



Semi-Permanent Hair Dyes: Using an empirical model to optimize formulation efficacy

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Introduction

Over the past few years, the demand for semi-permanent hair color products has increased. The most challenging aspects of formulating a performing and stable semi-permanent hair-coloring product are shelf stability, color deposition, and color retention after repeated shampooing. In order to speed up the formulation process, it helps if several variables, such as the need for a solvent system, can be established at the beginning of the process. Thus, formulators can focus on the most difficult issues and offer consumers a product they can trust. The aim of this work is to create a predictive model that indicates whether a solvent system is required when formulating with basic dyes. It correlates the dyes solubility with the overall color performance (color deposition and color retention) according to the shade to be developed.

Methodology

The water solubility of the dyes was determined at room temperature with 12% of solvent, in order to have a homogeneous solution without any insolubilized dyes. Solubility Indexes (SI_{dyes}) were then classified into high, moderate, low and very low solubility.

The overall hair color performance of 24 conditioner formulations with basic dyes was evaluated on bleached and yak hair tresses. The shades selected contemplate 13 commonly used basic dyes and 11 combinations thereof. The tresses were pre-washed with shampoo for 30 seconds (12% SLES, pH 5.5) followed by application of 3 g of a conditioner (with and without solvent) for 20 minutes on 1 g of bleached and yak hair to evaluate color deposition after one application. Subsequent 3, 5, 7 and 10 shampoo cycles (12% SLES, pH 5.5, 30 sec) were done to evaluate color retention. For visual observation of the color, pictures were taken using DinoLite microscope. The CIE $L^*a^*b^*$ coordinates were used to identify color differences in the first application and after repeated shampooing.

The empirical model was created using the SI_{dyes} and concentrations in formulation according to the shade to be developed (Equation 1). The equation provides a number that was then validated against hair color performance on hair tresses, in order to determine whether the solvent system provides better color performance.

$$SI_{shade} = \frac{\{(\% Dye\ 1 \times SI_{Dye1}) + (\% Dye\ 2 \times SI_{Dye2})\}}{(\% Dye\ 1 + \% Dye\ 2)}$$

Equation 1. Empirical Model to optimize formulation efficacy



Results

The solvent system consists of an optimized blend of ingredients (Propylene Glycol (and) Benzyl Alcohol (and) Quaternium-80) added into the water prior to the addition of the dyes. The addition of a solvent can be a key ingredient for improved hair color performance and formulation stability, but using it may not be necessary for all formulations as the opposite result may be observed. The aim of this study was to determine if the addition of the solvent system will be improving or affecting the hair color formulation.

Basic dyes are water soluble cationic molecules with high affinity to the hair. There are several basic dyes in the market with a broad range of water solubility. The solubility of the dyes in the formulation has an important impact on shelf stability, color deposition and color retention after shampooing. Formulating shades that often require the combination of dyes is specially challenging. The water solubility was considered as a variable for the empirical model to optimize formulation efficacy.

Figure 1 shows the Solubility Indexes Classification, from 5 (high solubility) to 2 (very low solubility). The dyes were grouped and classified into high (5-8% w/w), moderate (2-4% w/w), low (1% w/w) and very low (lower than 0.75% w/w) solubility.



Figure 1. Basic Dyes Solubility Index (SI_{dyes}) Classification.

The hair color performance of conditioners with basic dyes was evaluated for 11 shades, referred as Pantone Colors, in order to validate the empirical model according to Equation 1. SI_{shade} was calculated for the Pantone Colors in order to validate the empirical model against hair color performance on hair tresses. Figure 2 and 3 show the color deposition on bleached hair after one application and color retention after subsequent shampoo cycles for Pantone 1395C (Figure 2) and Pantone 2217C (Figure 3) respectively.

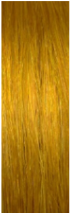
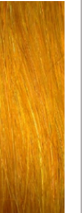
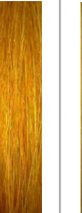
1 Application		After 3 shampoo cycles		After 5 shampoo cycles		After 7 shampoo cycles		After 10 shampoo cycles	
With 12% Solvent	Without Solvent	With 12% Solvent	Without Solvent	With 12% Solvent	Without Solvent	With 12% Solvent	Without Solvent	With 12% Solvent	Without Solvent
									

Figure 2. Color deposition after 1 application and color retention after 3, 5, 7 and 10 shampoo cycles for Pantone 1395C.

The SI_{shade} of Pantone 1395C was 2.66. For Pantone 1395C, formulation with solvent provided a more developed color after 1 application. After 10 shampoo cycles the color is lighter and yellower and the color retention with solvent is improved. The use of the solvent provided better color performance, with better color deposition and retention.



1 Application		After 3 shampoo cycles		After 5 shampoo cycles		After 7 shampoo cycles		After 10 shampoo cycles	
With 12% Solvent	Without Solvent	With 12% Solvent	Without Solvent	With 12% Solvent	Without Solvent	With 12% Solvent	Without Solvent	With 12% Solvent	Without Solvent
									

Figure 3. Color deposition after 1 application and color retention after 3, 5, 7 and 10 shampoo cycles for Pantone 2217C.

The SI_{shade} of Pantone 2217C was 3.84. For Pantone 2217C, formulation with solvent provided a slightly more developed color after 1 application. After 10 shampoo cycles the color is lighter and yellower, with no significant difference between formulation with and without solvent. The use of the solvent did not improve color performance for this shade.

As predicted, for high and moderate solubility dyes, the solvent system did not improve the overall color performance. For low solubility dyes, the solvent system provided better overall performance, with better color deposition and better color retention on hair. For the very low solubility dyes, the best color deposition was observed with solvent system; however, color retention was still an issue. The empirical model was validated against hair color performance and can be used to predict whether the solvent system is needed in formulation. For shades with SI_{shade} values lower than 3.0, a better color performance with solvent system is expected. For SI_{shade} values higher than 3.7, the solvent system is not expected to improve the color performance. For SI_{shade} values between 3.1 and 3.7, it is hard to conclude on the effect of the solvent system-for both color deposition and color retention.

Conclusion

We have demonstrated that the use of the solvent system has an important impact on hair color performance, affecting color deposition and color retention. Formulation requirements are different according to the shade to be developed, and the empirical model created can be used to predict whether the solvent is recommended or not – taking into account dye concentration and solubility. The results are formulation and pH dependent, and the concentration of the solvent system may also affect the hair color performance.

About the speaker



Raissa Bittar Mastello is an Application Technologist-Hair Specialist for Sensient Beauty North America. She is responsible for developing hair care and color application prototypes, assisting customers with formulation issues, and works to maximize the efficacy of Sensient's portfolio ingredients for hair color and care. Raissa began her career as a R&D scientist for Solvay, focusing on surfactants, emollients and actives for hair care products. As a scientist, she gained proficiency

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in hair care testing and sensory analysis. In 2017, she joined the R&D team in Sensient Brazil Hair Care Excellence Center, later transferring to Sensient Beauty North America Applications Team, based in New Jersey. Raissa received her Bachelor's degree in Pharmacy and Biochemistry from Universidade Estadual Paulista (UNESP) in São Paulo, Brazil in 2014.