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Original Article

Evaluation of Oxidizable Substance Interaction Associated with Orthodontic Clear Aligners and an Acrylic Material: A Preliminary *in vitro* Study

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Main Points

- All tested materials showed measurable interaction within 24 hours, although the extent varied among materials.
- The greatest interaction of oxidizable substances was observed in ClearQuartz, whereas SmartTrack exhibited the lowest levels.
- Potassium permanganate may be useful as a simple screening approach, but it does not identify or quantify specific compounds.

ABSTRACT

Objective: This study aimed to comparatively evaluate the interactions of oxidizable substances associated with different orthodontic aligner materials using potassium permanganate ($KMnO_4$).

Methods: In this study, materials from three different clear-aligner manufacturers (SmartTrack, ClearQuartz, and Scheu Dental CA Pro+) and one acrylic block were used. The materials were mechanically fragmented and exposed to $KMnO_4$, a strong oxidizing agent. Potassium permanganate solutions were prepared at six concentrations (1.24 mM, 0.62 mM, 0.31 mM, 0.16 mM, 0.08 mM, 0.04 mM) to establish a calibration curve (R^2=0.9999). Based on this calibration, 0.2 mM and 1 mM solutions were selected for the experimental phase. The color change was evaluated spectrophotometrically at 1, 4, and 24 hours to assess interactions with oxidizable substances.

Results: The amount of oxidizable substances interacting with $KMnO_4$ was estimated in mM. Oxidizable substances were detected in all samples (Acrylic Block 0.0723 mM, ClearQuartz 0.0826 mM, Scheu Dental CA Pro+ 0.0584 mM, SmartTrack 0.0271 mM); however, the estimated levels of oxidizable-substance interaction varied among samples. The highest level was observed in ClearQuartz at 24 hours.

Conclusion: Orthodontic aligner materials exhibit varying levels of interaction with oxidizable substances, particularly during the first 24 hours. The method may serve as a simple preliminary screening tool. Future studies should investigate the composition of the released substances using more sensitive analytical methods.

Keywords: Clear aligners, oxidizable substances, potassium permanganate, polymer degradation

INTRODUCTION

In recent years, clear aligners have been widely used in orthodontics as an alternative to traditional fixed appliances.[1] These clear aligners should be used for at least 22 hours per day to deliver sufficient force to achieve optimal orthodontic treatment outcome. The number of companies producing clear aligners is increasing. As the number of companies increases, clear aligner treatments and the materials used are also evolving.[2,3]

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Bisphenol A (BPA) is an industrial chemical used in the production of polycarbonate plastics and epoxy resins.[4] Bisphenol A is a well-known endocrine disruptor with hormone-like effects. Due to its estrogen-like structure, BPA may cause hormonal imbalance.[4] In addition, BPA can cause oxidative stress, deoxyribonucleic acid damage, apoptosis, and immune system suppression.[5-7] Recent studies have also examined possible relationships between BPA exposure and some types of cancer.[5-7]

Clear aligners used in orthodontics are generally manufactured from thermoplastic materials based on polyurethane, such as ClearQuartz (Straumann Group, Switzerland) and SmartTrack (Align Technology, USA), or polyethylene terephthalate glycol, such as CA Pro+ (Scheu Dental, Iserlohn, Germany).[8,9]

Despite growing evidence of chemical leaching from aligner materials, most analytical techniques for identifying specific compounds require advanced instrumentation and are not always practical for routine screening.[10] Potassium permanganate ($KMnO_4$), a strong but non-specific oxidizing agent, has been proposed as a simple method for estimating total oxidizable substance interaction associated with thermoplastic polymers by measuring discoloration resulting from oxidation-reduction reactions.[10]

In a previous study, BPA release from three commercially available orthodontic aligner brands was evaluated in artificial saliva, artificial gastric fluid, and ethanol.[11] Samples were analyzed using high-performance liquid chromatography (HPLC)-tandem mass spectrometry, and all brands released BPA, with great variability.[11] In another study, four different clear aligners were sectioned and immersed in glass vials containing ethanol at different concentrations, and the leached substances were detected by gas chromatography-mass spectrometry (GC-MS).[12]

However, there is ongoing debate about whether other components of clear aligners degrade due to oral temperature, salivary enzymes, and mechanical abrasion, releasing of a variety of oxidizable products over time.

