Quantification and evaluation of chemical footprint with four methods: A case of the dyeing and printing process of a polyester dress

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ABSTRACT – REZUMAT

Quantification and evaluation of chemical footprint with four methods: A case of the dyeing and printing process of a polyester dress

The textile printing and dyeing industry, with huge chemical demand, has a negative impact on the ecosystem. Chemical footprint quantifies the toxic impacts of chemical pollutants by assessing their behaviour in the environment. In this paper, four methods were used to calculate and evaluate the chemical footprint of a polyester dress printing and dyeing process. The chemical footprint of the printing and dyeing process of a polyester dress, calculated with USEtox, Assessment of Mean Impact, Score System, and Strategy Tool, was 1585.51 PAF×m^3×day, 14089.04 l, 331, and 75, respectively. Scouring, colouring, pretreatment, and printing were identified as the major procedures contributing, with the antifoaming agents and the chelating disperse agents as the major auxiliaries contributing. The results of the Strategy Tool are limited in their representativeness of environmental load. Compared to other methods, AMI ensures that the evaluation results are scientific while maintaining user-friendliness.

Keywords: *chemical footprint, polyester, printing and dyeing, toxic effects, environmental impact*

Cuantificarea și evaluarea amprentei chimice cu patru metode: un studiu de caz privind procesul de vopsire și imprimare a unei rochii din poliester

Industria de imprimare și vopsire a materialelor textilelor, cu o cerere enormă de produse chimice, are un impact negativ asupra ecosistemului, amprenta chimică cuantificând impactul toxic al poluanților chimici prin evaluarea comportamentului acestora în mediu. În acest articol, au fost utilizate patru metode pentru a calcula și evalua amprenta chimică a unui proces de imprimare și vopsire a unei rochii din poliester. Amprenta chimică a procesului de imprimare și vopsire a unei rochii din poliester, calculată cu USEtox, Assessment of Mean Impact, Score System și Strategy Tool, a fost de 1585,51 PAF×m^3×zi, 14089,04 l, 331 și, respectiv, 75. Spălarea, colorarea, pretratarea și imprimarea au fost identificate ca fiind principalele procese care contribuie la acest impact, iar agenții antispumanți și agenții dispersanți chelatori au fost identificați ca fiind principalii adjuvanți care contribuie la acest impact. Rezultatele Strategy Tool sunt limitate în ceea ce privește reprezentativitatea lor pentru impactul asupra mediului. În comparație cu alte metode, AMI asigură faptul că rezultatele evaluării sunt științifice, menținând în același timp ușurința în utilizare.

Cuvinte-cheie*: amprenta chimică, poliester, imprimare și vopsire, efecte toxice, impact asupra mediului*

INTRODUCTION

The practice of dyeing is among humanity's most ancient crafts and represents an essential component of the modern textile industry [1]. It serves to enhance the value of products, provides employment, and improves the well-being of people. Concurrently, the textile printing and dyeing industry is a chemical-intensive industry in which chemicals play a pivotal role. It employs over 8,000 chemicals and produces over 700,000 tons of synthetic dyestuffs globally yearly [2, 3]. Some of the textile auxiliaries used in the manufacturing process are released into the environment in the form of wastewater and waste gases, which have the potential to negatively impact the natural environment and ecosystems [4].

Increasing environmental issues and consumer awareness of sustainable products are forcing governments to implement control policies and compelling manufacturers to re-examine all aspects of dyeing processes in search of environmentally friendly technologies to reduce the negative environmental impact of production [5]. While current guidance on chemical risk assessment in production systems is aimed at facilitating the implementation of management activities, chemical footprint (ChF) is based on a life cycle assessment and presents a new solution for chemical risk assessment in the textile field from the perspective of quantifying toxic impacts [6, 7]. Tian et al. analysed the toxic impacts of chemicals emitted during the production of one kilometre of fabric using the Institute of Public and Environmental Affairs database, and the results revealed that mass and toxicity analyses differ in their ranking of the toxic impacts [8]. Qian et al. performed a ChF assessment on 1 kg of cotton woven fabric from yarn to finished fabric, and they identified the production processes and the pollutant sources that contribute most to the ChF [9]. Qian et al. evaluated the ChF of VOCs in the production of polyester fabrics, identified the pollutants with the most significant contribution to ChF at each process stage, and pointed out the direction of improvement in the dyeing and finishing process to reduce the toxic impact of VOCs [10].

The use of some chemicals has been neglected in some ChF studies due to issues such as the confidentiality of textile auxiliaries by their manufacturers and the lack of data on textile chemical use and characterisation factors, so researchers in the field have gradually introduced methods to improve the feasibility of ChF studies [11]. In this paper, we used four methods to quantify ChF in the printing and dyeing process of a polyester dress. We compared these four methods in terms of feasibility and evaluation results. This study not only provides a reference for polyester textile manufacturers to identify priority pollutants and reduce the toxic impact of chemicals, but also guides the selection and optimisation of methods for subsequent ChF studies.

