Quantification of Color Variation of Various Esthetic Restorative Materials in Pediatric Dentistry

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Ab s t rac t

Aim of study: The goal of this paper is to find an association between the staining capacity of dental restorations used in pediatric patients and food items and to develop an optimum model to predict the most informative factor that causes the highest amount of color change through machine learning algorithms.

Background: Color changes in restorative materials occur as a result of intrinsic and extrinsic factors, such as the type of restorative material, food items used, polished status of the material, and time interval.

Materials and methods: This was an "*in vitro* study" conducted at Aligarh Muslim University, Aligarh, Uttar Pradesh, India. The study included 200 specimens, that is, 40 in each group A (orange juice), group B (Amul Kool Café), group C (Pepsi), group D (Amul Kesar Milk), and group E (artificial saliva). The materials were glass ionomer cement (GIC), resin-modified glass ionomer cement (RMGIC), microhybrid composite resin, and nanohybrid composite resin. These were further divided into polished and unpolished groups. The optimum modeling of the prediction of color change in materials by different effective factors was done by machine learning decision tree. We applied two algorithms: Chi-square automatic interaction detector (CHAID) and classification and regression tree (CART). In prediction modeling in the decision tree by CHAID and CART, color change is taken as the dependent variable, and group (type of restorative material), food items, time interval, and polished status are taken as independent variables.

Results: The various beverages caused significant color variation due to different pigmentation agents. The agent that caused the highest color change was Kool Café. The Kesar Milk had the lowest pigmentation capacity. The greatest color variation was found on Glasionomer FX-II submerged in Pepsi and the least on Ivoclar Te-Econom Plus in Kesar Milk. The mean absolute error for the training dataset in the CART model and CHAID model is 0.379 and 0.332, and for the testing data set, it is 0.398 and 0.333, respectively. Therefore, the prediction of color change by the CHAID model is optimum, and we found that the restorative materials have a maximum predictor importance of 0.86 (86%), time interval 0.07 (7%), food items 0.04 (4%), and polished status has the least importance, that is, 0.03 (3%).

Conclusion: The staining capacity of restorative material highly depends on the material itself, the initial time interval, and least on the food items used. **Clinical significance:** The clinical performance of dental restorations could be affected by various beverages consumed by children. This study thus provides important clinical insights into esthetic dentistry by offering valuable information on long-term color stability and the effect of polishing on common esthetic restorative materials used in pediatric dentistry.

Keywords: Chi-square automatic interaction detector, Classification and regression tree, Color change, Esthetic restorations, Machine learning. *International Journal of Clinical Pediatric Dentistry* (2024): 10.5005/jp-journals-10005-2905

INTRODUCTION

The restoration is one of the treatment modalities for managing dental caries, and restorative dental materials are in high demand nowadays. Due to newer developments in restorative dentistry and the increasing demand for improved esthetic dental restorative materials, extensive research and development have been conducted around the globe to find ideal dental restorative materials for children as well as adults.¹ A wide variety of newer esthetic restorative materials are available to the pediatric dentist, including glass ionomer cements (GICs), resin-modified glass ionomer cements (RMGICs), and composite resins. However, the success or failure of any dental esthetic restoration in the oral cavity depends on the esthetic outcome and its maintenance over a long period, considering the continuous exposure of restorative materials to saliva, fluids, and food intake, which can lead to a change in the color of the restorative material.^{[2](#page-10-3)}

Glass ionomer cement was developed by Wilson and Kent in the 8th decade of the 20th century. Glass ionomer cement is very common in pediatric dental clinics due to its desirable properties, such as the release of fluoride, which acts as an anticaries agent, and its adhesion to tooth structure. The major disadvantages of GICs are their high technique sensitivity when applied in the oral cavity and their susceptibility to deterioration by organic acids, which are continuously released from the microbial biofilm

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and food degradation in the oral cavity. 3 Resin-modified glass ionomer cements was introduced in the market in the late 1980s, offering advancements in the physical properties of traditional GICs.[4](#page-10-1) Composite resins, developed in the 1970s, have since

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been available for direct esthetic restorations of both anterior and posterior teeth. Polymer composites are commonly used as esthetic restorative materials due to their excellent appearance and minimal susceptibility to microbial attack.^{[5](#page-10-4)}

