable classification. Overlaps occurred between polyamide 6 (PA 6) and polyamide 6.6 (PA 6.6), which are chemically closely related. Another spectral similarity could be observed for polymethyl metacrylate (PMMA) and polyvinylidene fluoride (PVDF), although these materials are chemically highly different. Apart from this, general problems occurred only with dark grey or black coloured samples, where the pigments significantly reduce the reflectivity and superimpose their own spectral characteristics on the sample, thus obscuring the polymer absorptions. Therefore, such samples are difficult to classify from their reflection spectra. Nevertheless, all these samples were included in the further investigations to assay the potentials and limits of on-line classification of polymers with spectral imaging.

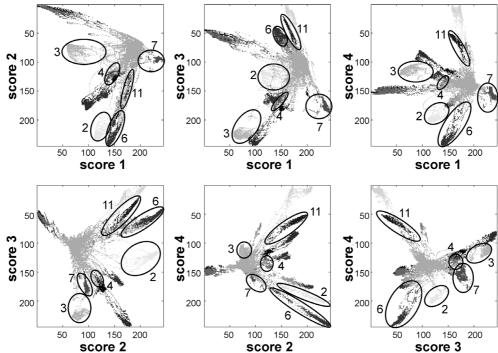


Figure 5. PCA feature space plots of the initial training set, plotting the first four scores against each other. Selected classes have been highlighted to increase intelligibility. The labels correspond to the classification given in Table 1, the medium-grey pixels in the centre of the score plots represent the spectral information from the hyperspectral image that does not belong to a sample.

Table 1. Initial training set.

	Material	Colour	Thickness (mm)	Training class
POM	Polyoxymethylene	natural	20	2
PE-HD	Polyethylene, high-density	natural	20	3
PVC-U	Polyvinylchloride, unplasticised	transparent	5	4
PA 6	Polyamide 6	natural	5	5
PVDF	Polyvinylidenfluoride	natural	12	6
PE-antistat.	Polyethylene, anti-statically modified	black	6	7
PVC-C	Polyvinylchloride, chlorinated	transparent	8.5	8
PA 6.6	Polyamide 6.6	natural	5	9
PMMA	Polymethylmethacrylate	white	3	10
PP-S	Polypropylene, modified	white	11	11
PVC-E	Polyvinylchloride, expanded	white	8	12
PETP	Polyethyleneterephthalate	white	5	13
PC	Polycarbonate	transparent	12	14
PP	Polypropylene	natural	6	15
PTFE +25%GF	Polytetrafluoroethylene, filled with 25% glass fibres	white	20	16
PS	Polystyrene	white	6	17

#### Pre-processing

For a stable classification, and to get comparable datasets, a suitable data pre-processing proved to be essential. As a first step, the acquired spectral data were standardised through a dark current subtraction and white reference scaling to obtain the actual reflectance data. Another function usually performed during pre-processing in a real-time systems is to reduce the amount of data to the necessary minimum, e.g. by spectral range selection or data binning, thus reducing the necessary processing time and speeding up the classification. This is of particular importance for high-resolution systems, in particular in the visible range. However, for the NIR spectral imager used in this work, the low resolution of the NIR camera rendered an additional data re-

duction unnecessary. Further data enhancement involved normalisation, typically following the Euclidean Distance (L2) norm algorithm, and/or calculating the first or second derivative, using the standard Savitzky–Golay algorithm. Finally, two of the investigated classification algorithms (LDC and QDC) required a principal component analysis (PCA) to be performed during pre-processing, to reduce the dimensionality of the data to between five and 15 principal components.

#### Classification algorithms

A number of different classification algorithms have been evaluated with the pre-processed data from the training set samples. The classifications were performed within Matlab® (The MathWorks

Inc., USA), using a Spectral Imaging toolbox providing the following classifiers: Linear and Quadratic Discriminant Classifier (LDC, QDC),<sup>17</sup> Fisher Linear Discriminant Classifier (FLDC)<sup>17</sup> and Spectral Angle Mapper (SAM).<sup>18</sup> Additionally, an unsupervised fuzzy-k-means classification algorithm<sup>17</sup> was investigated.

The classifiers were tested in an initial stage with normalised, differentiated and differentiated normalised data. The LDC and FLDC algorithms and the unsupervised fuzzy-k-means clustering showed an unsatisfactory performance in each instance. The remaining algorithms, QDC and SAM, which appeared to be more promising, were subjected to a more detailed investigation.

