Supporting Information

Establishment of an efficient and accurate thermal stability evaluation method based on machine vision and its application in PVC thermal degradation

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1. Experimental

1.1. Materials

Tung-maleic anhydride (TMA, acid value: 269.02 mg KOH/g), 3-amino-1,2,4-triazole (Atz, 96%, Aladdin), para-aminobenzoic acid (PABA, 99%, Aladdin), epichlorohydrin (99%, Shanghai Lingfeng), triethylbenzylammonium chloride (98%, Aladdin), sodium hydroxide, calcium oxide (98%), acetone (99.5%, Chinese medicine Shanghai style), methanol (99.5%, Aladdin), tetrahydrofuran (THF, 99%, Aladdin), N,N-dimethylformamide (DMF, 99.5%, Aladdin), petroleum ether (60-90 °C), PVC (PVC, S-1000, Shandong Qilu, China) were purchased commercially.

1.2. Synthesis of Tung oil derived amide epoxidized esters (TOAEE)

TOAEE was synthesized according to the references.[1] A reaction vessel containing TMA (31.68 g) was placed into an oil bath at 25 °C. PABA (6.68 g) was dissolved in acetone (70 mL) and slowly added to the vessel while continuously stirring. The reaction mixture was kept at 55 °C for 4 hours. The solvent was then removed through reduced pressure distillation and the resulting product was vacuum-dried at 70 °C for 24 hours, yielding a light-yellow slimy product (ABTMA). ABTMA (16.67 g), epichlorohydrin (25.97 g), and benzyltriethyl ammonium chloride (0.07 g) were added to a flask equipped with a reflux condenser, a thermometer, and a stirrer. The reaction was maintained at 110°C for 2 hours. After cooling the mixture to 60°C, sodium hydroxide (1.12 g) and calcium oxide (1.57 g) were added. The mixture was stirred at 60°C for 3 hours and then filtered using celite and filter paper. The excess epichlorohydrin was removed and recycled using a rotary evaporator. A yellowish viscous resin (TOAEE) was obtained with an epoxide equivalent weight of 701 g mol^{-1} (theory: 692.72 g mol^{-1}). The synthesis route of TOAEE is shown in Scheme 1a.

1.3. Synthesis of P-Atz_3

P-Atz_3 was synthesized according to the reference.[2] PVC (18 g), Atz (10.8 g), and DMF (180 ml) were combined in a flask and reacted at 85°C for 4 hours, resulting in a white viscous solution. The viscous solution was then washed multiple times with a 10wt% methanol aqueous solution and dried in an oven at 60°C for 24 hours to yield a white transparent flake solid (P-Atz_3). The synthesis route of P-Atz_3 is shown in Scheme 1b.

1.4. Preparation of PVC films

In this experiment, a mixture of THF, P-Atz_3, and TOAEE was prepared in different mass ratios of 5:1, 5:2, 5:3, and 5:4. The mixture was dissolved at 65°C and poured into a Petri dish for drying at room temperature for 48 hours. The resulting P-Atz_3/TOAEE films were named S1, S2, S3, and S4. Additionally, reference thin films were prepared using the same method with P-Atz_3 and PVC/TOAEE (mass ratio 5:3), named Sa and Sb, respectively. The specific composition of each film is provided in Table S1.

Table S1. Different formulations for PVC samples[a]

Samples	P-Atz_3	TOAEE	PVC	$CaSt_2$/ $ZnSt_2$
S1	4.17	0.83	0.00	-
S2	3.57	1.43	0.00	-
S3	3.13	1.88	0.00	-
S4	2.78	2.22	0.00	-
Sa	5.00	0.00	0.00	-
Sb	0.00	1.88	3.13	-
CZ41	-	-	5	0.15

[a] The mass ratio of $CaSt_2$ salt and $ZnSt_2$ salt is 4:1.

1.5. Characterization

FT-IR Characterization. The FT-IR spectra were obtained on a Nicolet iS10 FT-IR (Nicolet Instrument Crop., USA) infrared spectrophotometer. The experiment was performed within 400-4000 cm^{-1} with KBr as a reference.

Thermal stability test. The thermal stability of prepared PVC samples was determined by Congo red test and discoloration test. The static thermal stability time (T_s) could be obtained by heating the PVC film on a heat stability tester at 180 °C according to the standard ISO 182-1-1990. The thermal aging test of the PVC sheet (20 mm × 20 mm pieces) was tested at 180 °C according to the ISO 305:1990(E) standard.

The thermogravimetric analysis test. The thermogravimetric analysis (TGA) and differential thermal analysis (DTG) was together performed on an American TGA5500 instrument with a heating rate of 10 °C/min from 35 to 600 °C under nitrogen (100 mL/min).

Machine vision based thermal stability test. Machine vision analysis utilizes the high-definition camera C33 (Shenzhen Oni Electronics Co., Ltd.) as the monitoring equipment for machine vision. The programming language used is Python, along with the machine vision development software in OpenCV. The machine vision experiment is designed as follows: the high-definition camera C33 (Shenzhen Oni Electronics Co., Ltd.) is employed to monitor the color change method and the Congo red method experiment. Once the experimental image data for the color change method and Congo red method are obtained, OpenCV is utilized to convert the selected areas of the PVC film sample and Congo red test paper into respective RGB values. To minimize the impact of uneven color change and deformation, the image of the PVC film sample and Congo red test paper should be selected from areas with uniform color (Fig. S1). In order to reduce errors, it is recommended to preprocess the image with mean filtering before performing numerical conversion. Mean filtering is a process in which the pixel values in a specific area of an image are averaged and then replaced with this average value. The calculation formula for mean filtering is represented as $f = \frac{1}{M}\sum_{i,j \in N} g(i,j)$. In this formula, f denotes the final result value of filtering, N represents the target area, and M is the number of pixels in the target area N. The extent of filtering depends on the size of N. The color values of PVC film samples and Congo red test paper were obtained through the Congo red test and color change test, and their color change patterns in different color spaces were analyzed. The key factors considered were monotonicity, change amplitude, and fluctuation.

