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Advancing produced water quality via integrated mechanical vapor recompression: Chemical and toxicological characterization, hazard identification and mitigation

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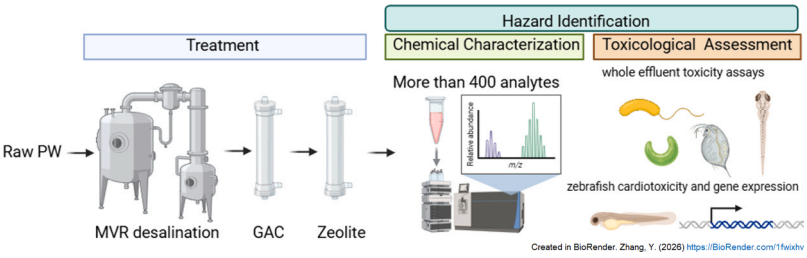
HIGHLIGHTS

- Pilot-scale MVR distillation demonstrated robust salinity reduction.
- The distillate still caused adverse impacts on all the tested aquatic organisms.
- GAC and zeolite polishing reduced PW pollutants to non-toxic levels.
- Toxicity reductions aligned with the removal of potential chemical stressors.
- Integrated treatment mitigated all adverse effects, including sublethal ones.

GRAPHICAL ABSTRACT



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ABSTRACT

This study evaluated Permian Basin produced water (PW) treatment through an advanced treatment train comprising mechanical vapor recompression (MVR) distillation, granular activated carbon (GAC), and zeolite adsorption. More than 400 analytes, including volatile and semivolatile organics (VOCs and SVOCs), inorganic ions, heavy metals, radionuclides, pesticides, dioxins, furans, and per- and polyfluoroalkyl substances (PFAS) – were quantified. Whole effluent toxicity (WET) tests were conducted across four trophic levels using *Vibrio fischeri*, *Raphidocelis subcapitata*, *Ceriodaphnia dubia*, and zebrafish (*Danio rerio*). In zebrafish, developmental endpoints and transcriptional responses of genes were assessed to detect sub-lethal effects. MVR distillation reduced total dissolved solids by 99.95%, total organic carbon by 89%, and total petroleum hydrocarbons by 92%. However, reductions in bulk organic parameters did not consistently reflect decreases in individual VOCs and SVOCs. Several hydrophilic VOCs (e.g., acetone, 2-propanol, 2-butanone) exhibited limited removal or even net increases during distillation. Caproic, propionic, and valeric acids (86.5, 123 and 198 mg/L) exceeded several toxicity thresholds for aquatic species. Untreated and distilled PW induced acute and chronic toxicity across all test species, with untreated PW causing 100% mortality in zebrafish embryos and the distillate resulting in 58–67% developmental abnormalities (edema, scoliosis, and impaired posture). In contrast, post-treatment with GAC and zeolite reduced most constituents to below detection limits and eliminated observable toxic effects. Zebrafish developmental and gene expression analyses confirmed the absence of significant perturbations

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following final treatment. This integrated chemical and biological assessment demonstrates that advanced multi-barrier treatment can effectively mitigate PW toxicity, supporting its potential reintegration into the hydrological cycle.

1. Introduction

Managing produced water (PW), the main by-product of oil and gas extraction, presents major environmental challenges and raises concerns over recent increases in seismic activity related to current disposal practices ([1-3]). The Permian Basin, the most productive oil and gas region in the United States, exemplifies these challenges due to the substantial volume and complex composition of its PW. Investigations have identified diverse organic compounds, elevated concentrations of dissolved salts, heavy metals, and radionuclides, which may present significant public health and ecological risks without adequate treatment [4,5]. The reuse of treated PW purified through advanced treatment processes is considered a strategic solution that could mitigate water scarcity in oil and gas-producing regions while addressing critical management and environmental challenges ([2,6,7]).

Recent studies have explored the feasibility of desalinating PW with thermal processes. Tarazona, Yeinner et al. (2024) evaluated the performance of a pilot-scale low-temperature thermal distillation technology in meeting criteria for the potential surface water discharge scenarios [7]. Building on those findings, Tarazona, Y. et al. [8] examined the integration of thermal distillation with established technologies, such as granular activated carbon (GAC) and zeolite, to mitigate potential stressors and produce a non-toxic effluent. Van Houghton et al. [9] evaluated a multi-stage treatment process incorporating coagulation/flocculation, a membrane bioreactor (MBR), GAC adsorption, ion exchange, and membrane distillation (MD). Their findings demonstrated the system's effectiveness in reducing contaminant levels to meet potential effluent discharge limits. These results were further validated through cytotoxicity testing with MCF-7 cells, which showed increased survival rates in MD effluents. A recent study also demonstrated that a pilot-scale multistage fractional freeze desalination (FD) coupled with seawater reverse osmosis (SWRO) process achieved approximately 99% removal of dissolved ions and 93.5% removal of total organic carbon (TOC) from PW in the Permian Basin [10,11]. Whole effluent toxicity (WET) assays and human cell line studies further confirmed that this multistage treatment process effectively produced purified PW with no adverse effects on the tested aquatic organisms or human cells [11]. Irrigation with this treated PW resulted in crop yields and soil health metrics comparable to those obtained using freshwater [12]. Delanka-Pedige et al. [13] conducted both targeted and non-targeted chemical analyses of effluents from photocatalytic membrane distillation (PMD) and vacuum membrane distillation (VMD). Their study integrated a chemical identification workflow with in-silico tools to explore correlations between detected compounds and their potential impacts on key receptors, including mammals (genotoxicity, mutagenicity, endocrine disruption) and aquatic organisms (acute and chronic toxicity). Collectively, these studies have: (i) enhanced understanding of PW quality; (ii) demonstrated the capacity of multiple treatment approaches to mitigate salinity and other chemical stressors; and (iii) established the effectiveness of available treatment technologies for producing purified PW with water quality potentially suitable for key reuse scenarios, including surface water discharge and irrigation of selected crops.

Despite these advancements, fundamental knowledge gaps persist regarding the chemical safety of thermally desalinated PW. Previous research has focused on a limited set of chemical analytes, raising concerns about whether such characterization efforts can adequately evaluate the quality of PW and ensure the chemical safety of thermally treated PW, particularly given the potential for unknown organic compounds to partition into the distillate [7,13]. Furthermore, most toxicological evaluations of PW effluents have primarily relied on conventional acute and chronic endpoints or in-silico toxicity predictions, which are often insufficient for comprehensive hazard identification. Although these tests can capture the effects of PW-associated chemicals on mortality, reproduction, and growth inhibition, they fail to detect subtle molecular and physiological perturbations arising from low-dose exposures or from complex and largely unidentified chemical mixtures present in PW [14,15]. To address these limitations, this study systematically characterizes raw, thermally desalinated, and polished PW from the Permian Basin by assessing effluents from a treatment train designed to mitigate known and unknown stressors. We applied a multi-tiered targeted analytical approach encompassing more than 400 analytes, including conventional water quality parameters, volatile and semi-volatile organic compounds (VOCs and SVOCs), heavy metals, volatile fatty acids, ammonia, dioxins, furans, pesticides, herbicides, surfactants, polychlorinated biphenyls, per- and polyfluoroalkyl substances, and radionuclides. This comprehensive analytical framework enables detailed tracking of less-studied constituents throughout each treatment stage, providing a more robust characterization of PW quality and treatment performance. Among aquatic models, zebrafish embryos are widely used in environmental toxicology because of their genetic similarity to higher vertebrates and their rapid, transparent embryonic development, which enables high-throughput, sensitive detection of effects from both known and unknown stressors [16–18]. Given its relevance to both environmental and human health assessments, our study used zebrafish embryo exposures as a high-resolution tool for hazard identification. The approach enables detection of developmental, molecular, and sub-lethal effects that standard toxicity assays may not capture, while evaluating the effectiveness of the treatment train in producing water suitable for potential surface discharge. By monitoring embryonic development and analyzing gene expression associated with endocrine regulation, phase I and II biotransformation, and oxidative stress, we aim to identify early molecular indicators of toxicity that conventional endpoints may overlook, thereby providing an unparalleled assessment of the biological safety of thermally desalinated PW. Overall, this study addresses the key knowledge gaps by integrating broad-spectrum targeted chemical analysis with WET testing across four trophic levels and zebrafish developmental and transcriptional screening. Physicochemical properties were used to analyze the target chemical results and to infer compound behavior during the desalination. Together, these lines of evidence extend water quality evaluation beyond conventional criteria and provide a state-of-the-art, effects--based assessment that reduces uncertainty associated with uncharacterized compounds, enabling a comprehensive evaluation for treatment performance and PW suitability for reuse.

2. Materials and methods

2.1. PW collection and treatment

The PW used in this study was sourced from an existing saltwater disposal well (SDW) near Big Spring, Texas. After transport to the pilot location, PW was stored in three 500-barrel (bbl, 79.5 m^3) storage tanks, where it remained without any additional processing before treatment. Based on the findings from our previous studies ([7,8]), the thermal distillate often has residual ammonia and VOCs. Therefore, raw PW underwent a sequential treatment involving mechanical vapor recompression (MVR) distillation, GAC, and zeolite to ensure the removal of hazardous compounds. A description of the units is provided below.

2.1.1. MVR distillation

During PW desalination using the pilot-scale MVR system (Figure S1), the initial heat was provided by a natural gas-powered burner, which heated a tube within a boiler at 230–260°C. The system used a mechanical positive-displacement type compressor to increase the temperature of the vapor generated in the distillation vessels. This compressed vapor was then used as the heat source for further vaporization of the feed water. The system operated within a differential pressure range of 3–14 psi, with water processing capacity increasing with the applied pressure. Evaporation and condensation temperatures varied as a function of operational pressure, ranging from 93 to 110°C (200–230 °F) for evaporation and 110–121°C (230–250 °F) for condensation under a vacuum pressure of −24.6 psi (-50 inHg). Condensed distillate temperatures were approximately 35°C (95 °F) in winter and 46°C (115 °F) in summer. Estimated energy requirements range from 18.87 to 31.45 kWh/m^3 of water processed. The unit operated at an average feed flow rate of 17.7 m^3 /d (3.24 gallons per minute, GPM), with a total dissolved solids (TDS) concentration of approximately 170,000 mg/L. This MVR unit typically achieves a water recovery rate of 30–40%, with a recovery rate of 32% observed during the sampling event. Samples were collected before and after the distillation unit for characterization, and additional distillate samples were collected specifically for conducting bench-scale post-treatment.

2.1.2. Post-treatment with GAC and zeolite

After distillation, the pH of the distillate was 10.2, resulting from elevated ammonia concentrations, and was subsequently adjusted to an operational pH of 8.5 by using diluted sulfuric acid. The distillate was then processed sequentially in two identical polyvinyl chloride (PVC) columns with GAC (12 ×40 Prewashed Virgin Coconut Shell activated carbon, EnviroSupply & Service Inc., California) set up in parallel to allow for duplicate testing of treatment performance. Each packed GAC column was operated in up-flow mode at a flow rate of 14 L/d, and maintained an empty bed contact time (EBCT) of 0.94 h using a peristaltic pump (Cole-Parmer). Samples were collected from each column at various time intervals to monitor treatment performance over time. Following GAC treatment, the water was further processed in two identical columns packed with clinoptilolite (Winston Zeolite, St. Cloud Mining), also set up in parallel for duplicate testing. The packed zeolite columns were operated in up-flow mode at a flow rate of 14 L/d, with an EBCT of 0.94 h, using a peristaltic pump (Cole-Parmer). Effluent samples were taken from both columns at different time intervals to evaluate the treatment performance of the zeolite. Additional information on the columns and materials is provided in Table S1, and the column setup is shown in Figure S2. After treatment, samples were collected for characterization.

