AI-Assisted Screening and Experimental Evaluation of Chelating Agents for Oxygen-Reinforced Alkaline Peroxide Bleaching of Eucalyptus Kraft Pulp

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Abstract

Artificial intelligence (AI)-assisted evidence screening was employed as a decision-support approach to prioritize chelating agents for oxygen-reinforced alkaline peroxide (EOP) bleaching of eucalyptus kraft pulp. Candidate agents were assessed using predefined technical, environmental, and practical criteria, and AI-generated information was verified against relevant literature and researcher assessment prior to experimental evaluation. Ethylenediaminetetraacetic acid (EDTA) served as the industrial reference, while diethylenetriaminepentaacetic acid (DTPA), ethylenediamine-N,N'-disuccinic acid (EDDS), and 1-hydroxyethylidene-1,1-diphosphonic acid (HEDP) were evaluated as alternative chelating agents. During preliminary screening, DTPA produced the highest mean ISO brightness and lowest mean Kappa number, whereas EDDS produced the highest mean pulp viscosity. Subsequent dosage evaluation identified 0.02–0.03% DTPA on an oven-dry pulp basis as the preferred range, providing a favorable balance among ISO brightness, Kappa number, pulp viscosity, and chelant dosage under the investigated conditions. At an identical dosage of 0.05%, DTPA and EDTA produced comparable observed bleaching responses. Overall, DTPA was identified as the most promising alternative among the chelating agents evaluated. The findings demonstrate the potential value of integrating AI-assisted evidence screening with literature verification, researcher-led assessment, and experimental evaluation as a structured approach for candidate prioritization in pulp-bleaching research.

Keywords: *Artificial intelligence; Chelating agents; Chemical screening; Hydrogen peroxide bleaching; Eucalyptus kraft pulp*

1. Introduction

The pulp and paper industry continues to seek bleaching technologies that improve pulp quality while reducing chemical consumption and environmental impacts. In elemental chlorine-free bleaching sequences, oxygen-reinforced alkaline peroxide (EOP) bleaching contributes to residual lignin removal and brightness development while reducing the chemical demand of subsequent bleaching stages [1-2].

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Hydrogen peroxide (H_2O_2) is an effective oxidizing agent for pulp bleaching; however, its performance is strongly influenced by transition metals such as iron (Fe), manganese (Mn), and copper (Cu), which can catalyze peroxide decomposition and thereby reduce bleaching efficiency [2,4]. Chelating agents are therefore used to control transition metals and improve peroxide stability. Ethylenediaminetetraacetic acid (EDTA) and diethylenetriaminepentaacetic acid (DTPA) are established chelating agents in pulp bleaching, while alternatives such as ethylenediamine-N,N′-disuccinic acid (EDDS) and 1-hydroxyethylidene-1,1-diphosphonic acid (HEDP) have also been investigated with respect to bleaching performance and environmental characteristics [5,7,9].

Selection of an appropriate chelating agent nevertheless requires consideration of multiple factors beyond metal-binding capacity, including hydrogen peroxide compatibility, alkaline stability, environmental profile, commercial availability, industrial application experience, and economic feasibility. Conventional experimental screening of numerous candidates and dosage levels can require substantial laboratory evaluation. Artificial intelligence (AI)-assisted evidence synthesis offers a structured approach for organizing and comparing heterogeneous information during preliminary candidate selection, provided that AI-generated information is verified against reliable literature and interpreted by researchers [3].

Recent AI and data-driven applications in pulp bleaching have focused primarily on process modeling, monitoring, and operational optimization rather than on evidence-assisted prioritization of chelating agents. Accordingly, the research gap addressed in this study is the integration of structured AI-assisted evidence screening with researcher verification and sequential experimental evaluation for chelating-agent selection. The methodological contribution is therefore not the development of a new AI algorithm or an autonomous chemical-selection system, but the use of AI as a decision-support tool within a researcher-controlled screening and validation workflow.

The objective of this study was to apply an AI-assisted, researcher-verified screening framework to prioritize candidate chelating agents for EOP bleaching of eucalyptus kraft pulp and subsequently evaluate the selected candidates experimentally. The experimental investigation comprised preliminary screening, dosage-response evaluation, identification of a preferred DTPA dosage range, and direct comparison of DTPA with the industrial EDTA reference. Through this integrated approach, the study aimed to assess the technical potential of DTPA as an alternative chelating agent under the investigated EOP bleaching conditions.

2. Materials and methods

2.1. Raw materials and chemicals

Industrial eucalyptus kraft pulp was collected from an operating pulp line at Thai Paper Company, Thailand, and used for all laboratory experiments. EDTA was used as the industrial reference chelating agent, while DTPA, EDDS, HEDP, MGDA, and GLDA were considered as potential alternatives during the AI-assisted screening (Table 1). NaOH, H_2O_2, and O_2 were used in the EOP bleaching experiments. The industrial-grade chemicals used in the bleaching experiments were obtained from Thai Paper Company and used as received without further purification. DTPA, EDDS, and HEDP were obtained from local chemical suppliers in Thailand and were also used as received.