METHODS AND DATA

System boundary and data

ChF accounting begins with the definition of the functional unit. The functional unit selected for this study is a 100% polyester dress, and the basic information about this dress is presented in table 1. The system boundary of this case is then determined based on the functional unit; this entails defining the starting and ending points of the evaluation range within the production process. Figure 1 depicts the system boundary of the polyester dress. In this study, the dyeing process encompasses scouring, alkali weight reduction, colouring, reduction clearing, and finishing, while pretreatment, printing, reduction clearing, and finishing are included in the printing process. The chemicals within the system boundary are limited to those dyes and auxiliaries that are used directly, with the chemicals used indirectly to produce the dyes and auxiliaries excluded from the system boundary. The input and output data for textile chemicals within the system boundary are collected from the Mistra Future Fashion Consortium (http://mistrafuturefashion.com/).

Table 1

BASIC INFORMATION ABOUT THE EVALUATED POLYESTER DRESS

Property	Part	
	Cover part	Under part
Mass (g)	241	231
Textile material	100% polyester	100% polyester
Dtex (g/10000 m)	119/114 (warp/weft)	114

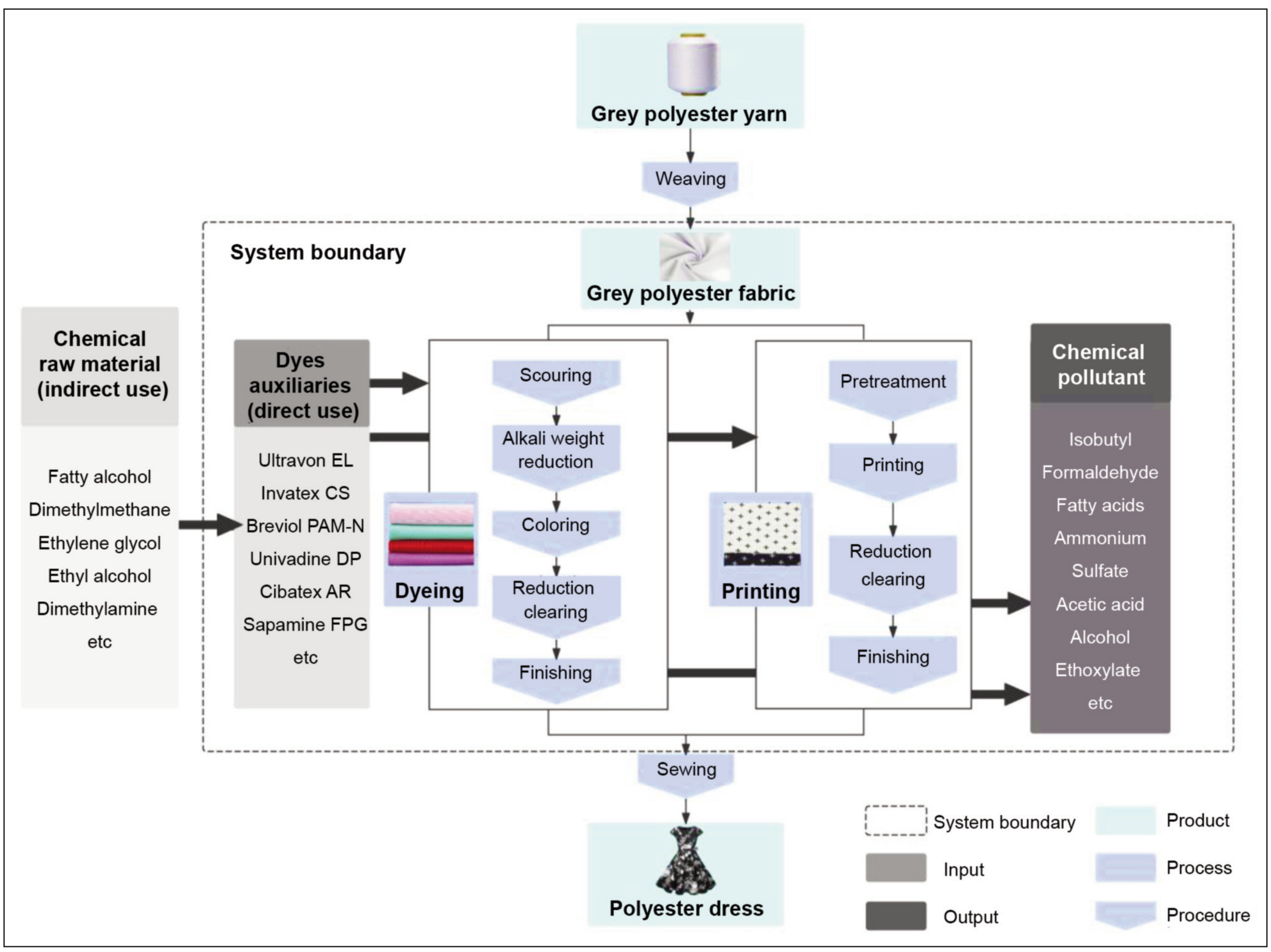

Fig. 1. System boundary of the evaluated polyester dress

Methods

The toxic impacts of chemicals input and output in the wet treatment of the polyester dress were evaluated by four methods: USEtox, the Assessment of Mean Impact (AMI), the Score System, and the Strategy Tool.

USEtox is an environmental model developed jointly by the United Nations Environment Program (UNEP) and the Society for Environmental Toxicology and Chemistry (SETAC), which assesses the toxic impacts of chemical pollutants emitted into the environment by quantifying three steps: environmental fate, exposure and effects [12]. Each chemical is assigned two highly integrated characterisation factors (CF), representing the hazards to humans and ecosystems, respectively. The ChF can be calculated using USEtox as shown in equation 1.

$$ChF_j = 290 \times \sum_{i=1}^{n} Q_{ij} \times FF_i \times XF_i \times EF_i = \\ = 290 \times \sum_{i=1}^{n} Q_{ij} \times CF_i \qquad (1)$$