The Quadratic Discriminant Classifier (QDC) is a conventional statistical classifier. During the training of the QDC model, the probability density functions of the individual training classes in the principal component space are estimated from the training data. Normally distributed data are assumed, and the distribution parameters (average, covariance) are estimated with maximum-likelihood estimation. The algorithm assigns the spectrum to the class with the highest likelihood. Assignments with a likelihood below a certain threshold value are rejected and classified into a common rejection class. The introduction of this threshold increases the robustness of the classification considerably. By adjusting the rejection threshold, the tolerance of the classification against sample deviations and modifications can be optimised.

The Spectral Angle Mapper (SAM) is a simple mapper algorithm without involving statistical evaluation. It chooses the class with either the smallest angle or the minimal dot product between the sample spectrum and the class reference spectrum. During training, reference spectra for the single classes are defined, in this work by calculating averaged spectra over small areas on the surfaces of the training set samples. A global threshold angle or individual class threshold angles allow an optimisation of the generalisation property of SAM, thus determining how tolerant the classifier is against sample deviations and chance variations of the spectra. For the present application, a global threshold angle of 17.5° was used. All spectra not falling into any of the cones defined by this angle and the single reference spectra

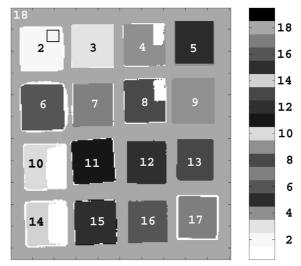


Figure 6. QDC classification results, shown for the initial training set. The algorithm is trained on a small spot, as indicated by the black rectangle in the left upper sample. The samples and assigned class labels correspond to Table 1.

were assigned to a common rejection class (class 1). The classification performance could be increased even further when using individual threshold angles for the different classes.

#### **Results and discussion**

#### Training phase

Figure 6 shows examples of the classification result obtained with the QDC algorithm for the training set. The classifier was trained on small, homogeneous regions of each polymer sample, as indicated by the small square in the illustration. In the classification result image, white pixels indicate spectra where no safe classification is possible as the likelihood is smaller than the chosen rejection threshold. Such inhomogeneities in the classification could be observed primarily with thin, semi-transparent samples in areas where the spectra are corrupted by adhesive paper labels on the rear side of the sample.

In a direct comparison, both algorithms proved to be equally capable of correctly classifying the samples, using normalised, differentiated and differentiated normalised data. With normalised differentiated data, the classes were best separable and hence the most stable classification results could be obtained. This proved in particular true in subsequent experiments, where, without changing the training, the illumination conditions were changed and the classification repeated using the training set samples. Both algorithms proved to be inert against changing illumination conditions when evaluating differentiated normalised data, whereas in particular the QDC produced a number a of false classifications when applied to the other data sets.

#### Evaluation phase

In addition to varying illumination conditions, for an application as a classification detector in automated separation systems, the robustness over a number of other variable parameters is crucial. To test that, both classifiers were evaluated with around 150 different samples with differing characteristics. The size and shape, the colour, the sample thickness, which is particularly important for (semi)transparent samples, the material quality and manufacturer, and the surfaces properties, e.g. the roughness, were varied. Additionally, non-polymer samples, such as pieces of wood or metal, were introduced at random. A typical evaluation sub-set, consisting of 20 different samples, is listed in Table 2. Figure 7 shows the corresponding classification using the SAM classification algorithm.

The comparison of the reference training classes (ground truth) to the classification results, as listed in Table 2, allows a number of conclusions to be drawn. First, chemically similar or (nearly) identical polymers, although stably classified into different classes during the training, fall together under these conditions. This is the case, for instance, for the different polyamides (classes 5 and 9), where a homogeneous sample is classified as if it has an inset (Figure 7), for polyvinyl chloride and some of its modifications (classes 4, 12 and occasionally 8), and for polypropylene and its derivatives (classes 11 and 15). However, as all these chemically related polymers falling in common classes can also be recycled together, this is not critical for the intended application. More critical is one case where two chemically different polymers, namely polyvinylidene fluoride (class 6) and polymethyl methacrylate (class 10), are spectrally so similar that sometimes false classifications occur. This occurs regularly with the QDC, but

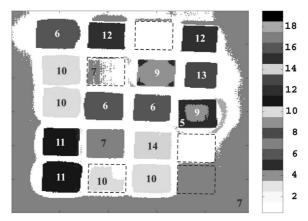


Figure 7. Spectral Angle Mapper (SAM) classification results for an example evaluation sub-set. The sample description and the assigned classifications are listed in Table 2.

sometimes also with the SAM. In case both substances are present in the feed, a cross-contamination of the fractions cannot be ruled out completely.