Table 1. Candidate chelating agents considered for AI-assisted screening

Chelating agent	Abbreviation	Screening status
Ethylenediaminetetraacetic acid	EDTA	Selected
Diethylenetriaminepentaacetic acid	DTPA	Selected
Ethylenediamine-N,N′-disuccinic acid	EDDS	Selected
1-Hydroxyethylidene-1,1-diphosphonic acid	HEDP	Selected
Methylglycinediacetic acid	MGDA	Not selected
L-Glutamic acid N,N-diacetic acid	GLDA	Not selected

Note: Candidate chelating agents were identified through literature review, industrial-practice assessment, and AI-assisted screening. Selected candidates were advanced to laboratory evaluation.

2.2. AI-Assisted screening and candidate prioritization

AI was used as a decision-support tool for evidence screening, synthesis, and preliminary prioritization of candidate chelating agents rather than as an autonomous selection method. Perplexity AI, ChatGPT, Microsoft Copilot, and Gemini Enterprise were used for literature discovery, evidence synthesis, structured candidate comparison, and cross-checking. Final decisions regarding candidate selection and experimental evaluation were made by the researchers.

Candidates were evaluated using seven predefined criteria: metal-binding capacity toward iron (Fe), manganese (Mn), and copper (Cu); hydrogen peroxide compatibility; alkaline stability; environmental profile; commercial availability; industrial application experience; and economic feasibility. The same criteria were applied across all candidate comparisons.

A representative structured prompt was: “Compare EDTA, DTPA, EDDS, HEDP, MGDA, and GLDA as potential chelating agents for peroxide-based bleaching of eucalyptus kraft pulp using the seven predefined criteria. Provide a qualitative comparative assessment supported by traceable published or technical sources, identify insufficient or conflicting evidence, and do not infer unsupported values or performance.” Minor wording adjustments were made where necessary for individual AI platforms.

AI-generated information was treated as preliminary evidence and cross-checked against relevant literature and technical information. Unsupported, inconsistent, or insufficiently documented statements were excluded. Candidate prioritization was qualitative rather than based on a numerical weighted score. The overall ranking was derived from an integrated assessment of verified evidence across the seven criteria together with researcher judgment. EDTA was retained as the industrial reference, whereas candidates considered technically and practically suitable were advanced to laboratory evaluation. The resulting comparative assessment is presented in Table 4.

Because no parallel conventional screening workflow was conducted, no quantitative claims were made regarding reductions in screening time, experimental cost, chemical consumption, or manpower attributable to AI assistance.

2.3. EOP bleaching procedure

The selected chelating agents were evaluated using industrial eucalyptus kraft pulp under identical oxygen-reinforced alkaline peroxide (EOP) bleaching conditions. All chemical charges were calculated on an oven-dry (OD) pulp basis. The EOP operating conditions were maintained constant across treatments, while the chelating-agent type and/or dosage were varied according to each experimental stage. The fixed operating conditions are summarized in Table 2.

1. Pulp preparation. Eucalyptus kraft pulp was adjusted to 9% pulp consistency and preheated to 68 °C before chemical addition.
2. Chemical addition. NaOH (1.9% on OD pulp), H_2O_2 (0.48% on OD pulp), and the designated chelating agent were added to the pulp and thoroughly mixed to ensure uniform chemical distribution.
3. Oxygen application. The chemically treated pulp was transferred to a pressurized bleaching reactor. The reactor was sealed, and oxygen was applied at 1.5 bar.
4. EOP treatment. The pulp was treated at 68 °C for 90 minutes under the specified oxygen pressure with mixing/rotation throughout the treatment.
5. Pulp recovery. Upon completion of the EOP treatment, the reactor was cooled and depressurized before the treated pulp was recovered.
6. Washing and analysis. The treated pulp was filtered and thoroughly washed with deionized water before determination of Kappa number, ISO brightness, and limiting viscosity number according to the analytical methods described in Section 2.5.

Table 2. EOP bleaching conditions used in this study

Parameter	Value
Pulp consistency (%)	9
NaOH charge (% on OD pulp)	1.9
H_2O_2 charge (% on OD pulp)	0.48
Oxygen pressure (bar)	1.5
Temperature (°C)	68
Retention time (minutes)	90

Note: Chelating-agent type and/or dosage were varied according to the experimental stage; all other EOP bleaching conditions were maintained constant.

2.4. Experimental design

The experimental program was conducted as a sequential four-stage evaluation following AI-assisted evidence screening, literature verification, and researcher-led candidate prioritization. The overall study workflow is summarized in Figure 1, while the objectives, chelating agents, experimental conditions, and response variables for each experimental stage are presented in Table 3. In Stage 1, EDTA, DTPA, EDDS, and HEDP were evaluated under common bleaching conditions to compare their bleaching responses and identify candidates for further evaluation. Stage 2 examined the dosage-response behavior of DTPA and EDDS, with EDTA included as the industrial reference. Because the Kappa numbers obtained in Stage 1 were low and showed limited variation among treatments, Stage 2

focused on ISO brightness and pulp viscosity as the principal responses for dosage evaluation. Kappa number was reassessed in the subsequent stages. In Stage 3, DTPA and EDTA were compared directly at the same chelating-agent dosage under identical bleaching conditions. Finally, Stage 4 evaluated the DTPA dosage range using ISO brightness, Kappa number, and pulp viscosity, with EDTA retained as the industrial reference.