Owing to the increasing attention being paid to dental esthetics, research is essential to better understand the features of different restorative materials and to improve their physical attributes, such as color stability.^{[6](#page-10-5)} Daily exposure of the oral cavity to foods containing a variety of staining agents can alter the color or modify the exposed surfaces of restorative materials, leading to poor esthetic results[.7](#page-10-6)

In esthetic degradation of restorative materials, both intrinsic and extrinsic factors may be associated. Changes in the resin matrix and the coupling between the resin matrix and the filler particles induce discoloration. The intrinsic color of composite materials can also vary as a result of aging under various physicochemical conditions such as visible and ultraviolet irradiation, temperature fluctuations, and humidity.^{[8](#page-10-7)} Mechanical wear and chemical breakdown can produce surface roughening, reducing the shine of the restoration and increasing extrinsic stains. The yellowing of materials appears to be related to multiple factors.⁹

A digital spectrophotometer is used to evaluate color changes in tooth-colored restorative materials. According to the Commission Internationale de l'Éclairage L*a*b* color space (CIELAB), all colors in nature are created by combining three primary colors (red, blue, and green) in specific proportions. This approach is commonly utilized by researchers in dentistry to examine various materials in terms of color change.¹⁰

Gordon V Kass devised the Chi-square automatic interaction detector (CHAID) technology in 1980. CHAID is a tool for discovering the link between variables. CHAID analysis creates a predictive model or tree to help find how variables can best combine to explain the outcome in the given dependent variable.

One of the variants of the decision tree algorithm is classification and regression tree (CART). It can perform tasks such as regression and classification. Scikit-Learn employs the CART algorithm to train decision trees (also known as "growing" trees). CART was created by Richard Olshen, Jerome Friedman, Leo Breiman, and Charles Stone in 1984. It uses a predictive algorithm, which is used in machine learning to describe how target variable values can be anticipated based on other factors. It is a decision tree in which each fork is divided into predictor variables, and each node ends with a prediction for the target variable.

The formulated research hypothesis of the present study was: "Different solutions would not affect the color stability of toothcolored restorative materials and there would be no difference in the color stability among the different esthetic dental restorative materials used in the study."

MATERIALS AND METHODS

The study was approved by the Institutional Ethics Committee of the Faculty of Medicine (IECJNMC/442 dated 19.10.2021). The four esthetic restorative materials were evaluated for color stability: (A) RMGIC, (B) conventional GIC, (C) microhybrid composite, and (D) nanohybrid composite [\(Table 1](#page-1-0)). These materials were tested in the following liquid food products: (A) Amul Kool Café, (B) Amul Kesar Milk, (C) orange juice, (D) artificial saliva (taken as control), and (E) Pepsi ([Table 2\)](#page-1-1).

Sample Size

It was revealed from the literature survey that the expected standard deviation of color changes for group I (liquid solutions) and group II (restorative materials) is 1.2 and 1.6, respectively, with a mean difference of 1.8 between the two groups. When the given formula was used with OpenEpi, Version 3 software, it was found that the total sample size needed was 200, equally divided between the four restorative material groups, with 50 in each group.

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n = \frac{(\sigma_1^2 + \sigma_2^2)(Z_{1-\alpha/2} + Z_{1-\beta})^2}{\Delta^2}
$$

 $Z_{1-\alpha/2}$ = Two-sided *Z*-value (e.g., *Z* = 1.96 for 95% confidence interval) and $Z_{1-\beta} = 0.841$ for power = 80%.

Preparation of the Specimens

Two hundred test specimens were prepared using a customized Teflon ring mold with dimensions of 8 mm (inner diameter) and 2 mm (thickness). The GIC and RMGIC samples were prepared by inserting the restorative materials into the mold over a thick glass slab placed between two mylar strips and glass slabs, and were allowed to set for a period of time according to the manufacturers'

[Table 2:](#page-1-3) Liquid food items with ingredients used in the present research