2.2. Chemical and toxicological characterization

To evaluate the water quality through the treatment train, a comprehensive chemical and toxicological characterization was conducted on raw PW, distillate, and post-treated water following the GAC and zeolite processes.

2.2.1. Chemical characterization

The chemical characterization of the water samples included a comprehensive targeted scheme that covered over 400 analytes. Key conventional parameters such as pH, electrical conductivity (EC), TDS, and total suspended solids (TSS) were analyzed using standard methods (e.g., SM Methods 4500-H^+B, 2510B, 2540 C, and 2540D, respectively). Metals, including both total and dissolved concentrations, were determined using inductively coupled plasma mass spectrometry (ICP-MS) in accordance with SW846 Method 6010D. Organic compounds were characterized by analyzing volatile and semivolatile organic compounds (VOCs and SVOCs) using gas chromatography coupled with mass spectrometry (GC/MS) following SW846 Methods 8260D, 8270D, and 8270E. Furthermore, total and dissolved organic carbon (TOC and DOC) were assessed via oxidation using the SM Method 5310B. Pesticides and herbicides were characterized using GC following SW846 Method 8081B. Dioxins and furans were analyzed using high-resolution gas chromatography/high-resolution mass spectrometry (HRGC/HRMS) as per SW846 Method 8290 A. Per- and polyfluoroalkyl substances (PFAS) were analyzed using solid phase extraction followed by liquid chromatography coupled with tandem mass spectrometry (SPE LC-MS/MS) following EPA Method 537. Radiological parameters, such as gross alpha and beta radioactivity, were quantified using EPA Method 900. For a complete list of all the characterization methods used, please refer to Table S2, which details the standardized protocols employed in each analysis, including all the characterizations conducted, the respective methods used, and the number of analytes evaluated.

2.2.2. Whole effluent toxicity (WET) assessment

The toxicological assessment evaluated the ecological impact of the collected water samples across four trophic levels within freshwater ecosystems. Four representative species were used: *Raphidocelis subcapitata* (alga, producer), *Ceriodaphnia dubia* (invertebrate, primary consumer), *Danio rerio* (zebrafish, secondary consumer), and *Vibrio fischeri* (bacterium, decomposer). *R. subcapitata* (UTEX 1648) testing followed U.S. EPA guidelines for chronic WET tests (EPA-821-R-02–013) [19], using static nonrenewal exposures to assess growth inhibition over four days, with 24-hour interval measurements and four replicates per concentration. Acute toxicity for *C. dubia* followed U.S. EPA WET guidelines (EPA-821-R-02–012) [20], using a 48-hour static exposure to determine survival endpoints, with 20 replicates per concentration and neonates grouped in sets of five per 20 mL chamber. Zebrafish embryo toxicity testing (*D. rerio*) followed the Fish Embryo Toxicity (FET) test under OECD Method 236 [21], assessing survival endpoints such as coagulation, lack of somite formation, tail detachment, and heartbeat over a 96-hour exposure period with semi-renewal every 48 h. Each condition had 24 embryos, one per well in 3 mL of solution. Zebrafish use has received approval for research ethics from the Institutional Animal Care and Use Committee (IACUC) at New Mexico State University and a proof/certificate of approval is available upon request. Toxicity against *V. fischeri* (Strain NRRL B-11177) was assessed using luminescence inhibition as the endpoint after 5 and 15 min of exposure, using a Model 500 Analyzer (Azur Environmental, DE, USA), following the 81.9% Screening Test Protocol [22]. Each concentration and control had three replicates. Raw PW, MVR distillate, and post-treated water underwent acute and chronic toxicity testing following standard dose-response assessments using U.S. EPA WET guidelines, with PW concentrations ranging from 0% to 100% (0%, 6.25%, 12.5%, 25%, 50%, 100%). Maintenance and test dilutions were prepared using moderately hard reconstituted water (MHRW) with target concentrations of 96 mg/L $NaHCO_3$, 60 mg/L $CaSO_4{\cdot}2\,H_2O$, 60 mg/L $MgSO_4$, and 4 mg/L KCl. During testing, MHRW parameters were maintained at pH 7.4–7.8, hardness 80–100 mg/L (as $CaCO_3$), alkalinity 57–64 mg/L (as $CaCO_3$), and dissolved oxygen (DO) 7–9 mg/L. To avoid false positive toxicity results, low-ion content effluents, such as distillate and post-treated effluents, were remineralized to match the ion content of MHRW before exposure.

For the data analysis, acute and chronic toxicity endpoints were derived according to EPA guidelines (EPA 833-R-10–003, 2010) [23]. In compliance with federal and state regulations, WET data validity and reliability were assessed using the EPA WET Analysis Spreadsheet v2.1, considering only data that met test acceptability criteria (TAC). No observed effect concentration (NOEC) and lowest observed effect concentration (LOEC) values were determined through Dunnett's or Steel's Many-One Rank tests. Effluent concentrations causing 25% inhibition (IC_{25}) and 50% lethality (LC_{50}) were calculated using linear interpolation, Spearman-Karber, Trimmed Spearman-Karber, or Probit methods [23,24]. For detailed information on TAC, endpoints, and statistical methods, refer to the U.S. EPA guidelines [23].

2.2.3. Cardiotoxicity and gene expression alterations in early zebrafish development

Effluents that exhibited no significant adverse effects in the initial toxicological characterization across all tested species underwent further evaluation to detect potential subtle effects. In this assessment, *Danio rerio* (zebrafish) embryos were used to explore more nuanced impacts. Specifically, endpoints related to cardiac response, as well as alterations in gene expression linked to metabolism, endocrine disruption, and oxidative stress, were systematically assessed. Cardiac impairments were monitored in parallel with the zebrafish FET test across the entire concentration range (0%, 6.25%, 12.5%, 25%, 50%, 100%). From the total exposed population, 10 embryos were selected randomly for detailed cardiac analysis. Heartbeat measurements were conducted between 48 and 96 hpf (hours post-fertilization). Additionally, embryos were monitored for abnormal phenotypic development between 24 and 96 hpf. Observations included, among others, pericardial and yolk sac edemas, craniofacial malformations, scoliosis, and abnormal pigmentation of the embryos. To assess post-treated effluent effects on metabolism, oxidative stress, and endocrine function in *D. rerio*, the expression of 12 genes (*cyp19a1a*, *cyp19a1b*, *vtg1*, *ahr*, *pxr*, *cyp1a*, *cyp1b1*, *udpgt1a1*, *sod1*, *sod2*, *esr1*, *ar*) was evaluated after 7 days of exposure. Additional details about the set of genes studied are provided in Table S3. At 7 days of exposure, total RNA was extracted from pooled larvae (5 individuals per sample) exposed to MHRW and post-treated effluent, with 2 replicates for each group. RNA extraction used the PureLink® RNA Mini Kit (Invitrogen, Thermo Fisher Scientific) following the manufacturer's protocol for animal tissues, with homogenization by Fisherbrand™ 150 Homogenizer. RNA concentration was measured on a BioTek Epoch Microplate Spectrophotometer with a Take3 microvolume plate. RNA samples were DNase I-treated (Invitrogen, Thermo Fisher Scientific) to remove DNA prior to reverse transcription. cDNA was synthesized using the iScript™ cDNA Synthesis Kit (Bio-Rad) per the kit instructions. qPCR was performed with SsoAdvanced™ Universal SYBR Green Supermix (Bio-Rad) on a CFX Connect Real-Time system (Bio-Rad), with an initial denaturation at 95°C for 10 s, followed by 40 cycles of 95°C for 15 s and 60°C for 1 min. Relative fold gene expression was calculated using the ΔΔCT method [25], normalized to the housekeeping gene *elf1*. Significant statistical differences between controls (MHRW) and treated PW were assessed using the Mann-Whitney (Wilcoxon rank sum) test.

3. Results and discussion

3.1. Chemical characterization

3.1.1. Impact of treatment processes on conventional water quality parameters and key performance indicators

Table 1 and Figure S3 present conventional water parameters for raw PW, thermal distillate, and post-treated water and key performance indicators (KPIs) of the treatment processes. Changes in each parameter were assessed to evaluate treatment stage efficiency in addressing contaminants in the raw PW. Distillation reduced TDS by 99.95%, from 172,000 mg/L to 79.5 mg/L, with post-treatment causing a slight increase to 106 mg/L, which could be attributed to the introduction of major ions such as Na^+, Ca^{2+}, K^+, Mg^{2+}, and Cl^- during GAC and zeolite post-treatment [8]. TSS decreased from 165 mg/L to non-detectable levels (< 8 mg/L) after distillation, indicating a removal rate of > 95.15%. Hardness was reduced by 99.99%, from 25,000 mg/L to 2.44 mg/L after distillation, with a slight post-treatment increase to 7.93 mg/L, maintaining an overall reduction of 99.97%. Total alkalinity

Table 1
Distillation and post-treatment performance: removal efficiencies for general parameters, bulk organics, ions, and other analytes.