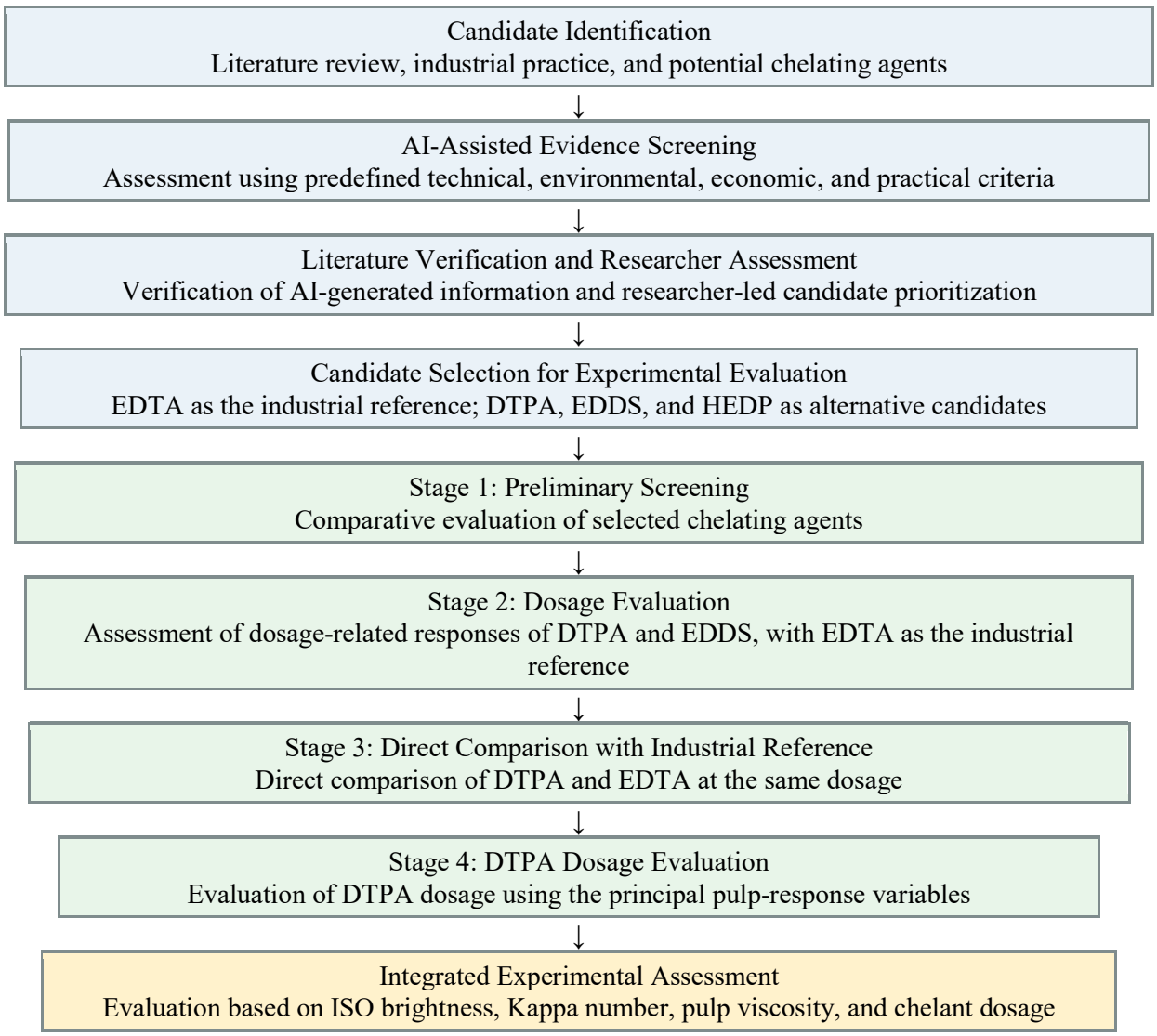


Figure 1. Overall workflow of AI-assisted screening and experimental evaluation of chelating agents for oxygen-reinforced alkaline peroxide bleaching of eucalyptus kraft pulp.