In light of the literature, the present study aimed to evaluate the interaction of oxidizable substances released from different brands of clear aligners and a conventionally used acrylic material, using a simple biochemical assessment method that can be performed under basic laboratory conditions. By comparing the interaction profiles of these orthodontic materials using a practical, accessible approach, this study sought to provide relevant insights into their potential chemical interactions and biocompatibility. The null hypothesis was that there would be no significant difference in the interaction of oxidizable substances among the tested materials.

METHODS

Orthodontic Material Selection

In this study, three thermoformed clear-aligner materials from different brands and one acrylic material commonly used in removable orthodontic appliances were evaluated. The clear aligner materials included ClearQuartz (Straumann Group, Switzerland), SmartTrack (Align Technology, USA), and CA Pro+ (Scheu Dental, Iserlohn, Germany). The aligners were obtained directly from the manufacturers. All samples were unused and had not been exposed to clinical conditions, and were removed from their original packaging immediately before testing without further processing. The acrylic material (Integra Orthodontic Acrylic, BGD, Türkiye) was fabricated in block form by an orthodontic laboratory in İstanbul, Türkiye.

Sample Solution Selection

Potassium permanganate was used to evaluate the interaction of oxidizable substances because of its simplicity, applicability as a preliminary screening method, and its well-established role as a strong but non-specific oxidizing agent.[10]

Oxidizable Substance Interaction Experiment

Preparation of Orthodontic Materials

The materials were mechanically fragmented with a slow-speed handpiece (KAVO, Biberach, Germany) fitted with a 12-blade tungsten carbide bur (Meisinger, Neuss, Germany) at 25,000 rpm (Figure 1). Fragmentation was performed to standardize the surface area of the specimens and enhance their interaction with the $KMnO_4$ solution in this preliminary screening model. This approach may increase the surface area and potentially overestimate interactions with oxidizable substances compared with those under clinical conditions. To prevent contamination, unused, a new sterilized bur was used for each material. A standardized sample weight of 1 g was prepared for each specimen.

Figure 1. Representative image of the fragmented ClearQuartz sample prepared for the potassium permanganate ($KMnO_4$) assay.

Potassium Permanganate Sample Preparation

Potassium permanganate solutions were prepared using distilled water (IsoLab, extra pure, 960.172). For calibration, six different concentrations (1.24 mM, 0.62 mM, 0.31 mM, 0.16 mM, 0.08 mM, and 0.04 mM) were prepared by serial dilution. Spectrophotometric measurements were performed at a wavelength of 525 nm. A calibration curve was constructed using these standard solutions, and linear regression analysis demonstrated an excellent linear relationship between concentration and absorbance (absorbance =2.578× Concentration + 0.0717; R^2=0.9999). The absorbance values obtained from the experimental samples were converted into Potassium permanganate concentrations using the rearranged calibration equation:

Concentration (mM) = (Absorbance - 0.0717)/2.578.

Based on the validated linear calibration range, 0.2 mM and 1 mM $KMnO_4$ solutions were selected for the experimental phase, as both concentrations fell within the calibration range and were suitable for the experimental conditions.[10]

Assessment of Discoloration

All experiments were conducted under controlled laboratory conditions at 37 °C. A fixed sample-to-solution ratio of 1 g of material per 100 mL of $KMnO_4$ solution was used for all groups to ensure consistency. All solutions were prepared in distilled water at approximately neutral pH (pH ≈ 7). A negative control consisting of $KMnO_4$ solution without any test material was included to determine baseline absorbance values.

Color change was evaluated spectrophotometrically at 1, 4, and 24 hours to assess interaction with oxidizable substances.

Ethical Approval and Consent

Ethical approval for this study was obtained from the İstanbul Kent University Ethics Committee (approval no: 2025-10, date: 10.12.2025). All procedures were conducted in accordance with relevant ethical guidelines and institutional standards. As no biological or patient-derived materials were used and the study was performed *in vitro*, informed consent was not required.

Statistical Analysis

This study was designed as a preliminary investigation to observe interactions between oxidizable substances in different orthodontic materials under standardized laboratory conditions. Each material was tested in 0.2 mM and 1 mM $KMnO_4$ solutions, and measurements were recorded after 1 hour, 4 hours, and 24 hours. Since the same experimental setup was monitored over time, the measurements reflect changes observed within each material group rather than the results of independent replicate experiments.