where ChF_j is the total ChF of procedure j (cases for human toxicity or PAF×m^3×day for ecotoxicity), Q_{ij} – the emission of substance i in procedure j, FF_i – related to the residence time of substance i in the corresponding environment (day), XF_i is represented by the fraction of substance i transferred to the receptor population in a specific time period (day^{-1} for human or dimensionless for ecotoxicity), the human toxicity. EF_i reflects changes in the probability of disease due to changes in the intake of substance i (cases/kg) and the ecotoxicity. EF_i reflects changes in the potential effect fractions of species in response to changes in concentration (PAF×m^3/kg), CF_i denotes the characterization factor that integrates the quantitative results of the three components of fate, exposure and effect of substance i in the environment (PAF×m^3×day).

AMI method characterises the average toxic impacts by considering the toxic effects of different classes of organisms as an alternative to species sensitivity distribution (SSD) curves for calculating ecological thresholds [13]. In this method, toxicity data from a minimum of three organism classes (vertebrates, invertebrates, plants) are required to represent each of the three base trophic levels in the food chain relationships. The ChF, based on this approach, represent the volume of water required to dilute the contaminant to a safe concentration. The ChF based on the AMI method can be expressed as equation 2.

$$ChF_j = \sum_{i=1}^{n} \frac{C_{i,j}}{HC_5(NOEC)_i} \cdot V \qquad (2)$$

where C_{ij} is the exposure concentration in the aqueous phase of substance i in procedure j (g/L), V – the volume of the water environment (L), $HC_5(NOEC)_i$ – the safe threshold for the aquatic ecosystem of substance i (mg/L), indicating that the vast majority of species in aquatic ecosystems are unaffected.

The concentration of the contaminant in the water environment is primarily determined by the fate process, so it can be expressed as equation 3.

$$C_i = \frac{Q_i \cdot F_i}{V} \qquad (3)$$

where Q_i is the mass of substance i emitted (g), F_i – the proportion of substance i that fate into the water environment, so equation 2 can be transformed into equation 4.

$$ChF_j = \sum_{i=1}^{n} \frac{Q_{i,j}}{HC_5(NOEC)_i} \cdot F_i \qquad (4)$$

The Score System is a semi-quantitative method by scores several major factors [14]. The following four criteria of the toxic impact are scored: A-amount of substance, B-biodegradability, C-bioconcentration factor and D-toxicity. Each criterion will be scored between 1 and 4. According to the Score System, the four scores are multiplied to obtain a toxic impact value for each substance. The value of 4 should be given to a criterion in the case of data missing for the criteria [15]. The scoring guidelines for the four criteria are presented in table 2.

The above three methods account for emitted substances; the data used for the calculation of the USEtox method, AMI method and Score System is found in table 2.