Table 3. Experimental design and research objectives

Experimental Stage	Objective	Chelating Agents Evaluated	Experimental Conditions	Response Variables
Stage 1: Preliminary Screening	To compare the bleaching responses of the selected chelating agents and identify candidates for further evaluation.	EDTA, DTPA, EDDS, and HEDP	Common EOP conditions using the same initial chelating-agent dosage.	ISO brightness (%ISO), Kappa number, and pulp viscosity (mL g^{-1})
Stage 2: Dosage Evaluation	To characterize the dosage-response behavior of DTPA and EDDS, with EDTA included as the industrial reference.	DTPA and EDDS, with EDTA as the industrial reference	DTPA: 0.02, 0.03, 0.05, and 0.07%; EDDS: 0.02, 0.05, 0.07, and 0.08%; EDTA: 0.03 and 0.05% on OD pulp.	ISO brightness (%ISO) and pulp viscosity (mL g^{-1})
Stage 3: Direct Comparison with Industrial Reference	To compare DTPA directly with EDTA at the same chelating-agent dosage under identical EOP conditions.	DTPA and EDTA	DTPA: 0.05%; EDTA: 0.05% on OD pulp.	ISO brightness (%ISO), Kappa number, and pulp viscosity (mL g^{-1})
Stage 4: DTPA Dosage Evaluation	To evaluate the DTPA dosage range using the three principal pulp-response variables.	DTPA, with EDTA as the industrial reference	DTPA: 0.02, 0.03, 0.04, and 0.05%; EDTA: 0.05% on OD pulp.	ISO brightness (%ISO), Kappa number, and pulp viscosity (mL g^{-1})

Note: All dosages are expressed on an oven-dry (OD) pulp basis. Stage 2 focused on ISO brightness and pulp viscosity following the low Kappa numbers observed in Stage 1.

Figure 1 summarizes the overall study workflow, while Table 3 provides the objectives, chelating agents, experimental conditions, and response variables for each experimental stage. The analytical methods used to determine ISO brightness, Kappa number, and pulp viscosity are described in Section 2.5, and the approach used for replicate measurements and data interpretation is described in Section 2.6.

2.5. Pulp property analysis

Following EOP treatment and washing, pulp samples were characterized by ISO brightness, Kappa number, and pulp viscosity to assess bleaching response, residual oxidizable material, and cellulose integrity, respectively. ISO brightness was determined according to ISO 2470-1:2016 by measuring the diffuse blue reflectance factor and reported as %ISO. Kappa number was determined according to ISO 302:2015 and used as an indicator of pulp bleachability and residual oxidizable material. Pulp viscosity was determined as the limiting viscosity number according to ISO 5351:2010 using cupri-ethylenediamine (CED) solution and reported in mL g^{-1}. The limiting viscosity number was

used as an indicator of cellulose integrity and the relative extent of cellulose degradation during EOP bleaching.

2.6. Data analysis and interpretation

All experiments were conducted in triplicate (n = 3), and results are reported as mean ± standard deviation (SD). Owing to the limited number of independent experimental replicates, the data were evaluated descriptively rather than used for inferential statistical comparisons among treatments. Differences were interpreted by considering the magnitude and consistency of ISO brightness, Kappa number, and pulp viscosity responses together with variability among replicate measurements. Small numerical differences were not interpreted as evidence of superior performance. Candidate selection and dosage assessment were based on the combined technical evaluation of bleaching response, residual oxidizable material, pulp-quality preservation, and chelant dosage under the investigated EOP conditions.

3. Results and discussion

3.1. AI-assisted screening and prioritization of candidate chelating agents

Artificial intelligence (AI) was employed as a decision-support tool for evidence screening and prioritization of potential chelating agents for oxygen-reinforced alkaline peroxide (EOP) bleaching of eucalyptus kraft pulp. Candidate chelating agents were initially identified through literature review, assessment of industrial practice, and AI-assisted evidence screening. The candidate pool comprised EDTA, DTPA, EDDS, HEDP, MGDA, and GLDA, as summarized in Table 1.

The candidates were assessed using the seven predefined criteria described in Section 2.2. The resulting qualitative AI-assisted assessment and screening outcomes are summarized in Table 4.

Table 4. Qualitative AI-assisted assessment of candidate chelating agents

Assessment Criterion	EDTA	DTPA	EDDS	HEDP	MGDA	GLDA
Metal-Binding Capacity	High	Very High	Moderate	Moderate	Moderate	Moderate
Hydrogen Peroxide Compatibility	Excellent	Excellent	Good	Good	Good	Good
Alkaline Stability	Good	Excellent	Moderate	Excellent	Good	Good
Environmental Profile	Moderate	Moderate	Excellent	Good	Excellent	Excellent
Commercial Availability	High	High	Moderate	High	Limited	Limited
Industrial Application Experience	Extensive	Extensive	Limited	Moderate	Limited	Limited

Assessment Criterion	EDTA	DTPA	EDDS	HEDP	MGDA	GLDA
Economic Feasibility	Moderate	High	Moderate	Moderate	Limited	Limited
Study Role	Industrial Reference	Alternative Candidate	Alternative Candidate	Alternative Candidate	Screening Candidate	Screening Candidate
Screening Outcome	Retained as Industrial Reference	Prioritized for Experimental Evaluation	Prioritized for Experimental Evaluation	Prioritized for Experimental Evaluation	Not Advanced	Not Advanced

The screening outcomes should not be interpreted as predictions of relative bleaching performance. The environmental profiles of chelating agents also differ considerably; EDDS has been reported to exhibit favorable biodegradation characteristics, whereas conventional synthetic chelants require consideration of environmental fate [8,10,15]. The bleaching responses of the prioritized candidates were subsequently determined experimentally, as described in Section 3.2.

