

Disperse dyeing affinity with different structural substituent effects

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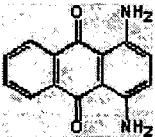

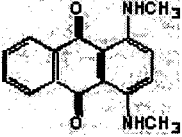
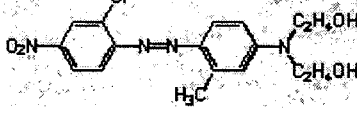
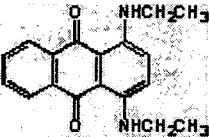
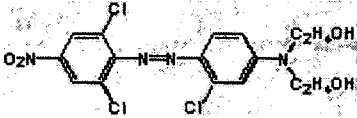
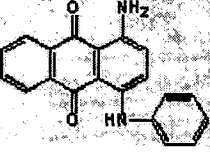

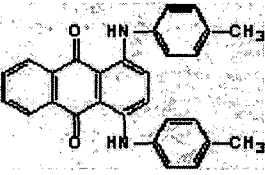

Adsorption properties of the 10 kinds of disperse dyes having different substituents were examined using several representative non-aqueous media on to poly(ethylene terephthalate) substrates. The dye adsorption amounts in pentane medium representing alkanes were much higher than those in the other non-aqueous media. In pentane medium, as the hydrophobicity of the dyes resulting from the substituents of dye molecules increased, the solubility of the dyes increased and the corresponding dye adsorption greatly decreased. This finding was coincident with the results from the previous study that the adsorption amount of disperse dyes on to substrates was inversely proportional to the solubility of the dyes. Furthermore, the hydrophobicity and the hydrophilicity of the dyes were discussed in terms of the electric dipole moments which obtained by a semiempirical method using molecular modeling software.

Experimental

Materials

The scoured and rinsed plain-weaved poly(ethylene terephthalate) fabrics (75denier/-36filaments, 10697yarns/inch, 705g/m³) were used. The dyes used were listed in Table 1. They were five anthraquinone and five azo disperse dyes having different substituents in the dye structures which could impart different levels of hydrophilic or hydrophobic characteristics to the dyes. Acetone extraction was carried out using a soxhlet extraction apparatus to purify the selected commercial disperse dyes and the purified dyes were then recrystallized in ethanol. As adsorption media, the 5 kinds of non-aqueous representatives were employed, namely acetone, benzene, methanol, tetrachloroethylene(perclene) and pentane.

Table 1. Disperse dyes used

Anthraquinone dyes		Azo dyes	
C. I. Name (Dye No.)	Structure	C. I. Name (Dye No.)	Structure
Disperse Violet 1 (V01)		Disperse Red 19 (R19)	
Disperse Blue 14 (B14)		Disperse Red 5 (R05)	
Solvent Blue 59 (B59)		Disperse Brown 1 (Br01)	
Disperse Blue 19 (B19)		Disperse Red 1 (R01)	
Solvent Green 3 (G03)		Disperse Orange 25 (O25)	

Adsorption

The disperse dyes (0.005g) were adsorbed on poly(ethylene terephthalate) (0.2g) using non-aqueous adsorption media (50ml) in sealed stainless steel pots at 130°C for 1 hr.

Solubility determination

In order to measure solubility of disperse dyes in non-aqueous media, an excess amount of the dyes was placed in 10ml of the solvents at 25°C for 48 hrs. The solutions were centrifuged to separate undissolved dyes and then filtered the solution out to eliminate undissolved dye solutes. The concentration of the dyes in this solution was measured spectrophotometrically and the solubility of the dyes in each media was then calculated.

Electric dipole moments of the dyes

In order to investigate the effect of substituent changes in the dye structures on solubility properties, a concept of the electric dipole moments of the dyes were considered and the values were theoretically obtained using molecular modeling software, CS Chem3D™ Pro (CambridgeSoft Co. USA). This electric dipole moment was computed by a semiempirical method using optional CS MOPAC system included in the molecular modeling software. To compute the dipole moments the standard parameters such as Austin Model 1 (AM1), closed shell and Mulliken charge population were selected.

Conclusions

10 kinds of disperse dyes having different substituents were examined to investigate the exhaustion properties towards poly(ethylene terephthalate) substrates in several non-aqueous media. The adsorption amount of the dyes in pentane medium representing alkanes was much higher than those in other media. In terms of substitution effect within dye structures, the solubility of the dyes in pentane increased with increasing hydrophobic substituents of the dyes. On the contrary, the adsorption amounts greatly decreased with increasing hydrophobic characteristics of the dyes. Dipole moments of the dyes decreased with substitution of the hydrophobic groups to the dye molecules. The decrease of dipole moment provided the increase of dye solubility in hydrophobic pentane. The dipole moment values obtained in this work might be different from those measured experimentally. However, this computation approach could be useful to explain the exhaustion properties of dyes in terms of solubility and adsorption.

References

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