Table 2

THE SCORING CRITERIA OF THE SCORE SYSTEM

Criteria			Score 1	Score 2	Score 3	Score 4
Amount of substance (kg/week)			<1	1–10	10–100	>100
Biodegradability	Surface water (%)		>60	10–60	<10	
	BOD/COD			>0.5		≤0.5
Bioconcentration	Bioconcentration factor (L/kg)		<100			≥100
	MW:500–1000 g/mol	Oil-water partition coefficient (P_{ow})	1000	≥1000		
		Water solubility (g/L)	>10	2–10	<2	
	MW<500 g/mol	P_{ow}	<1000	≥1000		
		Water solubility (g/L)	>100	2–100	0.02–2	<0.02
Toxicity	EC_{50} (mg/L)		>1000	101–1000	10–100	<10

Table 3

THE HAZARD LEVEL OF THE STRATEGY TOOL	
Hazard level	**Risk phrase**
Score 1	R20 R20/21 R20/21/22 R20/22 R21 R21/22 R22 R36 R36/38 R38 R50 R53
Score 3	R23 R23/24 R23/24/25 R23/25 R24 R24/25 R25 R34 R35 R36/37 R36/37/38 R37 R37/38 R41 R43 R48/20 R48/21 R48/22 R51/53 R52/53
Score 10	R26 R27 R28 R40 R42 R42/43 R45 R46 R48/23 R48/24 R48/25 R49 R60 R61 R62 R63 R64 R68 R50/53 R53

The Strategy Tool is a semi-quantitative method based on the available information in the Safety Data Sheets (SDS). According to the chemical risk phrases of the health and environmental hazards in the SDS, this method evaluates only the chemicals that are inputs to the production process. All relevant risk phrases were grouped into three levels. Substances with the highest level of risk phrase are scored 10, followed by 3 and 1, as shown in table 3. The number of exposure scenarios is also considered in the Strategy Tool, being set to the number of classified substances [16].

RESULTS AND DISCUSSION

USEtox results

Figure 2 presents the ChF results of a polyester dress with USEtox in the dyeing and printing process; the total ChF with USEtox was 1585.51 PAF×m^3×day, of which 459.73 PAF×m^3×day and 1125.88 PAF×m^3×day were for the dyeing process and printing process, respectively. The ChF values vary widely between procedures; the printing procedures contribute the most to ecotoxicity with a result of 1058.6 PAF×m^3×day, followed by colouring at 301.94 PAF×m^3×day, with both accounting for nearly 70% of the total. The smallest contributor to ChF is the reduction clearing procedure in the dyeing process, which is below 10 PAF×m^3×day. The ChF of the remaining procedures are within the same order of magnitude.

Compared to natural fibres, rayon, and nylon, polyester has no functional groups to give affinity for usual dyestuffs [17]. In the printing procedure, the dyestuff is mechanically fixed to the fibre surface by the paste. Due to the presence of a certain amount of surfactant in the paste, the surface tension between the gas and the liquid is relatively low, which makes the paste prone to bubbles when subjected to mechanical vibration and roller extrusion. A large quantity of antifoaming agents is used in the printing