3.2. Preliminary evaluation of alternative chelating agents

The bleaching performance of the selected chelating agents was evaluated under identical EOP bleaching conditions. ISO brightness, Kappa number, and pulp viscosity were used to assess bleaching response, residual oxidizable material, and cellulose integrity, respectively. The results are presented in Table 5 and were interpreted descriptively using the mean values and variability among three independent replicates (n = 3).

Table 5. Preliminary screening results of alternative chelating agents for EOP bleaching of eucalyptus kraft pulp

Chelating Agent	Kappa number (Mean ± SD, n = 3)	ISO brightness (%ISO, Mean ± SD, n = 3)	Difference from Control (%ISO)	Pulp viscosity (mL g^{-1}, Mean ± SD, n = 3)
Control (Blank)	1.09 ± 0.01	78.75 ± 0.20	0.00	539 ± 4
EDTA	1.10 ± 0.01	79.07 ± 0.25	+0.32	535 ± 4
DTPA	1.08 ± 0.01	79.66 ± 0.20	+0.91	534 ± 4
HEDP	1.14 ± 0.02	78.04 ± 0.30	−0.71	518 ± 5
HEDP (Alternative Grade)	1.16 ± 0.01	78.23 ± 0.30	−0.52	526 ± 5
EDDS	1.16 ± 0.01	78.38 ± 0.30	−0.37	545 ± 5

Note: Values are mean ± SD from three independent replicates (n = 3). Differences from the control were calculated from mean ISO brightness values for descriptive comparison.

As shown in Table 5, DTPA produced the highest mean ISO brightness (79.66 ± 0.20 %ISO) and the lowest mean Kappa number (1.08 ± 0.01) among the evaluated chelating-agent treatments. EDTA, the industrial reference, produced a mean ISO brightness of 79.07 ± 0.25 %ISO and a Kappa number of 1.10 ± 0.01. In contrast, EDDS produced the highest mean pulp viscosity (545 ± 5 mL g^{-1}), indicating a different response profile characterized by comparatively greater retention of pulp viscosity despite its lower bleaching response.

The favorable bleaching response observed with DTPA is consistent with its ability to complex transition-metal ions that can promote hydrogen peroxide decomposition. Control of these metal ions can improve peroxide stability and reduce undesirable oxidative reactions during peroxide-based bleaching [2,5].

Recent studies further show that oxidative bleaching and oxygen delignification must be evaluated through complementary responses such as Kappa number, ISO brightness, and pulp viscosity because improved delignification can be accompanied by changes in cellulose integrity [21–23].

Although the numerical differences among treatments were interpreted descriptively, the combined responses provided a practical basis for determining which candidates should proceed to the dosage-evaluation stage. DTPA was advanced because of its favorable combination of ISO brightness and Kappa number, whereas EDDS was retained because of its comparatively high pulp viscosity and distinct response profile. EDTA remained the industrial reference.

Because Kappa numbers remained low and varied only slightly among the Stage 1 treatments, Stage 2 focused on ISO brightness and pulp viscosity as the more discriminating responses for dosage evaluation. Kappa number was subsequently reassessed in Stages 3 and 4.

The Stage 1 results are consistent with the role of chelation in limiting metal-catalyzed peroxide decomposition and with previous studies involving DTPA and alternative chelating agents in pulp-treatment and peroxide-bleaching systems [2,5,6,13,16]. DTPA gave the highest mean brightness and the lowest mean Kappa number, while EDDS retained the highest viscosity, showing that bleaching response and cellulose preservation should be considered together. Recent kraft-pulp studies likewise evaluate bleachability using complementary optical, delignification, and pulp-quality responses [18,21,23].

The higher mean ISO brightness obtained with DTPA than with EDTA can also be interpreted from their metal-complexation characteristics. Both are aminopolycarboxylate chelants, but DTPA generally forms more stable complexes with transition metals relevant to peroxide decomposition, including Fe, Mn, and Cu [11,14]. Higher complex stability indicates stronger thermodynamic binding and can reduce the availability of catalytically active metal ions, thereby favoring more effective use of H_2O_2 for bleaching reactions [2,5]. This provides a plausible chemical basis for the higher mean brightness and slightly lower Kappa number observed with DTPA. However, because metal concentrations and residual H_2O_2 were not measured, this mechanism should be considered an interpretation rather than direct experimental confirmation.

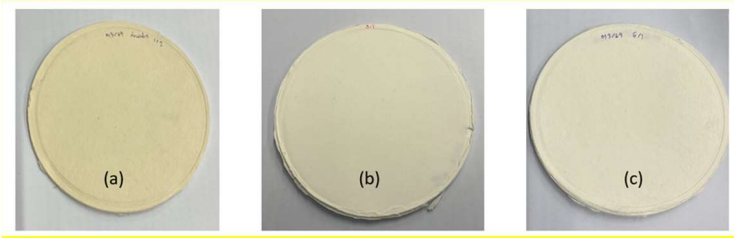


Figure 2. Appearance of eucalyptus kraft pulp sheets: (a) before bleaching, (b) after EOP bleaching with EDTA, and (c) after EOP bleaching with DTPA.