Analyte	Units	Raw PW	Distillate	Post-treated	R-D change (%)	D-P change (%)	R-P change (%)
TDS	mg/L	172,000	79.5	106	-99.95	+ 33.33	-99.94
TSS	mg/L	165	< 8.00	< 6.67	-95.15–100	-16.63–100	-95.96–100
pH	S.U.	6.1	10.2	8.2	-	-	-
Hardness	mg $CaCO_3$/L	25,000	2.44	7.93	-99.99	+ 225.00	-99.97
Alkalinity	mg $CaCO_3$/L	11,025	93.2	27.3	-99.15	-70.71	-99.75
TOC	mg/L	353.4	39.5	9.34	-88.82	-76.35	-97.36
DOC	mg/L	79.8	40.0	9.97	-49.87	-75.08	-87.51
HEM	mg/L	751	26.4	< 1.57	-96.48	-94.05	-99.79
TOX	µg/L	26,500	< 14.0	60	-99.95–100	-328.57	-99.77
TPH	mg/L	59.0	4.61	1.15	-92.19	-75.05	-98.05
GRO (C_6-C_{10})	mg/L	7.27	< 1.02	< 0.988	-95.97–100	-3.14–100	-86.41 – 100
DRO (C_{10}-C_{28})	mg/L	43.1	4.61	< 0.988	-89.30	-78.57–100	-97.71 – 100
ORO (C_{28}-C_{36})	mg/L	8.65	< 0.98	1.1500	-88.67–100	+ 17.35	-86.71
Na^+	mg/L	47,600	0.626	28.9	-100.00	+ 4516	-99.94
Ca^{2+}	mg/L	6350	0.916	2.88	-99.99	+ 214	-99.95
Mg^{2+}	mg/L	1270	0.052	0.43	-100.00	+ 724	-99.97
K^+	mg/L	349	< 0.106	1.90	-99.97–100	+ 1692	-99.46
Br^-	mg/L	550	0.071	0.116	-99.99–100	+ 63.15	-99.98
Cl^-	mg/L	72,100	1.50	27.2	-100.00	+ 1713	-99.96
F^-	mg/L	28.100	< 0.100	< 0.100	-99.64–100	N/A	-99.64 – 100
SO_4^{2-}	mg/L	226	< 0.200	8.86	-99.91–100	+ 4330	-96.08
PO_4^{3-}	mg/L	25.1	0.241	0.340	-99.04–100	+ 41.08	-98.65
Turbidity	NTU	39	5	1.4	-87.18	-72.00	-96.41
COD	mg/L	2220	142	64.0	-93.60	-54.93	-97.12
MBAS	mg/L	0.12700	0.112	ND	-11.81	+ 28.57	-37.01
TAN	mg N-NH_3/L	139	21	< 0.0508	-84.89	-99.76–100	-99.96–100
NO_3^-	mg N-NO_3 /L	< 0.0391	0.0871	0.116	-97.77	+ 33.18	97.03
NO_2^-	mg N-NO_2 /L	< 0.0293	< 0.0293	0.343	0.00	+ 1070	+ 1070
CN^-	µg/L	2.14	< 2.00	8.08	-6.54–100	+ 304	+ 276
H_2S	mg/L	< 5.00	< 5.00	< 5.00	N/A	N/A	N/A
S^{2-}	mg/L	< 0.0400	0.0406	< 0.0400	N/A	0.00	N/A
SiO_2	mg/L	31.2	< 0.370	14.7	-98.81–100	+ 3873	-52.88

R-D change (%): distillation removal efficiency, raw PW vs. distillate, – a percentage reduction with respect to raw PW feed; + percentage increment with respect to raw PW feed. D-P change (%): post-treatment removal efficiency, distillate vs. post-treated water, – a percentage reduction with respect to distillate; + percentage increment with respect to distillate. R-P change (%): complete treatment removal efficiency, raw vs. post-treated, – a percentage reduction with respect to raw PW feed; + percentage increment with respect to raw PW feed. N/A: not applicable as not detected in raw PW or distillate; The dilution factors of raw PW are 20 and 2 for COD and TOC analyses, respectively. The dilution factors of raw PW are 50 for K^+, Mg^{2+}, PO_4^{3-}, TAN and SiO_2, 100 for F^- and SO_4^{2-}, and 200 for Cl^-, 500 for Na^+ and Ca^{2+}.

decreased from 11,025 mg/L to 93.2 mg/L post-distillation, then further to 27.3 mg/L after post-treatment, representing an overall reduction of 99.75%.

These findings demonstrate the effective removal of calcium, magnesium, and bicarbonates, which are essential for reducing scaling potential and managing water chemistry for key reuse applications like cooling towers [26-28]. The pH increased significantly from 6.1 to 10.2 after distillation. This phenomenon, previously documented in thermal distillation processes with Permian Basin PW, is attributed to the reduction in overall ionic strength and residual ammonia levels (21 mg/L TAN) after distillation ([29–31,7]). These changes reflect the influence of distillation on the acidity/alkalinity balance, which is relevant for pH-dependent post-treatment units like adsorption and ion exchange, as it may impact the capital and operational costs during full-scale applications.

Regarding bulk organics, TOC was reduced from 353.4 mg/L to 39.5 mg/L (89%) after distillation, and further to 9.34 mg/L after post-treatment (97% overall reduction). Chemical oxygen demand (COD) decreased from 2220 mg/L to 142 mg/L (93%) after distillation and further to 64 mg/L post-treatment (97% overall reduction), demonstrating efficient removal of total and oxidizable organic matter. However, the residual TOC and COD observed after post-treatment indicate that some organic compounds in the thermal distillate were not fully removed by GAC. After 2 bed volumes (BV) of GAC columns, effluent TOC and COD concentration stabilized at around 10 and 65 mg/L, respectively (Figure S4). To assess the potential risks associated with these residual organics, a comprehensive chemical and toxicological evaluation of post-treated water was performed. Hexane extractable materials (HEM) decreased from 751 mg/L to 26.4 mg/L (96%) after distillation and to non-detectable levels (< 1.57 mg/L) after post-treatment (99.8% overall reduction).

Total petroleum hydrocarbons (TPH) were reduced from 59.0 mg/L to 4.61 mg/L after MVR distillation (92%) and further to 1.15 mg/L after post-treatment, achieving a 98% overall reduction. Gasoline range organics (GRO) decreased from 7.27 mg/L to non-detectable levels after distillation (<1.02 mg/L) and remained undetectable during post-treatment (< 0.988 mg/L). Diesel range organics (DRO) decreased from 43.1 mg/L to 4.61 mg/L (89%) after distillation, and to below method detection limit (MDL) after post-treatment (>97% reduction). Oil range organics (ORO) were reduced from 8.65 mg/L in the feed to near the MDL in both the distillate (< 0.98 mg/L) and the post-treated water (1.15 mg/L). These reductions demonstrate effective hydrocarbon removal across different C ranges, consistent with our previous findings, where TPH (C_6 to C_{35}) was reduced near MDL through combined low-temperature thermal distillation and GAC treatment [7,8].

Regarding major ions, sodium was reduced from 47,600 mg/L to 0.62 mg/L during distillation but increased to 28.9 mg/L post-treatment due to the zeolite ion exchange process. Calcium decreased from 6350 mg/L to 0.9 mg/L, rising to 2.9 mg/L during post-treatment. Magnesium dropped from 1270 mg/L to 0.05 mg/L after distillation, then increased to 0.43 mg/L post-treatment. Chloride decreased from 72,100 mg/L to 1.5 mg/L during distillation, with an increase to 27.2 mg/L post-treatment. Sulfate was reduced from 226 mg/L to non-detectable levels after distillation, then rose to 8.86 mg/L post-treatment. Phosphate concentrations dropped from 25.1 mg/L to 0.241 mg/L after distillation and showed no significant change after post-treatment (0.34 mg/L). TAN was reduced from 139 mg/L to 21 mg/L after MVR distillation (85%), then further to < 0.0508 mg/L post-treatment, achieving a minimal 99.96% overall reduction. The removal of ammonia in the distillate is attributed primarily to the ion exchange process in the zeolite columns, as the GAC column showed limited ammonia adsorption capacity (Figure S4), whereas zeolite columns showed a consistent complete ammonia removal (Figure S5). Regarding other parameters, H_2S levels remained undetectable across all samples, SiO_2 was reduced from 31.2 mg/L to < 0.370 mg/L after MVR distillation, then rose to 14.7 mg/L after GAC and zeolite post-treatment, suggesting its reintroduction during the post-treatment processes. Turbidity dropped from 39 NTU to 5 NTU after distillation and further to 1.4 NTU post-treatment, resulting in a total reduction of 96.41%.

The data in Table 1 and Figure S3 demonstrate that distillation and post-treatment processes effectively reduced most of the evaluated general parameters and KPIs. TDS, TSS, EC, and major ions like sodium, calcium, and chloride showed substantial reductions, underscoring distillation's effectiveness in addressing salinity and scaling potential. The treatments also removed organic contaminants significantly, including TOC, HEM, and TPH (C6 to C35), which are essential for reducing environmental and health risks associated with PW. Key toxic constituents, such as ammonia, were reduced to non-detectable levels, highlighting the effectiveness of the treatment for nonconventional pollutants. Collectively, these findings align with the previous studies on thermal distillation-based PW treatment ([7,32]) and underscore the overall effectiveness of the treatment processes for potential reuse applications. The following sections examine analytes that exhibited significant changes during treatment to provide a deeper understanding of water quality.

3.1.2. Impact of treatment processes on VOCs

Targeted analyses included a total of 92 VOCs for each sample. Fig. 1 and Table 2 show changes in VOC concentrations throughout the treatment process, from the feed through distillation and post-treatment. Table 2 highlights the detected analytes and provides a comparative summary of removal efficiencies at each treatment stage. Of the 92 targeted VOCs, 17 were detected in the feed PW, 14 in the distillate, and only one in the post-treated effluent. These results indicate that the treatment train achieved substantial overall VOC reduction, with the greatest removal occurring during post-treatment. Many VOCs were detected at concentrations below the laboratory reporting limit (RL) but above the MDL, including detections in the raw PW (2-butanone, n-hexane, and naphthalene) and the distillate (4-methyl-2-pentanone, 2-butanone, and naphthalene). These results were included in the analysis to support interpretation of contaminant presence and trends; however, due to the increased analytical uncertainty associated with measurements in this concentration range, the reported concentrations are considered estimates. For *n*-propylbenzene, distillation achieved an 84.23–100% reduction, with concentrations reaching non-detectable levels (<0.000429 mg/L), indicating that distillation alone was sufficient for complete removal. BTEX (benzene, toluene, ethylbenzene, and xylenes) compounds showed a significant reduction during distillation (85.86–95.21%), with concentrations in the distillate decreasing to 0.0213, 0.0236, 0.00234, and 0.0181 mg/L, respectively. Post-treatment further reduced concentrations of all BTEX to below detectable limits, achieving an overall removal efficiency of 98.15–100%. Considering the most stringent human health National Recommended Ambient Water Quality Criteria (AWQC) (benzene: 0.00058 mg/L; toluene: 0.057 mg/L; ethylbenzene: 0.068 mg/L) for the consumption of water and organisms, as well as the Maximum Contaminant Levels (MCLs) (benzene: 0.005 mg/L; toluene: 1 mg/L; ethylbenzene: 0.7 mg/L; xylenes: 10 mg/L) set by the EPA's National Primary Drinking Water Regulations (NPDWR) at 0.005 mg/L, the distillate still needs further treatment while the post-treated water meets all relevant criteria for the protection of human health [33,34]. Similarly, 1,2,4-trimethylbenzene showed an overall reduction of 98.60–100%, with removal across both treatment phases. These results highlight the effectiveness of the combined treatment in removing hazardous monoaromatic hydrocarbons, previously identified as potential stressors to *D. rerio* on PW distillates [7,8].