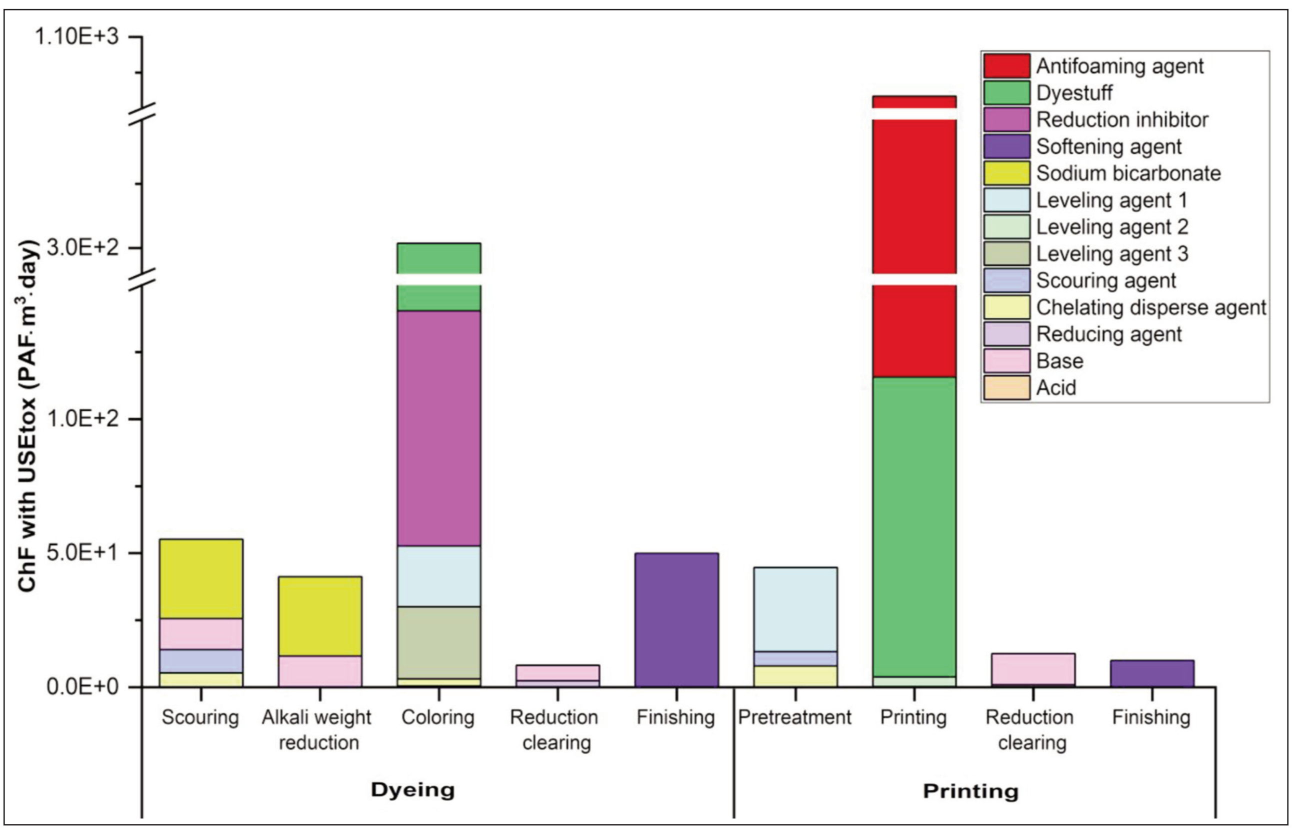

Fig. 2. Printing and dyeing process ChF of polyester dress obtained with USEtox

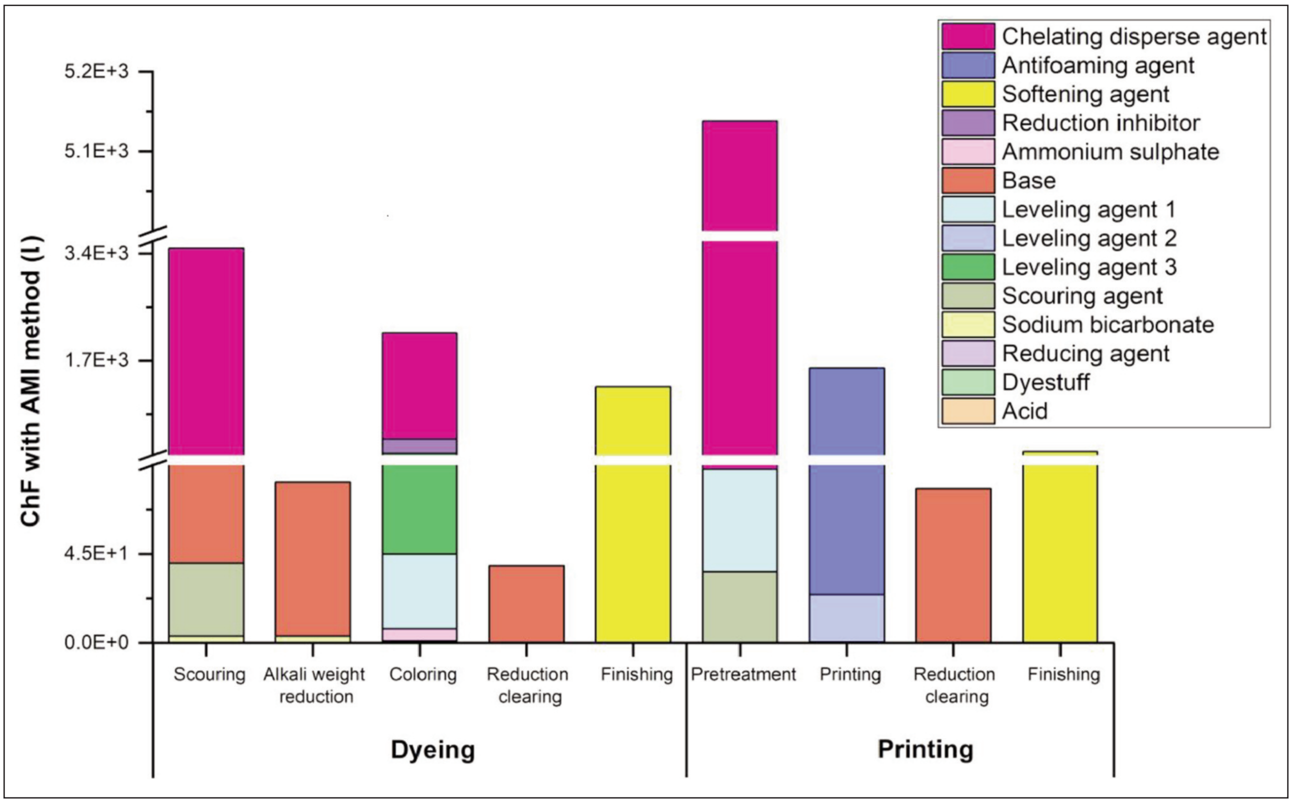

Fig. 3. Printing and dyeing process ChF of polyester dress obtained with USEtox

procedure to avoid problems such as blurred colours and uneven patterns by promoting liquid film drainage and destroying the film's elasticity, causing the bubble to burst [18]. In the dyeing procedure, as disperse dyestuffs are insoluble in water, it is necessary to use a large amount of levelling agent to make the dyestuffs and polyester come into contact quickly to improve the dyeing efficiency [19]. Reduction inhibitors help minimise reductive dye decomposition occurring during dyeing.

In the USEtox method, isobutyl acrylate had the most ecotoxicity impact on the environment among all the discharged chemical pollutants, accounting for 63.61% of the total ChF, followed by dyestuff, with a value of 273.52 PAF×m^3×day. Acetic acid and diethylene glycol monomethyl ether were the two substances that caused the least environmental load in this method, both less than 1 PAF×m^3×day. The isobutyl acrylate emissions from scouring agent, levelling agent 1 and antifoaming agent, 90.31% of which comes from the antifoaming agent in the printing procedure, which has the largest CF of any pollutant in this case. Although the CF of dyestuff is an order of magnitude smaller than the former, dyestuff is the main chemical for colouring and printing, and due to its minimal solubility in water, a large amount is needed to ensure the effect of the dyeing and