Figure 2 provides a qualitative visual comparison of eucalyptus kraft pulp before bleaching and after EOP bleaching with EDTA and DTPA. Both bleached samples appeared brighter than the

unbleached pulp, while the DTPA-treated sample showed a visually brighter appearance than the EDTA-treated sample. This qualitative observation was consistent with the instrumental ISO brightness measurements in Table 5, with mean values of 79.66 %ISO for DTPA and 79.07 %ISO for EDTA.

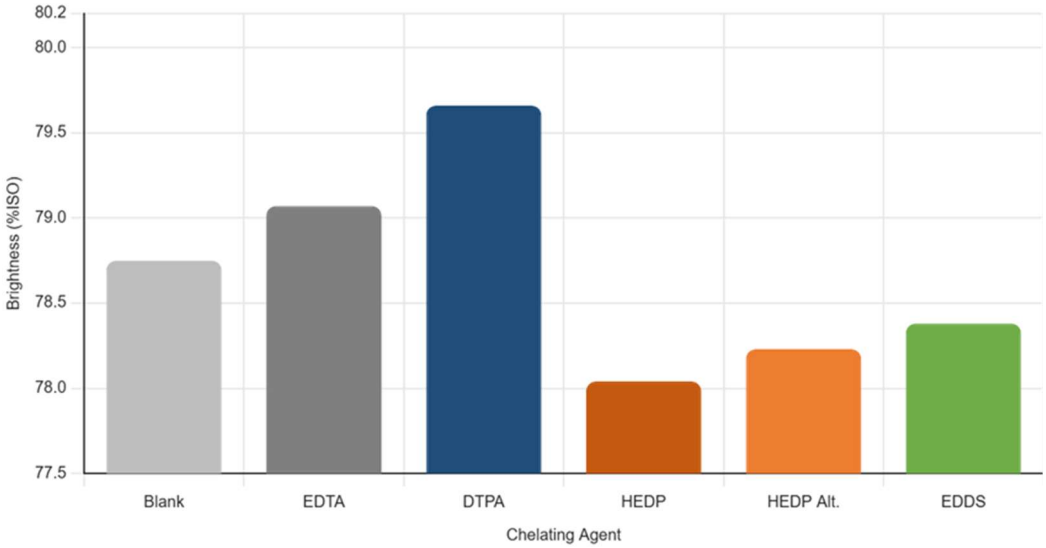


Figure 3. Effect of chelating-agent treatment on ISO brightness of eucalyptus kraft pulp following EOP bleaching.

Figure 3 illustrates the comparative ISO brightness responses of the evaluated treatments. DTPA and EDTA produced mean ISO brightness values above the control, whereas EDDS and both HEDP treatments produced values below the control. Because the numerical results are reported in Table 5, Figure 3 is presented primarily to visualize the relative treatment responses.

Table 6. Technical assessment and progression of chelating agents following preliminary screening

Chelating Agent	ISO Brightness Response	Kappa Number Response	Pulp Viscosity Response	Experimental Progression
EDTA	Above control	Similar to control	Similar to control	Industrial reference
DTPA	Highest mean	Lowest mean	Similar to EDTA	**Advanced to Stage 2**
HEDP	Below control	Above control	Lowest mean	Not advanced
HEDP (Alternative Grade)	Below control	Highest mean	Below control	Not advanced

Chelating Agent	ISO Brightness Response	Kappa Number Response	Pulp Viscosity Response	Experimental Progression
EDDS	Below control	Above control	Highest mean	**Advanced to Stage 2**

Note: The assessment is based on the descriptive experimental results in Table 5. ISO brightness, Kappa number, and pulp viscosity were considered collectively when determining progression to Stage 2; EDTA was retained as the industrial reference.

Overall, the preliminary evaluation identified DTPA and EDDS as appropriate candidates for further dosage evaluation based on their distinct response profiles. DTPA provided the most favorable combination of mean ISO brightness and Kappa number, whereas EDDS provided the highest mean pulp viscosity. Accordingly, DTPA and EDDS were advanced to Stage 2, with EDTA retained as the industrial reference.

3.3. Effect of chelating agent dosage on bleaching performance

Following preliminary screening, DTPA and EDDS were subjected to dosage evaluation, while EDTA was retained as the industrial reference. ISO brightness and pulp viscosity were used to evaluate bleaching response and cellulose integrity, respectively (Table 7). Because the dosage ranges differed among the chelating agents, the results were interpreted as individual dosage-response relationships rather than direct equal-dose comparisons.

Table 7. Effect of chelating-agent dosage on EOP bleaching performance of eucalyptus kraft pulp

Chelating Agent	Dosage (% on OD Pulp)	Brightness (%ISO, Mean ± SD, n = 3)	Pulp Viscosity (mL g^{-1}, Mean ± SD, n = 3)
EDTA	0.03	81.70 ± 0.25	552 ± 4
EDTA	0.05	80.75 ± 0.20	560 ± 4
DTPA	0.02	81.00 ± 0.20	579 ± 4
DTPA	0.03	81.20 ± 0.25	574 ± 5
DTPA	0.05	81.75 ± 0.20	554 ± 4
DTPA	0.07	79.90 ± 0.30	573 ± 5
EDDS	0.02	80.75 ± 0.25	576 ± 4
EDDS	0.05	80.15 ± 0.20	546 ± 4
EDDS	0.07	81.35 ± 0.25	548 ± 4
EDDS	0.08	81.05 ± 0.20	585 ± 5

Note: Values are mean ± SD from three independent replicates (n = 3). Dosage ranges were evaluated separately and were not intended as direct equal-dose comparisons.