2-Butanone showed a moderate reduction of 38.67% during distillation, followed by an additional 82.42–100% reduction in post-treatment, with final concentrations below detection limits (< 0.00828 mg/L). Similarly, 4-Methyl-2-pentanone similarly showed effective reductions across both treatment phases, with a final

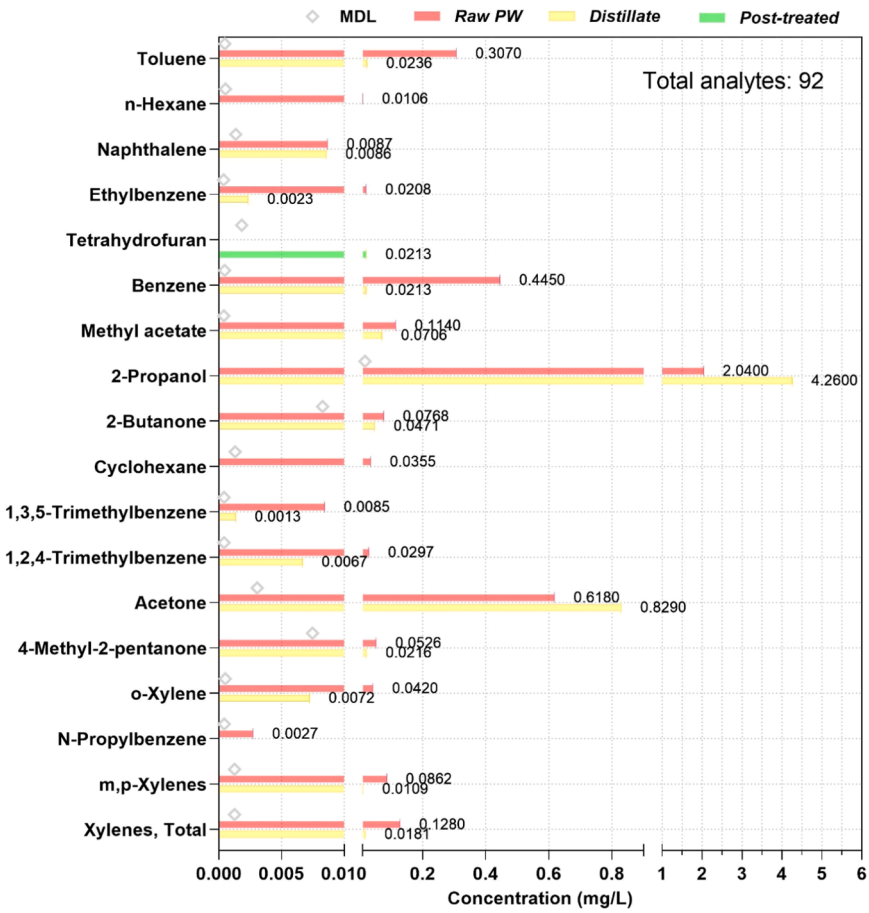

Fig. 1. Targeted characterization of VOCs in raw PW, MVR distillate, and post-treated water by GAC and zeolite; Out of 92 analyzed VOCs, 74 were not detected in all water samples.

Table 2
Distillation and post-treatment performance: removal of VOCs.

Analyte	Unit	Raw PW	Distillate	Post-treated	R-D change (%)	D-P change (%)	R-P change (%)
Xylenes, Total	mg/L	0.128	0.0181	< 0.00124	-85.86	-93.15–100	-99.03–100
m,p-Xylenes	mg/L	0.0862	0.0109	< 0.00124	-87.35	-88.62–100	-98.56–100
n-Propylbenzene	mg/L	0.00272	< 0.000429	< 0.000429	-84.23 – 100	0.00	-84.23–100
o-Xylene	mg/L	0.042	0.00724	< 0.000502	-82.76	-93.07–100	-98.80–100
4-Methyl-2-pentanone	mg/L	0.0526	0.0216	< 0.00749	-58.94	-36.68–100	-85.76–100
Acetone	mg/L	0.618	0.829	< 0.00307	+ 34.14	-99.63–100	-99.50–100
1,2,4-Trimethylbenzene	mg/L	0.0297	0.00668	< 0.000417	-77.51	-93.76–100	-98.60–100
1,3,5-Trimethylbenzene	mg/L	0.00845	0.00134	< 0.000411	-84.14	-69.93–100	-95.14–100
Cyclohexane	mg/L	0.0355	< 0.00129	< 0.00129	-96.37–100	0–100	-96.37–100
2-Butanone	mg/L	0.0768	0.0471	< 0.00828	-38.67	-82.42–100	-89.22–100
2-Propanol	mg/L	2.04	4.26	< 0.00523	+ 108.82	-99.88–100	-99.74–100
Methyl acetate	mg/L	0.114	0.0706	< 0.00401	-38.07	-94.32	-96.48–100
Benzene	mg/L	0.445	0.0213	< 0.000460	-95.21	-97.84–100	-99.90–100
Tetrahydrofuran	mg/L	< 0.00917	< 0.00183	0.0213	N/A	+ 1063	+ 132
Ethylbenzene	mg/L	0.0208	0.00234	< 0.000385	-88.75	-83.55	-98.15–100
Naphthalene	mg/L	0.00867	0.00858	< 0.00135	-1.04	-84.27–100	-84.83–100
n-Hexane	mg/L	0.0106	< 0.000517	< 0.000517	-95.12–100	0–100	-95.12–100
Toluene	mg/L	0.307	0.0236	< 0.000475	-92.31	-97.99–100	-99.85–100

R-D change (%): distillation removal efficiency, raw PW vs. distillate, – a percentage reduction with respect to raw PW feed; + percentage increment with respect to raw PW feed. D-P change (%): post-treatment removal efficiency, distillate vs. post-treated water, – a percentage reduction with respect to distillate; + percentage increment with respect to distillate. R-P change (%): complete treatment removal efficiency, raw vs. post-treated, – a percentage reduction with respect to raw PW feed; + percentage increment with respect to raw PW feed. N/A: not applicable as not detected in raw PW. The dilution factor for raw PW before analysis is 5.

concentration below MDL (< 0.00749 mg/L) and final removal efficiencies of 85.76–100%. Cyclohexane exhibited high removal efficiency, with distillation reducing its concentration from 0.0355 mg/L to below detection limits (<0.00129 mg/L), and post-treatment maintained below the detection limit of cyclohexane for a total reduction of 96.37–100%. Methyl acetate decreased from 0.114 mg/L to 0.0706 mg/L during distillation, followed by a further reduction in post-treatment to below detection limits (< 0.00401 mg/L), achieving an overall removal efficiency of 96.48–100%. During distillation, *n*-Hexane was effectively reduced to below detectable levels (< 0.000517 mg/L), achieving up to

95.12–100% reduction.

Despite the overall reduction in TOC, the concentrations of certain VOCs, such as acetone and 2-propanol, increased during distillation, indicating a greater tendency for these compounds to be recovered and concentrated in the distillate compared to other VOCs. To explore how the physical properties (molecular weight, hydrophobicity as log Kow, vapor pressure, boiling point, and solubility in Table S5) of VOCs impact their removal, pairwise correlations among multiple physical properties were analyzed using GraphPad Prism (version 10.6.1). Pearson correlation coefficients were applied based on data normality assessed by the Shapiro-Wilk test. Correlation matrices were generated, and statistical significance was evaluated using two-tailed tests ($p < 0.05$). Table S6 indicates that the molecular weight and hydrophobicity exhibit positive relationships (Pearson $r = 0.6746$ and 0.7909, respectively) with VOC removal by MVR, whereas the solubility shows a strong negative relationship (Pearson $r = -0.9567$) with the removal rate by MVR. Those results suggest that compounds with high molecular weights, high hydrophobicity, and low solubility tend to remain in the concentrate instead of transitioning into the gas phase. Specifically, acetone, 2-propanol, 2-butanone, methyl acetate, and 4-methyl-2-pentanone exhibited a greater tendency for carryover into the distillate, with changes ranging from a 59% decrease to a 109% increase, which may be attributed to their low hydrophobicity and high solubility. Surprisingly, although volatility can determine the transition of compounds into the gas phase, vapor pressure and boiling point are not the main drivers of recovery in the distillate (P value = 0.1969 and 0.0884, Table S6). For example, highly volatile compounds (vapor pressure at 25 °C > 95 mm Hg), including benzene, *n*-hexane, and cyclohexane, were not easily recovered in the distillate, with removals exceeding 95%. In contrast, several less volatile compounds (vapor pressure at 25 °C < 90 mm Hg), such as 2-propanol, 2-butanone and 4-methyl-2-pentanone, tended to be recovered in the distillate, exhibiting poor removals or even net increases in concentration (-59% to +108%). Similar behavior has been reported for membrane distillation units treating PW, in which 2-butoxyethanol (2-BE) exhibited higher mass transfer than acetic acid, ethylene glycol, and isopropyl alcohol, despite having a lower vapor pressure [35].

Overall, these results raise questions about volatility as the primary driver of compound partitioning in MVR distillation, suggesting that hydrophobicity and solubility may play a significant role under the tested conditions. Although volatility governs the transition of VOCs into the gas phase, intrinsic hydrophobicity may limit VOC carryover in the distillate. This rationale is consistent with the design and operation of the MVR system, where continuous mixing of vapor and brine is promoted to enhance heat and mass transfer. However, these conditions may favor the presence of hydrophilic VOCs in the distillate, as observed for 2-propanol, acetone, 2-butanone, methyl acetate, and 4-methyl-2-pentanone. Similar to other organics, post-treatment with GAC effectively reduced VOCs that increased during the distillation process. Specifically, acetone and 2-propanol were reduced to below detection limits (< 0.00307 mg/L and < 0.00523 mg/L, respectively), corresponding to overall removal efficiencies of approximately 99.50–100%. Interestingly, tetrahydrofuran (THF), which was not detected in either the feed or distillate, was identified in the post-treated water at a concentration of 0.0213 mg/L. Its presence after treatment suggests possible introduction during the post-treatment phase. Potential sources include leaching from polymeric components used in the post-treatment columns, such as tubing, seals, or sealants, or cross-contamination during sample handling and processing. This unexpected detection warrants further investigation to identify the specific source and implement corrective measures. Addressing this contamination is essential to maintain treatment integrity and prevent the reintroduction of trace pollutants in the final effluent, particularly when aiming to produce high-quality water suitable for unrestricted beneficial reuse.

The results demonstrate the effectiveness of the combined distillation and post-treatment processes in removing VOCs from raw PW. Distillation substantially reduced the concentrations of most VOCs, especially those with low solubility and high hydrophobicity. In contrast, hydrophilic and highly soluble compounds (log Kow < 1.5 and solubility >19,000 mg/L) exhibited poor removal or even increased concentrations after distillation, regardless of their vapor pressures (ranging from 20 to 232 mm Hg at 25 °C). These findings provide insights into the physical properties that govern the partitioning and removal of VOC from PW in thermal distillation. All VOCs detected in the distillate were subsequently reduced to non-detectable levels following post-treatment, achieving near-complete removal. These findings emphasize the critical importance of compound-specific monitoring in evaluating treatment performance and treated PW quality.

3.1.3. Impact of treatment processes on SVOCs

As summarized in Table S2, SVOCs were characterized using two methods: SW846–8270D SIM (16 targeted analytes) and SW846–8270E LL (64 targeted analytes). Using SW846–8270D SIM, 5 analytes were detected in both the feed and the distillate, and none were detected after post-treatment. Using SW846–8270E LL, 7 analytes were detected in the feed, 9 in the distillate, and 1 after post-treatment. SVOC concentrations were consistently lower than VOC concentrations and remained below 500 μg/L throughout the treatment train. Similar to VOCs, several SVOCs were detected between the MDL and RL in the feed PW (1,2-dichlorobenzene, 2-methylnaphthalene, 2-methylphenol, naphthalene, phenol, and pyridine) and in the distillate (2-methylnaphthalene, fluorene, naphthalene, and pyridine). These results were used to inform interpretation but are considered estimates.