printing process. A certain amount of acetic acid was used in the colouring and printing procedures; it mainly played a role in maintaining pH stability during the production process, and most of the acetic acid was neutralised in the reduction cleaning procedure [20]. Diethylene glycol monomethyl ether emission from levelling agent 2.

AMI results

The ChF results of the polyester dress with the AMI method in the dyeing and printing process are illustrated in figure 3. It can be seen from figure 3 that the total ChF with the AMI method is 14089.04 L, ecotoxic impact mainly occurs in pretreatment (36.48%), scouring (24.74%), colouring (15.19%), printing (11.22%) and finishing (9.12%) in the dyeing process. The toxic impact of alkali weight reduction and reduction clearing is much smaller than that of other procedures, both below 100 L.

The impacts of pretreatment, scouring, and colouring mainly come from the chelating dispersant agent. Chelating dispersing agents can combine with metal ions (Ca^{2+}, Mg^{2+}, Fe^{3+}) in water to form complexes that prevent metal salts from affecting the dyeing process, thus achieving the objective of improving the brightness and colour fastness of dyeing [21, 22]. In the AMI method, the largest contributor to ChF of all chemical pollutants is alcohols, C12-14, ethoxylated, accounting for 71.69% of the total ChF, followed by isobutyl acrylate, with 11.78%. The toxic impacts of Sodium sulfite (0.12 L), formaldehyde (0.14 L), diethylene glycol monomethyl ether (0.27 L), acetic acid (0.59 L), and dyestuff (0.64 L) are much less than other pollutants.