	Liquids	Ingredients
1	Orange juice (Real fruit juice, Dabur)	Water, orange juice concentrate (12.45%), sugar, vitamins, acidity regulator (Ins 330) and salt, organic acids such as citric, maleic, and ascorbic acids
2	Amul Kool Café (Amul, Gujarat)	Milk solids, coffee, sugar, permitted stabilizer, added flavors
3	Pepsi (PepsiCo, Inc., New York)	Carbonated water, high fructose corn syrup, caramel color, sugar, phosphoric acid, caffeine, citric acid, and natural flavors
4	Amul Kesar milk (Amul, Gujarat)	Toned milk, milk solids, sugar and artificial coloring and flavoring agents (kesar)
5	ICPA Wet Mouth Solution (ICPA)	Sodium carboxy methyl cellulose 0.5% w/v, glycerine 30% w/v in a flavored base

instructions. Composite samples were prepared similarly, with the restorative materials inserted into the mold over a thick glass slab placed between two mylar strips and glass slabs. The material was photopolymerized by a light emitting diode (LED) curing source light for 40 seconds at 800 mW/cm² (SmartLite Focus LED light cure, Dentsply Sirona). The light activation time was carried out in accordance with the manufacturer's instructions. Finishing and polishing were performed on only 25 standardized specimens of each restorative material using 1000-grit silicon carbide paper. The remaining 100 specimens (25 from each group) were left unpolished. Standardization was ensured using a digital electronic caliper.

Following preparation, the samples were immersed in distilled water for a whole day to rehydrate them. The baseline color measurements were taken using a digital spectrophotometer (VITA Easyshade V) after rehydration. The color parameters used for evaluations were based on lighting view geometry (d/10) and average daylight (D65: 6504 K). Readings were recorded using the CIELAB, and calibration was performed against a white reference.

Ten standardized specimens of each restorative material (five polished and five unpolished) were immersed in each liquid food product and the control solution, in specific containers, and stored at room temperature. The temperature was controlled using a thermostatically controlled incubator for 4 hours daily for 75 days continuously. All disks were subjected to color measurements using a spectrophotometer repeatedly by the same operator. The intraexaminer agreement of the data was tested by Cronbach's α at 0.98. All measurements were done at room temperature, with the baseline measurement on day 1 (T1), and then on day 7 (T7), day 15 (T15), day 30 (T30), day 45 (T45), day 60 (T60), and day 75 (T75).

Optimum Modeling for Forecasting

The optimum modeling was done using a machine learning decision tree. We applied two algorithms: CHAID and CART. CHAID analysis constructs a predictive model to help decide how factors should combine to best explain the outcome in the given dependent variable. CART, a variant of the decision tree method, is used for similar purposes.

Based on an attribute's threshold value, nodes in the decision tree divide into sub-nodes. The training set is the root node, which is divided into two by considering the best attribute and

[Fig. 1:](#page-2-2) Mean and standard deviation of color change in various restorative materials

threshold value. Additionally, the same rationale is used to divide the subgroups. This process continues until the tree reaches its final pure subset or has as many leaves as it can possibly have.

Machine Learning Method Accuracy

The accuracy of the predictive model is calculated using the mean absolute error and standard deviation. The collected data is divided into training (70%) and testing (30%) sets. A total of 1,400 rows of data were used, with 975 rows in the training set and 425 rows in the testing set.

The IBM Statistical Package for the Social Sciences (SPSS) software program (SPSS 16 Inc, Chicago, Illinois, United States) was used to analyze the data. The Shapiro–Wilk test was utilized to verify the data's normality. For color change, descriptive statistics such as mean, standard deviation, and standard error of the mean (SEM) were computed. Tukey's honestly significant difference (HSD) test was performed at the significance level (*p* < 0.05) with a 95% confidence interval after univariate analysis in the general linear model was used to evaluate the means of color change across various materials and solutions at baseline and at different time intervals. Significant values are reported up to two decimal places.

RESULTS

The overall mean and standard deviation of color change are as follows: GIC is 16.07 \pm 2.01, RMGIC is 14.73 \pm 1.45, microhybrid composite is 8.00 ± 0.96 , and nanohybrid composite is 8.11 ± 1.29 for all the liquid food products ([Fig. 1\)](#page-2-0). When comparing all the restorative materials, the mean differences in color change are: between GIC and RMGIC is 1.33; between GIC and microhybrid composite is 8.06; between GIC and nanohybrid composite is 7.95; between RMGIC and microhybrid composite is 6.73; between RMGIC and nanohybrid composite is 6.62; and between microhybrid composite and nanohybrid composite is –0.10 ([Table 3](#page-2-1)). These values are highly significant (*p* < 0.01). Thus, the sequence of color stability is microhybrid composite > nanohybrid composite > $RMGIC > GIC.$

When compared with the control solution, Wet Mouth, the overall maximum change in color was caused by Kool Café solution, with a mean difference of 0.35. This was followed by orange juice with a mean difference of 0.22, then Pepsi with 0.05, and the minimum color change was seen in Kesar Milk solution with a mean difference of 0.03. These values are highly significant (*p* < 0.01). The sequence of staining caused by solutions, from maximum to minimum, is Kool Café > orange juice > Pepsi > Kesar Milk for overall materials and time intervals.