Table S4 and Fig. 2 summarize SVOC behavior across the three treatment stages. Overall, removals during distillation were limited, whereas post-treatment effectively addressed residual SVOCs. During MVR distillation, with the exception of 1,2-dichlorobenzene, which was reduced to below the MDL, most SVOCs either increased in concentration or showed only slight reductions. Several compounds, including phenolic compounds (phenol, 2-methylphenol, 2,4-dimethylphenol, and 3- and 4-methylphenol), fluorene, and N-nitrosodiphenylamine, increased significantly during distillation. When interpreted in conjunction with the physicochemical properties compiled in Table S5, Pearson correlation analyses reveal that, when considered individually, the investigated physical properties do not adequately explain SVOC mass transfer into the distillate ($P > 0.05$; Table S6). Except for pyridine, the detected SVOCs have relatively low vapor pressures at 25 °C (<1.36 mm Hg) compared with VOCs (2.1–232 mm Hg), yet multiple SVOCs increased by orders of magnitude during distillation (Table S4 and Fig. 2).

Consistent with the trends discussed in Section 3.1.2, the observed SVOC behavior likely reflects additional mechanisms beyond those related to physical, chemical, and thermodynamic properties in Table S5. Contributing factors may include brine-vapor mixing and hydrodynamics within the MVR system, cross-contamination, and thermally driven transformation of organic compounds [35,36]. The continuously mixed configuration of the MVR unit promotes turbulent vapor-liquid conditions that enhance heat and mass transfer; however, it has been documented that turbulence can also increase aqueous phase carryover through fine droplet entrainment [37–39]. Under this hypothesis, if entrainment and carryover contribute materially, the distillate composition would be expected to skew toward more hydrophilic organics with limited volatility. This is consistent with the presence of 2, 4-dimethylphenol, methylphenol, phenols, and pyridine (log Kow <3, Table S4). In contrast, more hydrophobic compounds such as 1,2-dichlorobenzene, naphthalene, 2-methylnaphthalene, and fluorene (log K_{ow} > 3.3) generally occurred at lower concentrations in the MVR distillate (Table S5 and Fig. 2). However, the p-value of the Pearson correlation exceeds 0.05 ($P = 0.1069$), indicating that hydrophobicity may not play a dominant role in SVOC removal. Within this group, naphthalene showed minimal change during distillation, decreasing slightly from

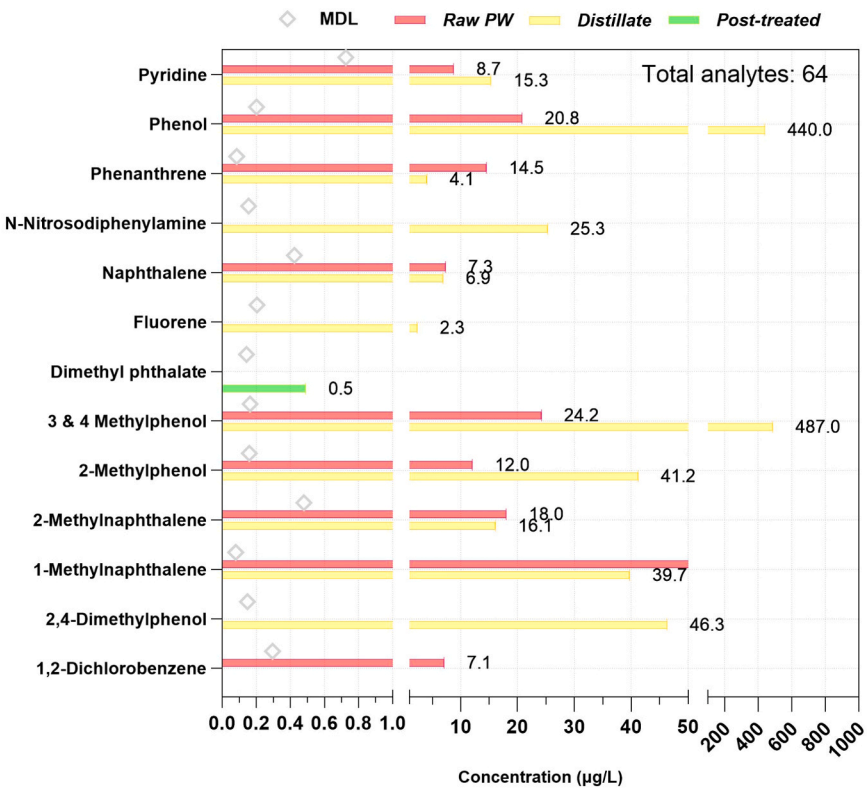

Fig. 2. Targeted characterization of SVOCs in raw PW, MVR distillate, and post-treated water by GAC and zeolite; Out of 64 analyzed SVOCs, 51 were not detected in all water samples.

7.30 µg/L in the raw PW to 6.86 µg/L in the distillate. These results align with previous findings [7], indicating that naphthalene was relatively persistent after MVR distillation. Similarly, 2-methylnaphthalene exhibited minimal variation, decreasing from 18.0 µg/L to 16.1 µg/L. Although a detailed mechanistic evaluation is beyond the scope of this study, these findings emphasize an important point. Bulk organic reductions during thermal treatment of PW do not necessarily predict the fate of individual constituents. Resolving the mechanisms that control actual compound separation will be essential for advancing thermally-driven PW desalination. This will require studies that link system design and operating conditions to analyte-specific physicochemical properties. This strategic work is needed to distinguish the relative contributions of compound properties and process-driven effects in governing the overall fate of the compounds.

Similar to THF, dimethyl phthalate was detected only after post-treatment, suggesting its potential introduction during these stages rather than originating from the PW itself. This observation aligns with the possibility of leaching from polymeric materials (e.g., PVC tubing and fittings) used in the GAC/zeolite column system. Phthalates, commonly employed as plasticizers, are known to migrate from plastic components into aqueous environments [40]. While no official AWQC has been established for THF, the detected concentration of 0.049 µg/L remains well below the recently proposed long-term freshwater water quality criterion of 13.7 µg/L [41].

Overall, MVR distillation alone frequently led to modest reductions and, in several cases, increases in SVOC concentrations in the distillate. Elevated levels of compounds such as phenols (including 2,4-dimethylphenol, 3- and 4-methylphenol, and phenol), N-nitrosodiphenylamine, and pyridine highlight the complex volatilization and partitioning behavior of these substances within the MVR unit. These findings are consistent with prior studies that emphasize the limitations of distillation alone in removing specific SVOCs from PW [7]. However, the combined treatment approach proved more effective: all SVOCs identified in the distillate (Table S4 and Fig. 2) were reduced to below detection limits following post-treatment with GAC and zeolite. These results demonstrate the effectiveness of the integrated treatment strategy to address SVOCs in PW.

3.1.4. *Impact of treatment processes on volatile fatty acids (VFAS)*

Table S7 and Fig. 3a illustrate changes in VFA concentrations throughout the treatment process. Acetic acid was the only VFA detected in the feed PW, decreasing markedly from 112 mg/L to below detection limits (< 3.2 mg/L) following distillation. Based on this initial profile, no other VFAs were expected in the distillate. However, caproic, propionic, valeric, and butyric/isobutyric were detected after distillation. While butyric/isobutyric acid appeared at a relatively low concentration (2.42 mg/L), the other VFAs were present at higher levels: caproic acid at 86.5 mg/L, propionic acid at 123 mg/L, and valeric acid at 198 mg/L in the distillate. During the MVR operation, a mechanical compressor failure caused lubrication oil to leak into the steam distillate conduit. Although all residual oil was manually removed before restarting the unit, the elevated VFA concentrations observed in the distillate indicate probable contamination from this incident, as these analytes were not detected in the raw PW. Although a food-grade lubricant blend was used in the compressor, residual organic acids may still reduce dissolved oxygen levels downstream of the discharge. While these compounds were not specific targets of the post-treatment process, GAC post-treatment nonetheless markedly reduced the acids introduced during the compressor failure: propionic, valeric, and butyric/isobutyric acids decreased to below detection limits (< 2 mg/L), and caproic acid declined to 7.35 mg/L. These findings underscore the complexity of scaling up technologies and highlight the value of comprehensive monitoring in detecting process deviations. This analysis not only identified the contamination source but also provided insights to optimize compressor design and improve operation and maintenance practices for commercial applications.

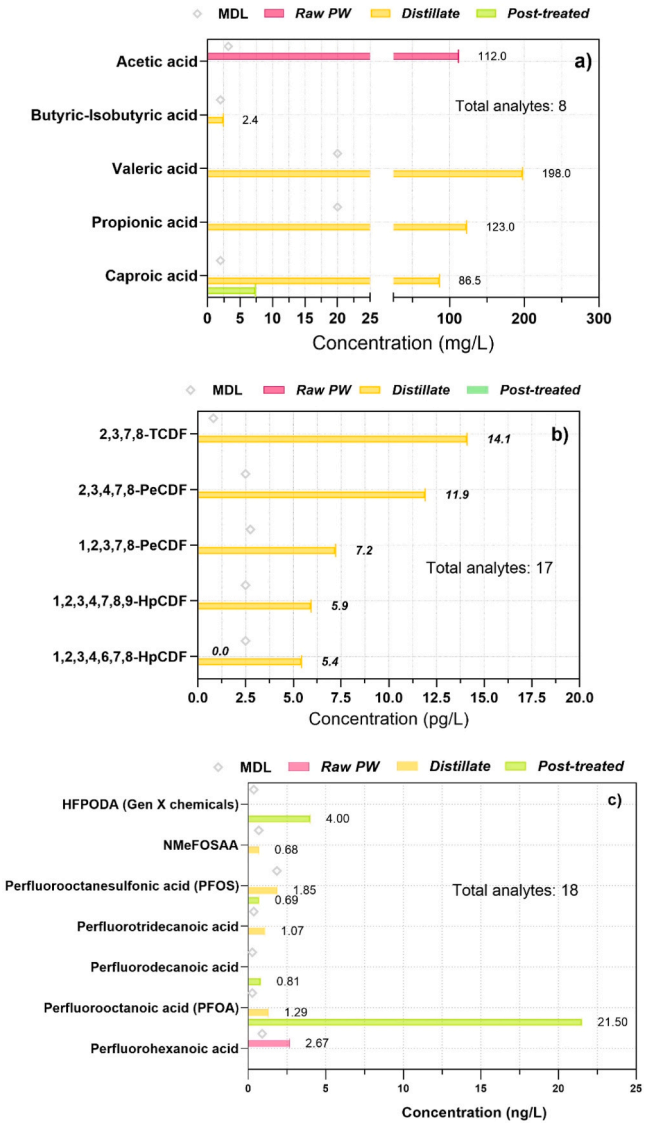

Fig. 3. Targeted characterization of VFAs (a), Furans (b) and PFAS (c) in raw PW, MVR distillate, and post-treated water by GAC and zeolite; Out of 8 analyzed VFAs, 3 were not detected in all water samples; Out of 17 analyzed dioxins and furans, 12 were not detected in all water samples. Out of 18 analyzed PFAS, 11 were not detected in all water samples.