DTPA exhibited a non-monotonic dosage response. Mean ISO brightness increased from 81.00 %ISO at 0.02% DTPA to 81.75 %ISO at 0.05%, but decreased to 79.90 %ISO at 0.07%. The highest mean pulp viscosity within the DTPA series was observed at 0.02% (579 mL g^{-1}). EDDS showed a similarly non-monotonic response, indicating that increasing chelant dosage did not consistently improve ISO brightness or pulp viscosity.

These responses are consistent with the role of chelating agents in controlling transition-metal ions that can promote hydrogen peroxide decomposition and undesirable oxidative reactions during peroxide bleaching. However, chelation effectiveness depends on the chelating agent, pulp characteristics, and bleaching conditions, which may contribute to the observed dosage-response behavior [2,5,9].

Hydrogen peroxide oxidation is influenced by reaction conditions, transition-metal availability, and lignin chemistry, while increases in oxidative treatment severity may also affect cellulose integrity and other pulp-quality properties [12,17,19–23].

The dosage producing the highest mean ISO brightness did not coincide with that providing the highest mean pulp viscosity. Although 0.05% DTPA produced the highest mean ISO brightness, 0.02–0.03% DTPA maintained relatively high brightness with higher pulp viscosity. Therefore, bleaching response, cellulose integrity, and chelant dosage were considered collectively rather than selecting a dosage based on maximum brightness alone.

The Stage 2 results supported further evaluation of the lower DTPA dosage range. Before this evaluation, DTPA and EDTA were compared directly at an identical dosage of 0.05% on OD pulp in Stage 3 to provide a controlled comparison with the industrial reference.

The non-monotonic dosage response indicates that increasing chelant charge did not produce proportional improvement after sufficient metal control was approached. Brightness and viscosity represent different responses, so their maxima need not occur at the same dosage. Recent peroxide/extraction and kraft-pulp studies similarly show that oxidative bleaching can improve brightness or lignin removal while requiring attention to yield, viscosity, and pulp preservation [19–23]. This supports selecting DTPA dosage from the combined response rather than maximum brightness alone.

The decrease in mean brightness at the highest DTPA charge further suggests that chelant effectiveness was not proportional to dosage once sufficient metal control was approached. After the accessible catalytic-metal fraction is adequately complexed, additional DTPA would not necessarily provide a corresponding increase in peroxide efficiency. Recent peroxide, extraction, and oxygen-delignification studies likewise show that increasing oxidative treatment severity does not necessarily yield proportional improvements in brightness or delignification and that cellulose or pulp-quality preservation must be evaluated concurrently [19–23].

3.4. Direct comparison of DTPA and EDTA

DTPA and EDTA were evaluated at an identical chelating-agent dosage of 0.05% on OD pulp under the same EOP bleaching conditions. ISO brightness, Kappa number, and pulp viscosity were evaluated to compare bleaching response and cellulose integrity.

Table 8. Direct comparison of DTPA and EDTA at an identical chelating-agent dosage

Chelating Agent	Dosage (% on OD Pulp)	Kappa number (Mean ± SD, n = 3)	ISO brightness (%ISO, Mean ± SD, n = 3)	Pulp viscosity (mL g^{-1}, Mean ± SD, n = 3)
EDTA	0.05	1.11 ± 0.03	81.88 ± 0.25	569 ± 4
DTPA	0.05	1.10 ± 0.04	81.50 ± 0.25	571 ± 3

Note: Values are mean ± SD from three independent replicates (n = 3). Both chelating agents were evaluated at 0.05% on an oven-dry pulp basis under identical EOP bleaching conditions.

The equal-dose comparison showed similar observed responses for DTPA and EDTA, with small numerical differences in ISO brightness, Kappa number, and pulp viscosity. EDTA produced a slightly higher mean ISO brightness (81.88 vs. 81.50 %ISO), whereas DTPA showed a slightly lower mean Kappa number (1.10 vs. 1.11) and slightly higher mean pulp viscosity (571 vs. 569 mL g^{-1}). These differences were interpreted descriptively and do not establish statistical equivalence or superiority of either chelating agent.

The comparable overall response at the same dosage supported further evaluation of DTPA at lower dosages in Stage 4 to identify a preferred dosage range under the investigated conditions. At the common 0.05% charge, DTPA and EDTA gave similar observed brightness, Kappa number, and viscosity profiles. This agrees with the established use of aminopolycarboxylate chelants for metal control in peroxide bleaching [2,5]. The result should not be interpreted as statistical equivalence; it simply shows no large deterioration when DTPA replaced EDTA under these laboratory conditions.