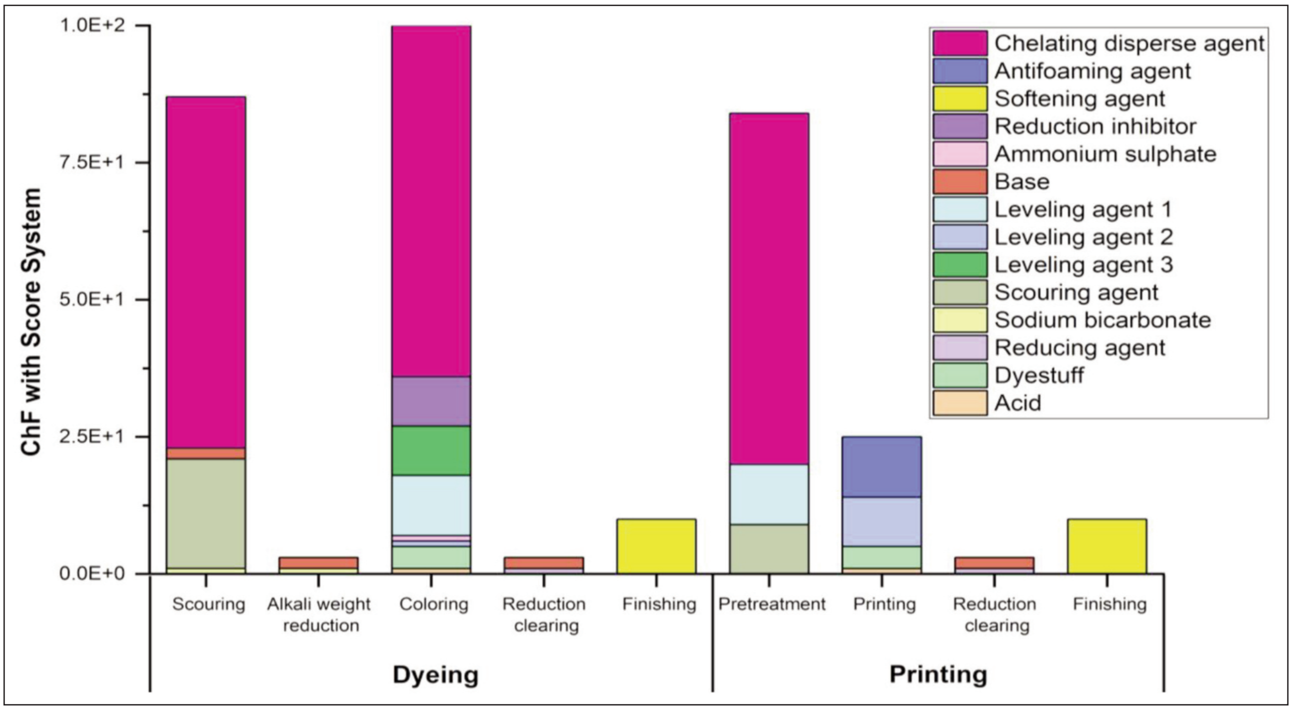

Fig. 4. Printing and dyeing process ChF of the polyester dress obtained with the Score System

Score system results

Figure 4 displays the toxic impact of the polyester dress in the dyeing and printing process (331). The Score System points out colouring (100), scouring (87), and pretreatment (84) as the three most significant procedures for environmental impacts, mainly because they all use chelating disperse agent in their production. The poor performance of the chelating disperse agent is due to the worst possible scores for bioaccumulation, biodegradability, and toxicity.

Strategy tool results

The ChF results with the Strategy Tool are illustrated in figure 5. Compared with the results of the previous