3.1.5. *Impact of treatment processes on dioxins and furans*

Dioxins and furans are known for their high toxicity, bioaccumulation, and environmental persistence, making their removal essential to ensure environmental safety in PW reuse [42,43]. Table S7 and Fig. 3b provide data on concentration changes of these analytes throughout the treatment process. Although dioxins were not identified in the samples, five furans were detected after distillation: 2,3,7,8-TCDF (14.1 pg/L); 2,3,4,7,8-PeCDF (11.9 pg/L); 1,2,3,7,8-PeCDF (7.21 pg/L); 1,2,3,4,7,8,9-HpCDF (5.93 pg/L) and 1,2,3,4,6,7,8-HpCDF (5.42 pg/L). Two phenomena may explain these findings: (i) these furans were present in the raw PW but went undetected due to matrix effects, such as high concentrations of other organic and inorganic compounds affecting ionization, elution, and promoting adduct formation [44]; or (ii) these furans may reflect in-process formation (co-distillation by-products) during MVR distillation. The presence of chlorinated organic compounds (e.g., 1,2-dichlorobenzene), inorganic chloride salts, and the elevated temperatures inherent to vaporization and vapor recompression may, in principle, create conditions associated with chlorinated furan formation ([42,45,46,43]). These findings represent a novel observation in PW desalination and underscore the need for systematic monitoring of process conditions and post-distillation water quality. Given that elevated temperatures, organic matter, and high chloride concentrations are intrinsic to the process, it is necessary to determine whether the detected furans represent an isolated occurrence or are promoted by MVR operating conditions. These results are consistent with recent studies on PW distillation, indicating that PW distillates may retain multiple residual constituents of concern at low concentrations [7,13]. Comprehensive characterization of PW effluents is therefore necessary not only to assess treatment performance but also to identify potential treatment artifacts, including co-distillation by-products and the introduction of new pollutants associated with in-process upsets. Although furans were detected after the MVR distillation process, post-treatment effectively reduced the concentration of all identified furans to below detection limits: 2,3,7,8-TCDF (<0.809 pg/L), 2,3,4,7,8-PeCDF (<2.49 pg/L), 1,2,3,7,8-PeCDF (<2.75 pg/L), 1,2,3,4,7,8,9-HpCDF (<2.49 pg/L), and 1,2,3,4,6,7,8-HpCDF (<2.49 pg/L). These results are consistent with previous findings on post-treatment of PW distillates with GAC, where most identified organics were reduced below MDL [8].

3.1.6. *Impact of treatment processes on PFAS*

PFAS are a large class of synthetic chemicals that have been widely used since the 1940s due to their unique physicochemical properties, including thermal stability, chemical resistance, and water- and oil-repellency. However, concerns about PFAS have escalated in recent years due to their environmental persistence, bioaccumulation potential, and adverse health effects such as cancer, liver and kidney dysfunction, immune suppression, and developmental toxicity [47–49].

Table S7 and Fig. 3c present PFAS concentrations across the feed, distillation, and post-treatment stages. Of the 19 PFAS monitored, only perfluorohexanoic acid (PFHxA) was detected in the raw PW, at 2.67 ng/L. Although PFAS have been used in oil and gas operations to enhance permeability, reduce interfacial tension, and improve wettability [50], their presence in the raw PW studied was limited. These findings are consistent with previous characterizations of PW from the Permian Basin, which have reported PFAS at concentrations below 1 ng/L: PFBS (0.17 ng/L), PFBA (0.31 ng/L), PFHxS (0.25 ng/L), NEtFOSE (0.98 ng/L), and PFTeDA (0.24 ng/L) [5]. After distillation, additional PFAS were detected, including perfluorooctanoic acid (PFOA, 1.29 ng/L), perfluorotridecanoic acid (PFTrDA, 1.07 ng/L), perfluorooctanesulfonic acid (PFOS, 1.85 ng/L), and N-methyl perfluorooctane sulfonamidoacetic acid (NMeFOSAA, 0.680 ng/L). Following post-treatment, PFOS (0.686 ng/L), perfluorodecanoic acid (PFDA, 0.812 ng/L), hexafluoropropylene oxide dimer acid (HFPO-DA, 4.00 ng/L), and PFOA (21.5 ng/L) were detected in the effluent. The substantial increase in PFOA and HFPO-DA (GenX chemicals) in the final treated water suggests potential contamination introduced during post-treatment. While identifying the exact source is beyond the scope of this study, possible PFAS sources include the materials and parts used in GAC and zeolite treatment systems (e.g., tubing, columns, sealing materials).

From a regulatory perspective, it is noteworthy that the raw PW met the MCLs under the NPDWR for PFOA and PFOS (each 4 ng/L), as well as for PFHxS, HFPO-DA, and PFNA (each 10 ng/L) [33]. However, in the post-treated thermal distillate, PFOA exceeded the MCL at 21.5 ng/L, and HFPO-DA was detected at the MCL of 4 ng/L. Although PFOA levels in the post-treated finished PW also exceeded the NPDWR MCL, they remained well below the EPA's recommended AWQC for aquatic life, which are 3.1 mg/L (acute) and 0.1 mg/L (chronic) [51,52]. As discussed, the significant increase of PFOA and HFPO-DA in the final post-treated water suggests potential introduction during post-treatment. This elevation not only leads to exceedance of the NPDWR MCL for PFOA but also highlights the broader challenges of managing PFAS. Identifying and controlling these contamination pathways is essential to maintain consistent water quality. Future efforts

should focus on improving post-treatment design, construction, and operational and maintenance practices to prevent PFAS introduction, ensuring compliance with emerging criteria while protecting public health.

3.1.7. Impact of treatment processes on pesticides, herbicides, polychlorinated biphenyls (PCBs), rare earth metals, and isotopic uranium

This study also included the characterization of other potential contaminants, such as pesticides (e.g., 4,4'-DDD, aldrin, dieldrin), PCBs, herbicides (e.g., pentachlorophenol, 2,4-D, dicamba), organophosphorous pesticides (e.g., malathion, diazinon), rare earth metals (e.g., dysprosium, neodymium, europium), and isotopic uranium species. Although these compounds are not expected in PW due to their lack of direct application in oil and gas extraction, they could be introduced through freshwater and brackish water sources used in extraction (e.g., pesticides, herbicides) or originate from geological formations (e.g., uranium). None of these analytes were detected in the tested water samples, indicating their absence or concentrations below the detection limits of the analytical methods. Therefore, these contaminants did not pose a significant concern in this study. These results emphasize the importance of site-specific assessments, as PW composition can vary greatly based on geological formations and extraction methods [2]. Table S8 summarizes more information on the characterization of herbicides, PCBs, rare earth metals and isotopic uranium.

3.1.8. Impact of treatment processes on radionuclides

Several radioisotopes derived from naturally occurring radioactive materials (NORM) have been identified in PW and present a unique challenge for PW management [2,5]. While various technologies can be used for NORM removal in PW, limited studies have documented NORM behavior in complete treatment trains for PW beneficial reuse [2].

Table 3 and Figure S6 illustrate the variations in radionuclide concentrations throughout the treatment process, spanning from the feed stage to distillation and post-treatment. As presented in Tables 3, 4 radioisotopes, including radium-226 (24.3 pCi/L), radium-228 (18.6 pCi/L), gross alpha particles (1320 pCi/L), and gross beta particles (563 pCi/L) were detected in the raw PW. The distillation process effectively removed all the radionuclides to a non-detectable level, while radium-226, radium-228, and gross alpha remained undetectable after post-treatment. A low concentration of gross beta activity (1.25 pCi/L) was detected in the final treated water, which remained well below the 50 pCi/L screening level used for routine monitoring decisions in vulnerable community water systems under the Radionuclides Rule [33]. The gross beta activities in the final effluent are likely from the trapped radionuclides in the GAC used in the post-treatment.

3.1.9. Impact of treatment processes on total and dissolved metals

Table S9 and Fig. 4 provide an in-depth view of the changes in concentration for a variety of metals, including total and dissolved concentrations, throughout distillation and post-treatment. As shown in Fig. 4, toxic and regulated metals and metalloids such as arsenic (As), cadmium (Cd), copper (Cu), chromium (Cr), lead (Pb), and zinc (Zn) were not detected in the raw PW. This contrasts with previous research on Permian Basin PW, where these metals were found at average concentrations of As (3.17 mg/L), Cd (0.47 mg/L), Cu (0.65 mg/L), and Cr (1.7 mg/L) [5]. These metals pose significant concerns due to their toxicity, environmental persistence, and stringent regulatory standards [8]. The absence of these contaminants in the raw PW collected in this study shows the variability of PW quality in the Permian Basin. The total and dissolved barium (Ba) concentrations in the raw PW decreased significantly from 30.3 and 31.0 mg/L to 0.00578 and 0.00540 mg/L after distillation, and further reduced to 0.00178 and 0.00495 mg/L, respectively, after post-treatment. These changes resulted in reductions exceeding 99.9%, with Ba concentrations in both the distillate and final effluent remaining below the NPDWR MCL (2 mg/L, as shown in Table S9 and Fig. 4) [33]. Total selenium (Se) remained below detection limits throughout the entire process. Dissolved Se was reduced from 0.745 mg/L to 0.0170 mg/L during distillation (97.72% reduction), with no significant changes after post-treatment (0.0125 mg/L), below the NPDWR MCL 0.05 mg/L [33].

In the raw PW, the total and dissolved aluminum (Al) concentrations were identified at 1.8 mg/L and < 1.76 mg/L, respectively. After distillation, both concentrations exhibited similar levels, with the total and Al concentration reduced to 0.0385 and 0.0390 mg/L, respectively. No significant alterations were observed after post-treatment, with concentrations of 0.0529 mg/L and < 0.0352 mg/L, respectively, for total and dissolved aluminum. Total iron (Fe) concentration decreased from 43.6 mg/L in the feed to 0.259 mg/L in the distillate, achieving a 99.41% reduction. Post-treatment further reduced total Fe to below detection limits (< 0.0283 mg/L), resulting in an overall reduction of 99.94%. Dissolved Fe, initially at 34.0 mg/L, was reduced to below the detection limit (< 0.0283 mg/L) after distillation, a concentration that did not change after post-treatment, achieving a total reduction of 99.92%. The total manganese (Mn) content in the feed decreased from 2.53 mg/L to 0.011 mg/L after distillation, resulting in a 99.57% reduction. There were no significant changes in total Mn levels after post-treatment, which was determined at 0.0135 mg/L. The dissolved Mn concentration also showed a similar trend, with 0.011 mg/L after distillation and 0.014 mg/L after post-treatment. Overall, Al, Fe, and Mn concentrations in the final treated water meet the requirements of drinking water regulations, indicating the effective management throughout the treatment strategy.