The second result is that both classifiers tend to identify dark coloured polymers falsely. This problem had already been indicated in the preliminary experiments, as the spectra show very little spectral features. The same is true for PTFE, which served as the white reference standard. Anyway, both algorithms classify such samples into the rejection class (RC), or into class 7, which belongs to a polymer filled with carbon black, but never into classes belonging to other polymers. Hence, the dark items simply pass through the classifier system and would be ejected by a sorter with non-polymer materials, without contaminating the clean polymer fractions. In case legal or economical requirements should necessitate sorting these polymers as well, a special classification procedure using an enhanced data acquisition would be necessary.

As the direct comparison of the classification performances shows, the SAM is the preferable method for this application. This can be attributed to the better generalisation capabilities of SAM, which enables this simple algorithm to perform better than the statistically more powerful QDC. Another advantage is the reduced processing time of the SAM in comparison to the QDC, which can be attributed to

Table 2. Example evaluation sub-set. False classifications into to incorrect (material) classes are shaded grey. The label RC (rejection class) indicates a classification that does not fall into any of the defined sample classes.

Mate- rial	Colour	Thickness (mm)	Ground truth class	Classification results	
				QDC	SAM
PVDF	natural	20	6	6	6
PVC	red	25	4	RC	12
Wood	natural	15	-	7	RC
PVC-E	white	15	12	RC / 12	12
PMMA	transparent	4	10	10 / 6	10
PP-S	grey	10	11	RC	7 / RC
PA 6	white	20	5	5/9	9/5
PETP	white	20	13	13	13
PMMA	white	3	10	6	10
PVDF	natural	5	6	6	6
PVDF	natural	5	6	6	6
PA 6.6	natural	20	9	5/9	5/9
PP	white	6	15	11 / RC	11 / 15
PVC	grey	5	4	7	7
PC	transparent	3	14	14	14
PP	grey	3	15	RC	RC
PP	natural	8	15	15	11 / 15
PMMA	transparent yellow	2	10	6 / RC	10
PMMA	Opaque white	3	10	6	10
PP-S	grey	5	11	6 / RC	7

two facts: (i) the SAM does not require a PCA during pre-processing and (ii) the algorithm is simpler. This time advantage is of great value for the envisaged real-time application.

#### Real-world samples

As a final step, real-world polymer waste fractions were investigated, using the imager set-up suspended over a conveyor belt transporting the polymer waste. The spectral data is pre-processed, involving normalisation and differentiation, and classified using the SAM algorithm. In the present configuration, this allows acquiring more than 50 image lines per second. As an example, the online classification of a packaging material fraction is shown in Figure 8. The single materials can clearly be identified, e.g. a polyethylene cap on a polyethylene terephthalate bottle. Also the size and shape of



Figure 8. On-line real-time classification results of the spectral imager, located over the conveyor belt in a prototype plastic waste sorter. The left image shows the waste stream as is, the right image the corresponding classification results.

the items are clearly discernible, allowing the precise control of, for example, an attached sorter unit.

#### Conclusion and outlook

Spectral imaging proves to be a valuable method for on-line, real-time classification of synthetic polymers. By applying suitable classification algorithms, the most abundant synthetic polymers can be identified with high reliability, independent of their shape or their pigmentation. Only materials that have only low and/or unstructured absorption bands in the investigated spectral range (e.g. PTFE), or where the content of filling materials with strong broadband absorptions (i.e. carbon black) is high, cannot be classified satisfactorily. The best classification results could be obtained by applying the Spectral Angle Mapper (SAM) method, supplemented by a threshold value, on the differentiated normalised data. The key advantage of this method is the significantly reduced computing time in comparison to methods dependent on principal component analysis, thus making real-time classification feasible. In addition to the classification, standard image processing algorithms can be applied to the classification result images, allowing, for example, the identification of polymer insets in other materials.

Ongoing work concentrates on expanding the application fields into other areas, e.g. to on-line real-time quality control, and on further optimising the data evaluation to increase the processing speed and thus the achievable resolution.

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