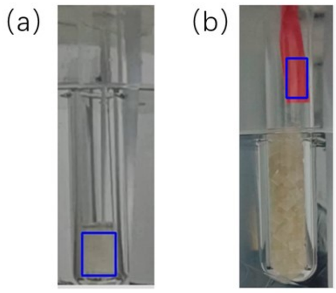

Fig. S1 (a) PVC film sample area selection; (b) Congo red test paper area selection.

2. Results and discussion

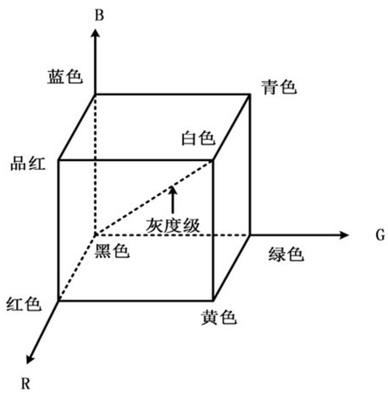

Fig. S2 RGB color space model.

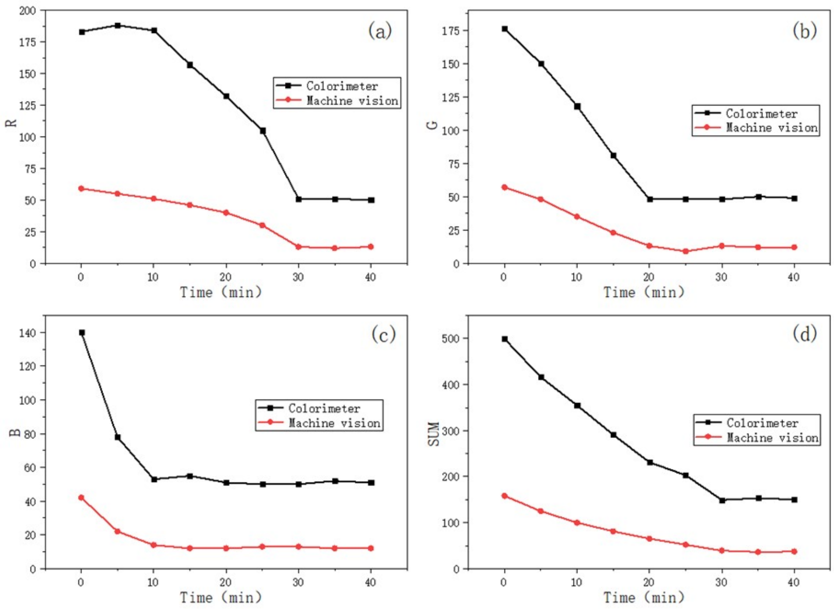

Fig. S3 RGB values of PVC samples in the color change method recorded by machine vision and color difference instrument.

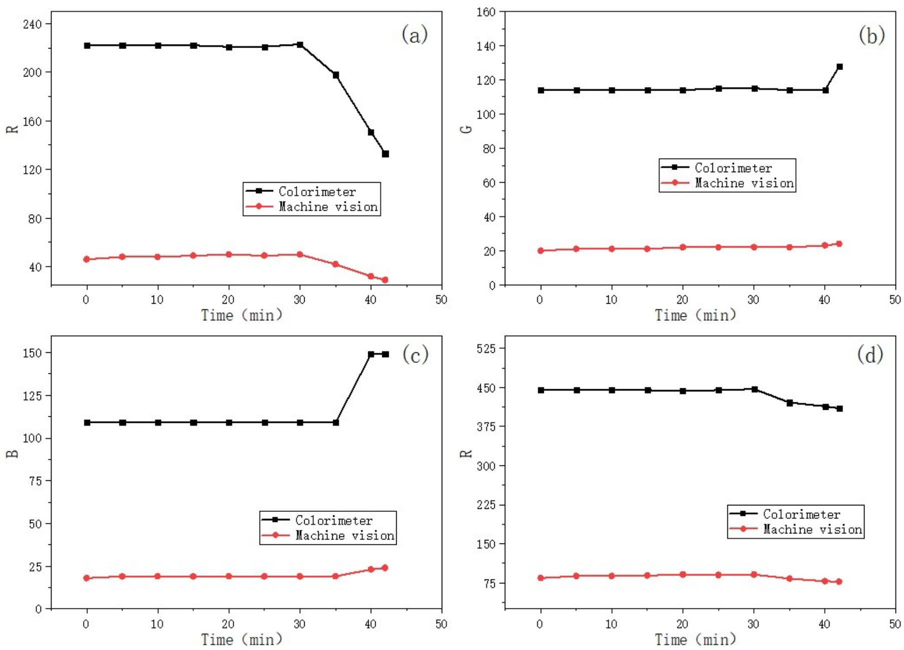

Fig. S4 RGB value of Congo red test paper in Congo red method recorded by machine vision and colorimeter.

Reference

1 M. Wang, S. H. Li, H. Y. Ding, J. L. Xia and M. Li, *New J. Chem.*, 2020, **44**, 4538-4546.

2 M. Wang, X. Z. Fan, Q. Bu, P. Y. Jia and S. Q. Yuan, *J. Renewable Mater.*, 2023, **11**, 2015-2031.