Changes in $KMnO_4$ concentration during the observation period were used to compare the behavior of the tested materials. Lower $KMnO_4$ values were associated with greater interaction with oxidizable substances. The purpose of this preliminary study was to identify general patterns and compare the materials under the same conditions.

Because independent replicate experiments were not conducted, statistical comparisons were not performed. The findings are therefore presented descriptively.

RESULTS

The fragmented material samples were exposed to 0.2 mM and 1 mM $KMnO_4$ solutions. Color change was measured spectrophotometrically (PG Instruments T80+, UK) at 1, 4, and 24 hours.

Oxidizable substances were detected indirectly in all samples, with variations across materials and time intervals. The amount of oxidizable substance interacting with $KMnO_4$ was estimated in mM from absorbance values using the calibration curve. Progressive discoloration over time was observed, corresponding to a decrease in $KMnO_4$ concentration and indicating increased interaction with oxidizable substances. The greatest change was observed in the ClearQuartz group at 24 hours, whereas the smallest change was recorded in the SmartTrack group. The quantitative results are presented in Table 1.

Table 1. Measured oxidizable substance levels (mM) calculated based on $KMnO_4$ reduction

Materials	1 hour concentration (mM)	4 hour concentration (mM)	24 hour concentration (mM)	Concentration level
Blank	1.00	1.00	**1.00**	1 mM
Acrylic Block	1.00	0.99	**0.94**	1 mM
ClearQuartz	0.96	0.89	**0.71**	1 mM
Scheu Dental	0.98	0.96	**0.89**	1 mM
SmartTrack	1.00	1.00	**0.98**	1 mM
Blank	0.20	0.20	**0.20**	0.2 mM
Acrylic Block	0.20	0.18	**0.12**	0.2 mM
ClearQuartz	0.17	0.16	**0.09**	0.2 mM
Scheu Dental	0.18	0.14	**0.12**	0.2 mM
SmartTrack	0.19	0.18	**0.17**	0.2 mM

Lower $KMnO_4$ concentration values indicate greater interaction of oxidizable substances.
$KMnO_4$, potassium permanganate.

In the 0.2 mM $KMnO_4$ solution, all materials showed progressive discoloration, indicating a reduction in $KMnO_4$ concentration (Figure 2).

In the 1 mM $KMnO_4$ solution, a similar trend was observed, with increasing discoloration over time. The greatest change occurred in the ClearQuartz group at 24 hours, whereas the SmartTrack group showed only minimal variation (Figure 3).

DISCUSSION

The use of clear aligners has increased substantially in recent years, and this trend has been accompanied by continuous developments in material composition. Clear aligners are thermoplastic materials thermoformed to fit three-dimensional dental models; their composition varies among manufacturers. As a result, their potential biological effects remain a subject of ongoing investigation.[8]

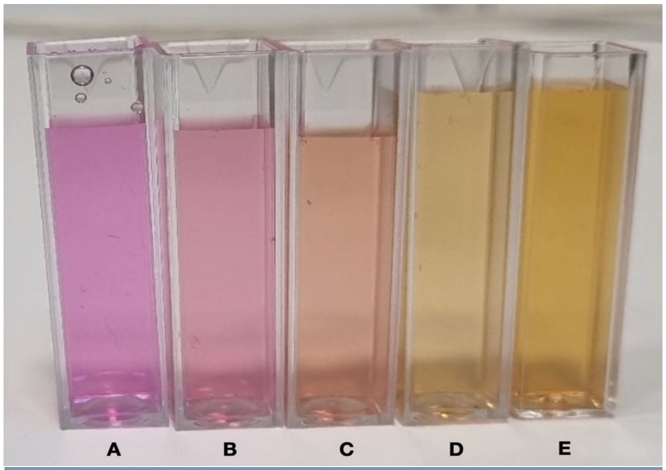

Figure 2. Representative appearance of the samples immersed in 0.2 mM potassium permanganate ($KMnO_4$) solution after 24 hours of incubation at 37 °C. From left to right: (A) Control, (B) SmartTrack, (C) CA Pro+ (Scheu Dental), (D) ClearQuartz, and (E) Acrylic block.