3.5 Evaluation of DTPA dosage range

Following the equal-dose comparison with EDTA, the lower DTPA dosage range identified in Stage 2 was evaluated further using ISO brightness, Kappa number, and pulp viscosity. DTPA dosages of 0.02–0.05% on OD pulp were evaluated, with EDTA at 0.05% retained as the industrial reference (Table 9).

Table 9. Evaluation of DTPA dosage range under identical EOP bleaching conditions

Chelating Agent	Dosage (% on OD Pulp)	Kappa number (Mean ± SD, n = 3)	ISO brightness (%ISO, Mean ± SD, n = 3)	Pulp viscosity (mL g^{-1}, Mean ± SD, n = 3)
EDTA	0.05	1.11 ± 0.03	81.88 ± 0.25	569 ± 4
DTPA	0.02	1.09 ± 0.02	82.10 ± 0.20	569 ± 4
DTPA	0.03	1.10 ± 0.03	81.80 ± 0.25	578 ± 5
DTPA	0.04	1.08 ± 0.02	81.55 ± 0.20	576 ± 4
DTPA	0.05	1.10 ± 0.04	81.50 ± 0.25	571 ± 3

Note: Values are mean ± SD from three independent replicates (n = 3). DTPA dosages of 0.02–0.05% were evaluated using the combined responses of ISO brightness, Kappa number, and pulp viscosity; EDTA at 0.05% was retained as the industrial reference.

The DTPA treatments showed relatively limited variation in bleaching response across the investigated dosage range. Mean ISO brightness ranged from 81.50 to 82.10 %ISO and mean Kappa number from 1.08 to 1.10. The highest mean ISO brightness was obtained at 0.02% DTPA (82.10 %ISO), whereas the highest mean pulp viscosity was obtained at 0.03% DTPA (578 mL g^{-1}). Increasing the DTPA dosage to 0.04–0.05% did not provide a consistent improvement across the three response variables.

Considering ISO brightness, Kappa number, pulp viscosity, and chelant dosage collectively, 0.02–0.03% DTPA was identified as the preferred dosage range under the investigated EOP conditions. This range maintained favorable bleaching responses while reducing the applied DTPA dosage relative to the higher levels evaluated. The preferred range represents a descriptive multi-response technical assessment rather than a mathematically or statistically determined optimum.

Overall, the Stage 4 evaluation indicated that 0.02–0.03% DTPA provided a favorable balance among ISO brightness, Kappa number, pulp viscosity, and chelant dosage under the investigated conditions. Higher DTPA dosages provided no consistent overall improvement. Together with the equal-dose comparison with EDTA, these findings support DTPA as a promising alternative chelating agent for the investigated bleaching system

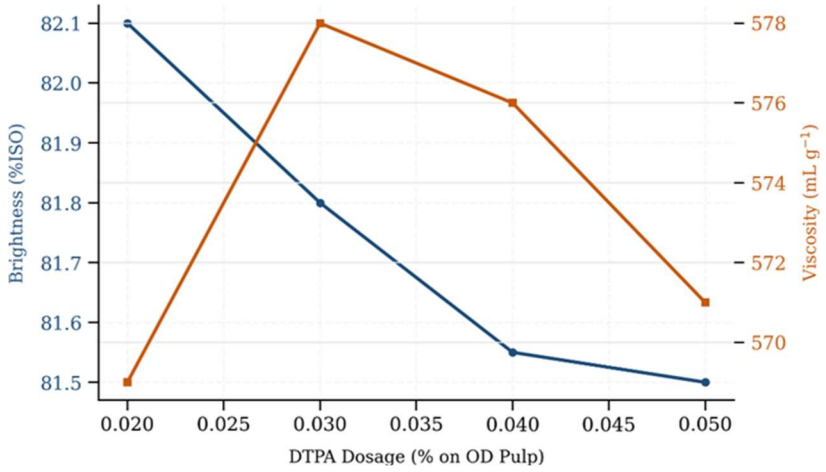


Figure 4. Effect of DTPA dosage on ISO brightness and pulp viscosity of eucalyptus kraft pulp following EOP bleaching.

4. Conclusion

This study demonstrates the applicability of an AI-assisted evidence-screening approach, integrated with literature verification, researcher-led assessment, and experimental evaluation, for prioritizing chelating agents for oxygen-reinforced alkaline peroxide (EOP) bleaching of eucalyptus kraft pulp. Among the candidates evaluated, DTPA exhibited the most favorable overall bleaching response, whereas EDDS provided the highest pulp viscosity.

A DTPA dosage of 0.02–0.03% on OD pulp was identified as the preferred range under the investigated conditions, providing a favorable balance among ISO brightness, Kappa number, pulp viscosity, and chelant dosage. At an identical dosage of 0.05%, DTPA and the industrial EDTA reference exhibited comparable observed bleaching responses. Overall, the findings support DTPA as the most promising alternative among the chelating agents evaluated in this study. Further mill-scale assessment of technical performance, economic feasibility, process compatibility, and environmental considerations is required before industrial implementation.

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Conflict of Interest

We declare no conflict regarding the publication of the study.

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