Total boron (B) decreased from 13.2 mg/L in the feed to < 0.0162 mg/L after distillation ($\geq$99.88% reduction) and remained below the MDL following post-treatment. Total phosphorus (P) decreased significantly from 5.40 mg/L in the feed to 0.08 mg/L after distillation (99.04% reduction), with a slight increase to 0.17 mg/L post-treatment. Dissolved phosphorus P showed a similar trend, decreasing from 8.20 mg/L to 0.08 mg/L during distillation, then rising to 0.11 mg/L post-treatment. The overall P reduction was 97.9%, indicating substantial removal during distillation, with minor increases likely due to desorption or ion exchange occurring during the GAC and zeolite post-treatments. Silicon (Si) concentrations were significantly reduced from 12.7 mg/L to below detection limits during distillation (< 0.173 mg/L).

Table 3
Distillation and post-treatment performance: Radionuclides.

Analyte	Unit	Raw PW	Distillate	Post-treated	R-D change (%)	D-P change (%)	R-P change (%)
Gross Alpha	pCi/L	1320	0.513*	0.827*	-99.96–100	N/A	-99.94–100
Gross Beta	pCi/L	563	0.148*	1.25	-99.97–100	+ 745	-99.78
Radium-226	pCi/L	24.3	0.103*	0.0295*	-99.58–100	N/A	-99.58–100
Radium-228	pCi/L	18.6	0.345*	0.699	-98.15–100	+ 103	-96.24

R–D change (%): distillation removal efficiency, raw PW vs. distillate, – a percentage reduction with respect to raw PW feed; + percentage increment with respect to raw PW feed. D–P change (%): post-treatment removal efficiency, distillate vs. post-treated water, – a percentage reduction with respect to distillate; + percentage increment with respect to distillate. R–P change (%): complete treatment removal efficiency, raw vs. post-treated, – a percentage reduction with respect to raw PW feed; + percentage increment with respect to raw PW feed. N/A: not applicable as not detected in raw PW.

*: either absent or present at a level too low to be measured. Negative values do not indicate negative radiation but reflect measurement uncertainty and background variability, with the true concentration likely near zero. The dilution factors for all the samples before analysis are 1.

Table 4
Dose-response assessment on *V. fischeri*.

	Sample ID	NOEC [%]	LOEC [%]	IC_{25} or LC_{50} [%, 95% C. I.]	Hypothesis test (S - NS)	Point estimate test	Effect at 100%	Toxicity reduction [%] [TR]
V. fischeri	Raw PW	< 6.25	6.25	5.71 (4.83–6.92)[IC]	S[DT]	LI	100	-
	Distillate	< 6.25	6.25	8.66 (8.09–9.29)[IC]	S[DT]	LI	97.6	2.4
	Post-treated	100	> 100	> 100 (N/A)[IC]	NS[DT]	LI	3.3	96.7
R. subcapitata	Raw PW	< 6.25	6.25	6.64 (6.43–6.88)[IC]	S[SMORT]	LI	99.9	-
	Distillate	25	50	38.79 (36.95–40.90)[IC]	S[DT]	LI	84.2	15.7
	Post-treated	100	> 100	> 100 (N/A)[IC]	NS[SMORT]	LI	-21.1	> 100
C. dubia	Raw PW	< 6.25	6.25	1.69 (1.69–1.69)[LC]	S[SMORT]	LI	100	-
	Distillate	50	100	63.73 (57.02 – 71.23)[LC]	S[SMORT]	SK	100	0.0
	Post-treated	100	> 100	> 100 (N/A)[LC]	NS[SMORT]	LI	0.0	100
D. rerio	Raw PW	< 6.25	6.25	1.69 (1.69–1.69)[LC]	S[SMORT]	P	100	-
	Distillate	6.25	12.5	19.17 (13.79–24.56)[LC]	S[SMORT]	P	100	0.0
	Post-treated	100	> 100	> 100 (N/A)[LC]	NS[SMORT]	P	-8.1	> 100

[IC]: concentration causing 25% inhibition (IC_{25}); [LC]: concentration causing 50% lethality (LC_{50}); 95% CI: 95% confidence upper and lower intervals; S: 100% sample concentration is statistically different from the control; NS: 100% sample concentration is not statistically different from the control; DT: Dunnett's Test.; SMORT: Steel's Many-One Rank Test; LI: Linear interpolation.; SK: Spearman-Karber; TSK: Trimmed Spearman-Karber; [TR]: reduction in toxicity (%) with respect to the Raw PW

However, Si levels sharply increased to 6.56 mg/L after post-treatment. This phenomenon has been documented previously in post-treatment of PW distillates with GAC and zeolite, where certain constituents, including Si, can be introduced due to complex interactions between the PW distillate and treatment materials [7]. Both total and dissolved strontium (Sr) were effectively managed throughout the treatment process. Total and dissolved Sr decreased from 3610 and 2900 mg/L to 0.161 and 0.144 mg/L after distillation, and further to 0.013 and 0.025 mg/L post-treatment, achieving an overall reduction of 99.99% for both species.

Similar to other pollutants, the treatment strategy effectively removed metals and nonmetals in PW, underscoring the importance of combining distillation with appropriate post-treatment methods. Although treated PW is not intended for reuse as a potential drinking water source, the findings highlight its potential for discharge to surface waters with stringent designated uses, including domestic supply.

3.2. Toxicological characterization

The toxicological characterization was consistent with the chemical characterization findings. Raw PW caused severe adverse effects across the tested concentration range in all species. Although MVR distillation substantially improved water quality, it resulted in only limited reductions in adverse effects across species. In contrast, post-treatment mitigated all evaluated toxicological endpoints, underscoring its role as a critical polishing barrier. The following sections present these toxicological results in detail.

3.2.1. Toxicological characterization: V. fischeri

The Microtox® *V. fischeri* acute toxicity test results for raw PW, MVR distillate, and post-treated water are shown in Fig. 5a. Additionally, Table 4 presents the statistical analysis and toxicity endpoints derived from the dose-response assessment. The raw PW exhibited significant toxicity to *V. fischeri*, with an NOEC below 6.25% and an IC_{25} value of 5.71%. Complete inhibition of bioluminescence was observed at 50% and 100% raw PW concentrations. As illustrated in Figure 14-A, even at the lowest concentration tested (6.25%), luminescence inhibition exceeded 20%. These findings underscore the high toxicity of raw PW to *V. fischeri*, emphasizing the importance of comprehensive treatment before discharge and the potential environmental impacts of raw PW spills and illegal dumping. For the distillate, the dose-response assessment showed similar effects on *V. fischeri*, with both the NOEC and LOEC remaining the same as in the raw PW at < 6.25%. This suggests that while the MVR distillation process effectively reduces salts, bulk organics, metals, and radionuclides, it may still leave some constituents at toxic concentrations in the distillate. These findings align with previous studies indicating that PW distillates can be toxic to *V. fischeri* due to residual constituents such as ammonia [7]. As presented in Fig. 5a, post-treatment proved highly effective in reducing toxicity to non-observable levels. No adverse responses were observed in the entire concentration range. These results demonstrate that the combination of distillation and post-treatment was successful in mitigating toxicity toward the bacteria *V. fischeri*.

3.2.2. Toxicological characterization: R. subcapitata

The *R. subcapitata* chronic WET results for raw PW, distillate, and final post-treated water are shown in Fig. 5b, with Table 4 providing the statistical analysis and toxicity endpoints from the dose-response assessment. Similar to *V. fischeri*, raw PW exhibited high toxicity to *R. subcapitata*, with complete growth inhibition observed at 25%, 50%, and 100% concentrations. As shown in Table 4, the LOEC was recorded at 6.25%, and the IC_{25} was 6.64%. Even low concentrations of raw PW severely impaired algal growth, with ~90% inhibition noted at 12.5% concentration at the 96-hour endpoint. These findings highlight the severe adverse effects that untreated PW can have on freshwater algae. The distillation process moderately reduced the toxicity of the raw PW *R. subcapitata*, as shown in Fig. 5b. No adverse effects were observed at distillate concentrations below 25% (NOEC: 25%). The IC_{25} for the distillate increased to 38.79%, indicating a significant reduction in toxicity compared to raw PW. However, adverse effects were still evident at the highest tested concentration (100%), where 84% growth inhibition was recorded. This is consistent with previous results [7], and demonstrates that although distillation effectively diminished the toxic impact on algae, it did not fully mitigate the adverse effects at higher concentrations. Post-treatment with GAC and zeolite effectively detoxified the PW for *R. subcapitata*, with no observable adverse effects even at full-strength effluent (NOEC: >100%). The overall toxicity reduction exceeded 100%, confirming that the integrated treatment approach successfully detoxified the PW for *R. subcapitata*.

3.2.3. Toxicological characterization: C. dubia

The acute WET results for *C. dubia* of the three waters are presented in Fig. 5c, with Table 4 detailing the statistical analysis and toxicity endpoints from the dose-response assessment. Exposure to raw PW resulted in dramatic adverse effects on *C. dubia*, with no survivors observed across the full concentration range tested. The complete mortality at the lowest concentration (6.25%) underscores the high levels of toxicants present in the raw PW and highlights the severe

Fig. 4. Targeted characterization of total and dissolved metals in raw PW, MVR distillate, and post-treated water by GAC and zeolite; Out of 59 analyzed metals, 32 were not detected in all water samples.

environmental impact that untreated PW spills can have on freshwater invertebrate populations. Distillation significantly reduced mortality in *C. dubia*, with the NOEC increasing to 50%, indicating a notable reduction in toxicity at concentrations below 50%. However, 100% mortality was still observed at full-strength distillate. These findings align with previous research showing that PW distillate caused 100% mortality in *C. dubia* neonates [7]. This outcome highlights that distillation alone is insufficient for fully mitigating toxic effects, emphasizing the need for post-treatment to achieve a non-toxic effluent. Consistent with the *V. fisheri* and *R. subcapitata* results, post-treatment completely mitigated the adverse effects on *C. dubia* (Fig. 5c).

3.2.4. Toxicological characterization: D. rerio

The zebrafish WET results for the three waters are presented in Fig. 5d, with Table 4 providing the statistical analysis and toxicity endpoints from the dose-response assessment. Similarly, raw PW exerted serious adverse effects on *D. rerio*. Complete mortality was observed across the full concentration range tested. These results demonstrate that even minor exposure to untreated PW (NOEC: <6.25%) can dramatically impact fish embryos and highlight the need to effectively manage PW to avoid incidental spills with the potential of impairing fish populations in receiving waters. As shown in Fig. 5c, distillation significantly reduced the toxicity of raw PW toward *D. rerio*. However, the LC_{50} value was estimated at approximately 19%, and complete mortality was observed at 100% concentration, demonstrating the limitations of the MVR distillation system in fully mitigating stressors present in raw PW. Consistent with other WET tests, post-treatment with GAC and zeolite effectively reduced mortality in *D. rerio* embryos, achieving a NOEC of 100%.