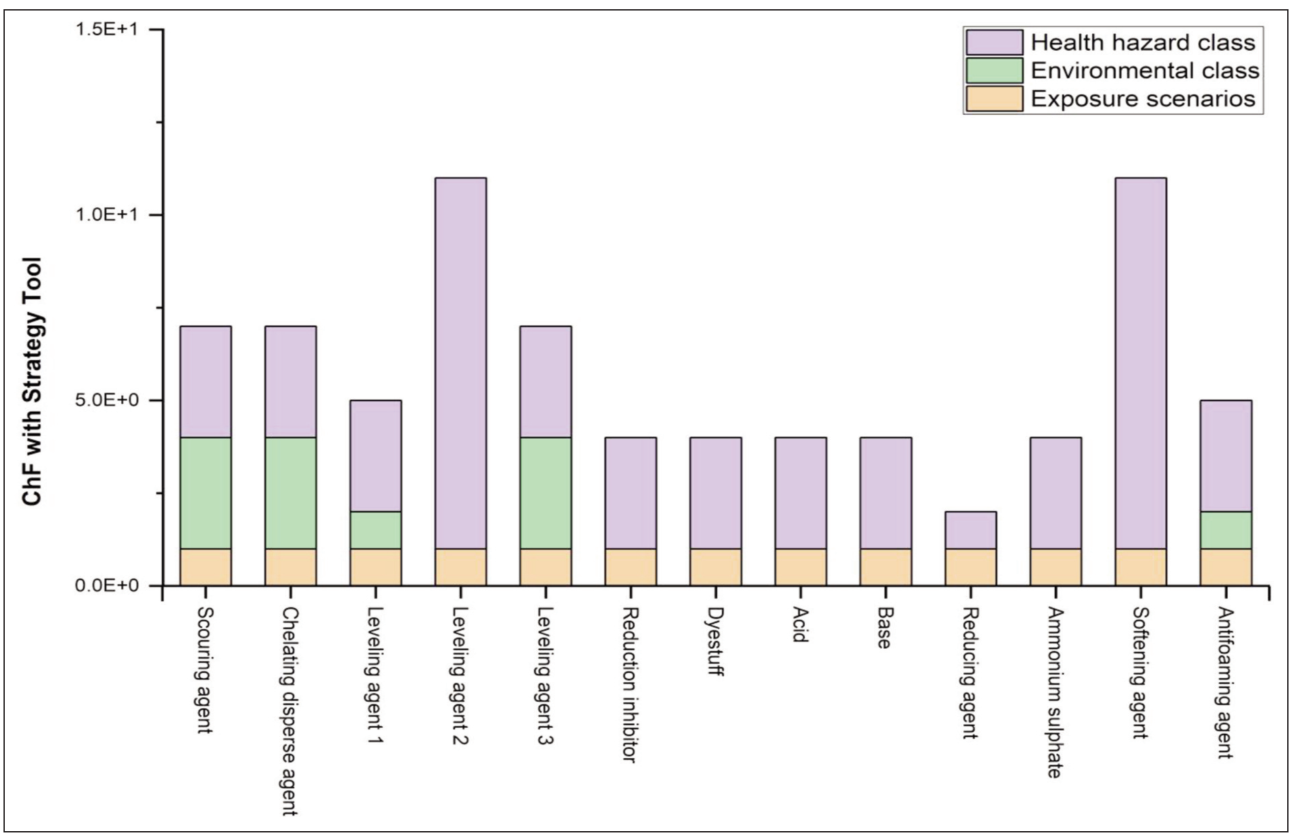

Fig. 5. Printing and dyeing process ChF of polyester dress obtained with the Strategy Tool

methods, the differences between the auxiliaries in this result are relatively minor. The Strategy Tool indicates that the levelling agent 2 and softening agent are the most significant textile auxiliaries based on health impact. If only environmental impact is considered, scouring agent, chelating disperse agent, and levelling agent 3 are the most important auxiliaries to be concerned about.

Comparison of the use and results from the methods

The four methods do not give a consistent assessment of chemicals in the dyeing and printing process. The difference in results can be explained by the difference in emphasis angle and embodiment scale of each method.

In the results with the Strategy Tool, the small difference in each of the auxiliaries is because this method mainly evaluates from the perspective of the type and number of auxiliaries used, and ignores the specific quality of chemicals used, which may lead to misguided assumptions that the choice of auxiliaries for each process is not important. The results of AMI and Score System are very similar in the order of the various processes, with the top three contributing procedures being scouring, colouring, and pretreatment, and the three least contributing procedures being alkali weight reduction and reduction clearing in dyeing and printing. The chelating disperse agent is the most influential auxiliary for both methods. These similarities show the commonality of the two methods in the assessment thread to a certain extent. However, the score of the chelating disperse agent in the result with USEtox is low, probably due to the uncertainty in the CF, which reflects the problem of excessive reliance on CF.

In terms of the assessment thread, both USEtox and AMI incorporate the persistence of chemical pollutants indirectly into the potential to cause harm, rather than treating persistence as a separate criterion like the Score System. The assessment thinking of the Strategy Tool is mainly classifying the risk of auxiliaries according to the risk labelling in the SDS, which focuses more on the protection of the people involved in the production and pays less attention to the environmental impacts caused by the chemical pollutants after production.

Regarding practical usability, the strategy tool is undoubtedly the most convenient method, especially for the auxiliary manager of the production side, but the cost is that the results are limited in science. Although the Score System is simple to use, its results do not accurately reflect the load in a specific area when compared to USEtox and AMI. USEtox is efficient enough for skilled ChF practitioners, and its main advantage is that it combines the fate results at different intervals with the ecotoxicity impacts, but the high integration of USEtox can inconvenience the ChF accounting process in the absence of CF. AMI is easier to use than USEtox in the quantification and evaluation of ChF, and it retains the science and efficiency of the fate results for chemical pollutants, but also gives the practitioner freedom in the core toxic effects.

CONCLUSIONS

The chemical pollutants emitted during the printing and dyeing process of the polyester dress have a serious impact on the environment. ChF accounting and evaluation can quantify the ecotoxicity impacts of chemical pollutants and identify the most important affecting procedures and auxiliaries. In this paper, four methods were used to calculate and evaluate the ChF of the polyester dress printing and dyeing process, and the practical usability and results of the four methods were compared. The ChF of the printing and dyeing process of a polyester dress calculated with USEtox, AMI, Score System, and Strategy Tool is 1585.51 PAF×m^3×day, 14089.04 L, 331, and 75, respectively. Scouring, colouring, pretreatment, and printing were identified as the major procedures contributing to ChF, with antifoaming agent and chelating disperse agent as the major auxiliaries contributing to ChF.

The two semi-quantitative methods, the score system and the strategy tool, are relatively easy to use, although the Strategy Tool is assessed on a more user-protective basis, so the results of the Strategy Tool are limited in their representativeness of environmental load. Compared to other methods, AMI ensures that the evaluation results are scientific while maintaining user-friendliness. Further investigation is desired on how the various approaches work together, and the combined results of various methods can be considered. It is important to explore the combination of user-friendliness and representativeness for the accounting and evaluation of ChF to guide the textile industry towards more green chemical management.

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