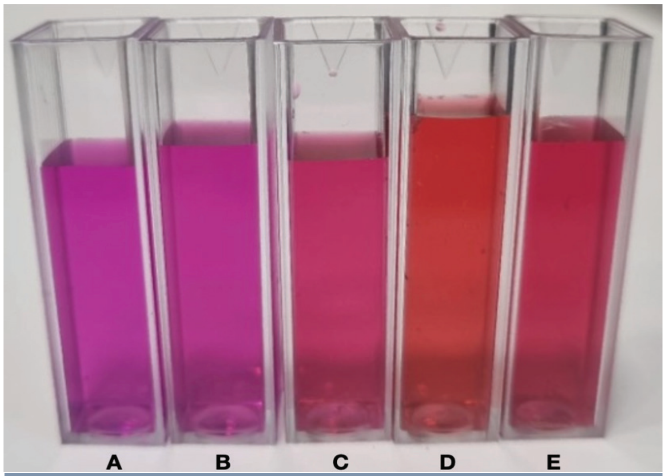

Figure 3. Representative appearance of the samples immersed in 1.0 mM potassium permanganate ($KMnO_4$) solution after 24 hours of incubation at 37 °C. From left to right: (A) Control, (B) SmartTrack, (C) CA Pro+ (Scheu Dental), (D) ClearQuartz, and (E) Acrylic block.

The present *in vitro* study demonstrated that all tested orthodontic materials reduced $KMnO_4$ within the first 24 hours, indicating the presence of oxidizable substances capable of reacting with the oxidizing agent under the experimental conditions. These findings highlight the importance of considering the early chemical behavior of orthodontic materials, as even initial interactions may contribute to cumulative biological exposure during treatment.

Furthermore, the results emphasize the potential value of simple biochemical evaluation methods for providing clinically relevant information about the chemical stability and biocompatibility of materials routinely used in orthodontic practice. The increase in discoloration over time reflected the reduction of $KMnO_4$. Since $KMnO_4$ is a strong but non-specific oxidizing agent, the observed discoloration should be considered an indicator of overall oxidizable load rather than a direct measurement of specific monomers or degradation products.[10,12]

Although $KMnO_4$ is not present in the oral environment, it was selected as a strong, non-specific oxidizing agent to estimate the overall oxidizable load associated with orthodontic materials. Similar approaches have been used in polymer research as preliminary screening tools to assess chemical reactivity. This approach differs from conventional methods used in previous studies, in which materials are incubated in artificial saliva, gastric fluid, or organic solvents such as ethanol, followed by compound-specific analyses using techniques such as HPLC or GC-MS.[11,12]

Compared with these established methodologies, the $KMnO_4$ method offers a simple and inexpensive screening approach that does not require sophisticated instrumentation. This may enhance its applicability as a preliminary assessment tool in material comparison studies.[10] However, unlike immersion models that allow identification and quantification of specific leached compounds, such as BPA, the $KMnO_4$ method provides only indirect and non-specific information on overall interactions with oxidizable substances.[11,12]

In a previous study, three commercially available clear aligner systems (SmileDirect, Invisalign, and Essix Ace) were immersed in artificial saliva, artificial gastric fluid, and ethanol, and BPA release was quantified using HPLC-tandem mass spectrometry. Samples were analyzed using HPLC-tandem mass spectrometry, and BPA release was detected in all materials.[11] These findings are consistent with the present results and suggest that clear aligner materials may exhibit oxidative reactivity under experimental conditions.

In another study, materials from four clear aligner systems (Invisalign, Eon, SureSmile, and Clarity) were evaluated in ethanol at different concentrations, and leaching was detected by GC-MS. A total of eleven different chemical compounds were identified.[12] These findings support the presence of multiple leachable substances in clear aligner materials and are consistent with the present results. Although the current method does not allow identification of specific compounds, the observed permanganate reduction may reflect interactions with the overall oxidizable substance.[13,14]

Azhagudurai et al.[13] reported measurable amounts BPA release from four different clear aligner materials in an ex vivo setting, with the highest release occurring within the first 24 hours. These findings indicate that the initial period of aligner wear is critical for chemical leaching; this is consistent with the present results, which show greater permanganate consumption at earlier time points.