In the prediction modeling using the CHAID model, color change was taken as the dependent variable, with material (type of restorative material), food items, time interval, and polished status as independent variables. We found that material had the highest

[Table 3:](#page-2-3) Distribution of mean and standard deviation of color change in different restorative materials

Restorative materials N Mean Standard deviation Standard error				
GIC	50	16.07	2.01	0.10
RMGIC	50	14.73	1.45	0.08
Microhybrid composite	50	8.00	0.96	0.05
Nanohybrid composite	50	8.11	1.29	0.07

predictor importance at 0.86 (86%), followed by time interval at 0.07 (7.0%), food items (solution) at 0.04 (4%), and polished status had the least importance at 0.03 (3.0%) [\(Figs 2](#page-3-0) and [4\)](#page-7-0).

In the prediction modeling using the CART model, where color change was the dependent variable and material (type of restorative material), food items, time interval, and polished status were independent variables, we found that material had the highest predictor importance at 0.8945, followed by food items at 0.0488, time interval at 0.0377, and polished status had the least importance at 0.02 ([Figs 3](#page-3-1) and [5](#page-9-0)).

The mean absolute error for the training dataset in the CART model is 0.379 and for the testing data set is 0.398. In contrast, the CHAID model has a mean absolute error of 0.332 for the training data set and 0.333 for the testing data set, which is lower. Therefore, the prediction of color change by the CHAID model is optimum.

Dis c u s sio n

The development of restorative materials has been attributed to a rise in patient demand for enhanced aesthetics. Resin restorative materials are a major concern due to their propensity to discolor, necessitating restoration renewal. Color stability thus gains equal importance with other physical or mechanical attributes.¹¹

In the present research, for unpolished and polished conventional GIC, the maximum color change was seen in Pepsi, and the minimum color change was seen in orange juice. This change can be attributed to the acidic effect of Pepsi, which caused softening and dissolution of the glass particles surrounding the matrix. This produced a rough surface, increasing the surface area for the adsorption of pigments and potentially causing staining[.12](#page-10-14) Similar results were reported by Adusumilli et al.,^{[1](#page-10-2)} which concluded that carbonated drinks showed the highest color change among immersion media for GIC. Shalan et $al.^{13}$ concluded that cola beverage showed the maximum color change, while chocolate milk and orange juice showed the minimum color change for GICs.

In the present study, unpolished and polished RMGIC showed the maximum color change in Amul Kool Café. The minimum color change for unpolished RMGIC was seen in Pepsi, and for polished RMGIC, it was seen in Amul Kesar Milk. These alterations could be explained by the materials' high surface texture or high-water absorption rate, which both increase staining susceptibility.^{14,15} The study conducted by Tunc et al.¹⁶ concluded that chocolate milk caused the maximum color change in RMGIC, which is in accordance with this study. In contrast, Penumatsa¹⁷ concluded that RMGIC showed the least color change in chocolate milk and the maximum color change in ice candy.

In the present study, the maximum color change for unpolished and polished microhybrid composite was seen in Pepsi, and the minimum color change for unpolished and polished microhybrid composite was seen in Amul Kesar Milk. Filler particles in microhybrid composites typically have a size of no >1 µm. As a result, these materials have a high filler loading, which produces low polymerization shrinkage and high mechanical characteristics while preserving a smooth surface upon polishing.^{18[,19](#page-11-2)} While inorganic glass fillers can only absorb water on the surface of a material, the resin matrix of composite materials can absorb water from the environment into most of the substance's structure.^{[20](#page-11-3)} Excessive water sorption might shorten the lifespan of a resin composite by hydrolyzing the silane, expanding and plasticizing the resin component, and promoting the creation of microcracks.²¹ Similar results were seen in a study conducted by Bansal et al., 22 22 22 where Coca Cola caused the highest discoloration and surface roughness in resin composites. A study conducted by Usha et al.⁷ concluded that microhybrid composites showed the maximum color change in turmeric powder and the least in saffron extract and tandoori powder. Since saffron is the main coloring agent in Amul Kesar Milk, this study is in accordance with the present study.