In a similar study, BPA leaching from both thermoformed clear retainer materials and acrylic resin was investigated. Detectable BPA release was observed in both groups, particularly under thermal and mechanical stress. These findings are comparable with the present results and further support the oxidative reactivity observed in orthodontic materials.[14]

The method used in the present study is intended as a comparative screening approach rather than a definitive analytical technique.

Clinical Relevance

From a clinical perspective, immersion models using artificial saliva may better simulate the oral environment by incorporating factors such as of saliva and temperature on material degradation.[11,13] In contrast, the $KMnO_4$ method does not directly simulate the oral environment, but it may provide a simple way to compare the oxidative behavior of different materials.

It should also be considered that some immersion methods, particularly those using ethanol, may increase substance release because of their strong extraction effect.[12] Unlike compound-specific analytical methods, the $KMnO_4$ approach provides indirect information about the overall interaction between the tested material and the oxidizing solution.

Clear aligners and acrylic orthodontic appliances remain in prolonged contact with the oral environment during clinical use. The present findings indicate that orthodontic materials may exhibit oxidative behavior, particularly during the initial phase of use. Although the biological effects of these substances were not directly evaluated, the material-dependent differences observed in leaching behavior may still provide preliminary insight into materials' behavior. However, the present findings cannot be directly translated to clinical conditions. These findings also highlight the importance of continued research and material development to improve the chemical stability and biocompatibility of orthodontic appliances.

Study Limitations

The present study has some limitations that should be considered when interpreting the findings. First, $KMnO_4$ is a non-specific oxidizing agent; therefore, the observed reduction reflects the total oxidizable content rather than the release of specific monomers or degradation products. In addition, the method may overestimate substance release by including reactions with residual particles or polymer surface oxidation.

Another limitation is that the materials were mechanically fragmented into small particles before testing to standardize the surface area and enhance interaction with the $KMnO_4$ solution. While this approach allowed a controlled comparison between materials, it may have increased the effective surface area and led to an overestimation of oxidizable substance interactions compared with intact aligners used under clinical conditions.

Additionally, the experiments were conducted *in vitro* using distilled water, which does not adequately simulate the complex oral environment, including salivary composition, temperature variations, and mechanical forces. Therefore, the findings should be interpreted as preliminary screening results rather than a direct representation of clinical behavior.

Although immersion techniques remain the gold standard for identifying and quantifying specific leachables, the $KMnO_4$ method may still be useful as a practical, complementary tool for preliminary screening and comparative evaluation of material behavior. Future studies combining both approaches under clinically relevant conditions could help clarify material biocompatibility and degradation processes.

Despite these limitations, the $KMnO_4$ method remains a simple and practical approach for the initial evaluation of the interaction of oxidizable substances in orthodontic materials. Further studies under clinically relevant conditions, supported by more advanced analytical techniques, are needed to identify the specific compounds involved and better understand their possible biological effects.

CONCLUSION

Within the limitations of this preliminary *in vitro* study, all tested orthodontic materials demonstrated measurable interactions with $KMnO_4$, indicating the presence of oxidizable substances. The extent of interaction varied among the investigated materials, with ClearQuartz exhibiting the highest interaction with oxidizable substances and SmartTrack showing the lowest interaction levels under the tested conditions.

These findings suggest that clear aligners and acrylic orthodontic materials may differ in their chemical reactivity and potential degradation behavior. Although the $KMnO_4$ method does not identify or quantify specific compounds, it may serve as a simple, practical, and accessible preliminary screening approach for the comparative evaluation of orthodontic materials. Future studies should investigate the composition of the released substances using more sensitive analytical methods.

Ethics

Ethics Committee Approval: Ethical approval for this study was obtained from the İstanbul Kent University Ethics Committee (approval no: 2025-10, date: 10.12.2025).

Informed Consent: As no biological or patient-derived materials were used and the study was performed *in vitro*, informed consent was not required.

Footnotes

Author Contributions: Concept – M.K., B.İ.B., A.K., G.B., S.B., Y.G.; Design - M.K., B.İ.B., A.K., G.B., S.B., Y.G.; Data Collection and/or Processing - B.İ.B., A.K., G.B.; Analysis and/or Interpretation - B.İ.B., A.K., G.B.; Literature Search - M.K., B.İ.B., A.K., G.B., S.B., Y.G.; Writing - M.K., B.İ.B., A.K., G.B., S.B., Y.G.

Conflict of Interest: No conflict of interest was declared by the authors.

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