In the present study, the maximum color change for unpolished and polished nanohybrid composite was seen in Amul Kool Café, and the minimum color change for unpolished and polished nanohybrid composite was seen in Amul Kesar Milk. The filler particles in nanohybrid composites typically have a size of about 1 nm. Triethylene glycol dimethacrylate (TEGDMA), which is present in nanohybrid composite, causes greater water sorption and, as a result, a lower degree of color stability. Stain is most likely to penetrate through microcracks and microvoids at the interface between the filler and the matrix. 23 23 23 The surface roughness resulting from wear or chemical deterioration can also impact gloss, which in turn can intensify extrinsic staining.^{[24](#page-11-7)} Similar results were seen in a study carried out by Ozera et al.,²⁵ who concluded

[Fig. 3:](#page-3-2) Prediction importance of CART model **[Fig. 2:](#page-3-3)** Prediction importance of CHAID model

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that coffee, which is also a constituent of Amul Kool Café, caused the maximum color change in nanohybrid composites. A study conducted by Usha et al. 7 7 concluded that nanohybrid composites showed the maximum color change in turmeric powder and the least in saffron extract and tandoori powder. Since saffron is the main coloring agent in Amul Kesar Milk, this study is in harmony with the present study.

A study conducted by Savas et al. 3 concluded that RMGIC is more color stable than conventional GIC. Mohan et $al.^{21}$ and Lopes et al. $²$ $²$ $²$ found that composites are more color stable than</sup> conventional and RMGICs due to their hydrophobic nature, which shows greater stain resistance than hydrophilic materials like GICs. In contrast, Penumatsa¹⁷ found that RMGICs show more resistance to staining than nanocomposite resins. Kathiria et al.^{[26](#page-11-9)} stated that GICs have high water content, which prevents water from being absorbed into the bulk of the material, making it less susceptible to color change. Their study concluded that composites showed more color change than GIC. Similar results were seen in a study performed by Bezgin et al. 24 24 24 Faghihi et al. 27 27 27 concluded that nanohybrid composite resin had a greater color change in comparison to GIC.

A study conducted by Tunc et al.¹⁶ concluded that GIC is the most color stable, followed by composite resins, with RMGICs being the least color stable. In contrast, Tan et al. 28 28 28 and Ulusoy et al. 12 concluded that nanohybrid composites are more color stable than RMGICs.

Assaf et al.^{[8](#page-10-7)} reported that microhybrid composites are more color stable than nanohybrid composites. However, Curtin et al. 23 23 23 and Alkhadim et al.⁹ found that nanohybrid composites are more color stable than microhybrid composites.

Elwardani et $al.^{29}$ $al.^{29}$ $al.^{29}$ concluded that Coca-Cola caused the highest color change, followed by orange juice. Majeti et al.^{[30](#page-11-13)} and Deljoo et al.³¹ found that coffee resulted in the greatest color change in restorative materials. Savas et al.^{[3](#page-10-0)} reported that chocolate milk caused the most staining, with cola and orange juice following.

Polishing the restorative materials showed greater color stability than unpolished materials in our study. This finding is supported by Deljoo et al.³¹ and Beltrami et al.,^{[32](#page-11-15)} where polished specimens exhibited lower discoloration compared to unpolished specimens.

According to the results, the research hypothesis that "different solutions would not affect the color stability of tooth-colored restorative materials and that there would be no difference in the color stability among the different esthetic dental restorative materials used in the study" was rejected.

There are certain limitations to the study. As this is an *in vitro* study, masticatory and other forces were not considered, which may also affect color stability in the long run.

CONCLUSION

- Within the limits of this current study, it was concluded that microhybrid composite was the most color-stable restorative material, followed by nanohybrid composite, RMGIC, and GIC, which was the least color-stable when immersed in various beverages.
- The maximum staining in all restorative materials was caused by Kool Café, followed by orange juice, Pepsi, with Kesar Milk causing the least staining.

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