The toxicological assessment of PW effluents demonstrated significant risks to each trophic level when untreated, underscoring the necessity of a robust, multi-stage treatment approach. The changes in toxicity following distillation highlight the varying sensitivities of different aquatic organisms to PW contaminants and emphasize the need for comprehensive post-treatment to achieve non-toxic effluent. While distillation partially reduced toxicity, full detoxification was only achieved through post-treatment, which was essential for mitigating adverse effects across all tested organisms (bacteria, algae, freshwater

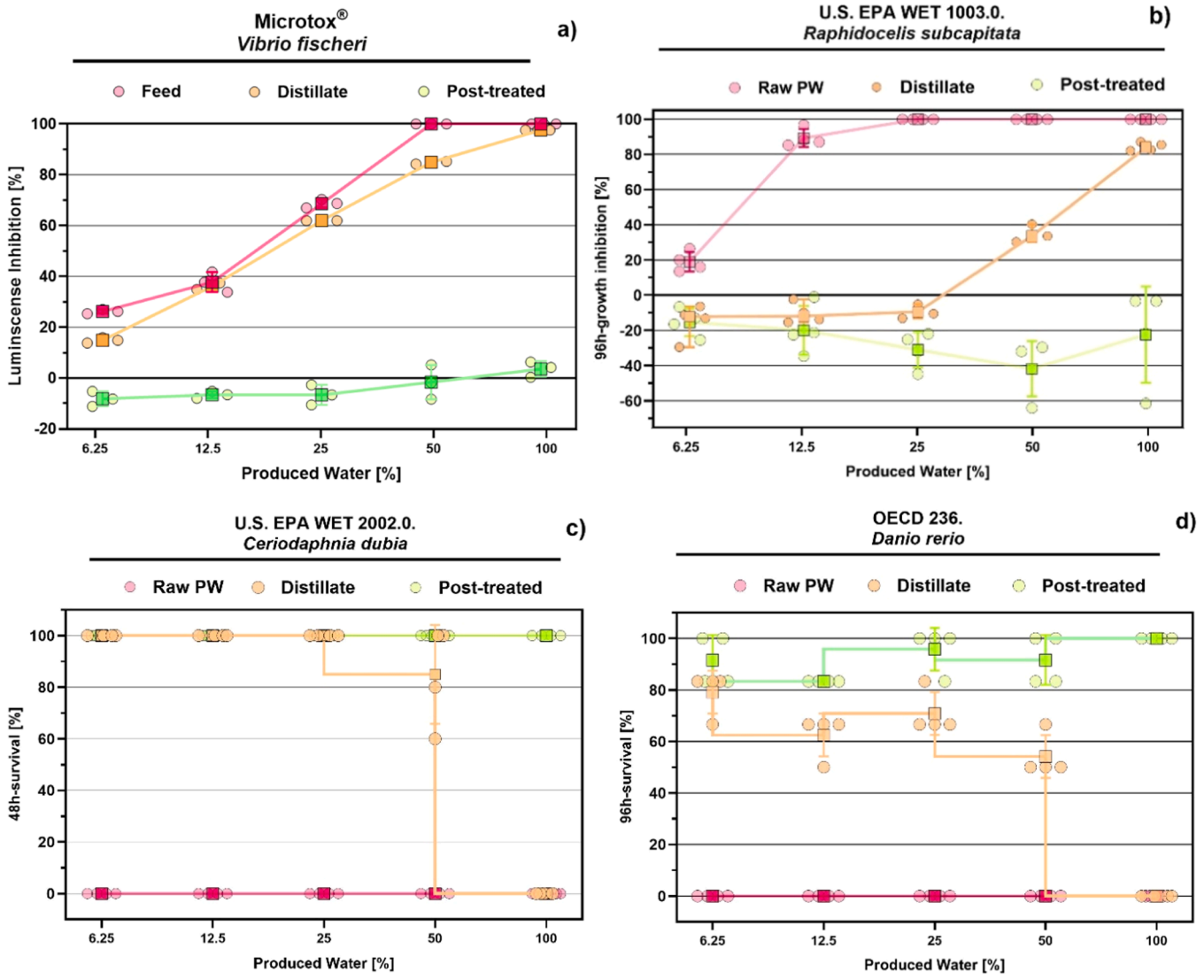

Fig. 5. Toxicological characterization of raw PW, MVR distillate, and post-treated water by GAC and zeolite: *V. fischeri* (a), *R. subcapitata* (b), *C. dubia* (c) and *D. rerio* (d). *V. fischeri*: 3 experimental replicates, 15 min of exposure time; ***R. subcapitata*:** 4 experimental replicates, 96 h of exposure time; ***C. dubia***: 20 experimental replicates grouped in 4 groups of 5 replicates (4 ×5), 48 h of exposure time; *D. rerio*: 24 experimental replicates grouped in 3 groups of 8 replicates (3 ×8), 96 h of exposure time; Error bars: standard deviation in; C: controls; ns: effects not significantly different from the control.

invertebrates, and fish).

3.2.5. *Cardiotoxicity and teratogenic effects on early stages of D. rerio*

Fig. 6 illustrates the cardiac response of zebrafish embryos to different concentrations of the three waters, measured as heartbeats per minute (bpm) over a period of 96 h. Overall, the control groups consistently maintained a baseline heartbeat rate between 130 and 180 bpm. Exposure to raw PW resulted in severe impairment of embryonic development, including the cardiac system. No survivors were observed, and no heartbeats were documented for the raw PW exposure group (Fig. 6a). Exposure to the distillate resulted in concentration-dependent changes in cardiac activity. At 100% concentration, there was a significant reduction in heart rate at 48 h, 72 h, and 96 h. In particular, at 96 h, no heartbeats were observed at this concentration. Lower distillate concentrations (50%, 25%, 12%, and 6%) exhibited bpm rates comparable to the control, indicating that the compounds in the distillate were not impairing the embryos' heart response at these doses (Fig. 6b). Consistent with previous results, no observable cardiac alterations were noted for the post-treated water. After GAC and zeolite treatment, the PW showed cardiac responses similar to those of the control group (130–180 bpm) across all tested concentrations (Fig. 6c). Consistent with previous sections, this indicates that the post-treatment processes effectively reduced the constituents causing cardiac alterations observed in the 100% distillate test (0 bpm), highlighting the potential of the integrated treatment train to improve overall water quality.

To offer a visual assessment of the developmental impacts associated with the three waters at 100% concentration, Fig. 6d provides images of the microscopic observations conducted during the FET test. Exposure to raw PW resulted in a cessation of normal developmental progression, significantly deviating from the typical embryonic stages observed in zebrafish. In accordance with previous findings, these observations demonstrate that the raw PW studied contains compounds in concentrations that disrupt normal embryogenesis. While there is a noticeable improvement in the developmental outcomes of the embryos exposed to the distillate compared to raw PW in the first 48 h, issues such as scoliosis and pericardial/yolk sac edemas occurred at 72 and 96 h, indicating that the distillation process does not eliminate all harmful components. 38% and 67% of embryos had pericardial or yolk sac edemas when exposed to 50% and 100% distillate, while scoliosis was observed in 58% of embryos after exposure to 100% distillate

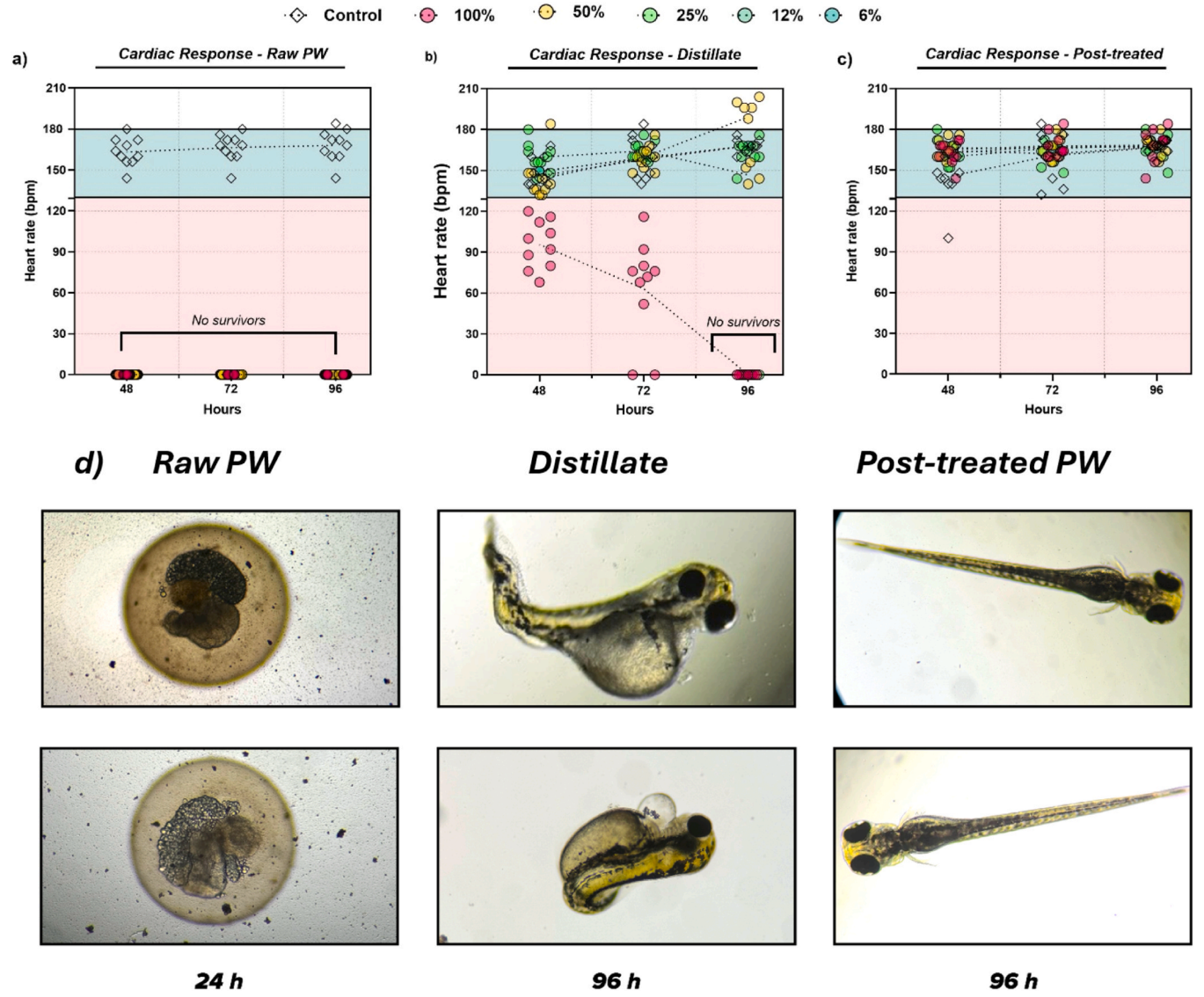

Fig. 6. Cardiac responses of zebrafish embryos following exposure to (a) raw PW, (b) MVR distillate, and (c) post-treated water treated with GAC and zeolite; (d) representative microscopic observations after exposure. Heartbeat rates were measured in 10 randomly selected embryos per treatment at 48, 72, and 96 h of exposure.

(Figure S7a and b). Moreover, more than 60% of larvae had the impaired posture (side-lying instead of upright) after exposure to 50% and 100% distillate (Figure S7c). This partial treatment still poses a risk to normal embryonic development and is consistent with the results of the FET test and the cardiac responses, where at 96 h, the embryos exposed to the distillate exhibited no signs of cardiac function. After post-treatment, the embryos exhibit markedly improved development, with more typical morphology and no evidence of developmental alterations. All the abnormal features observed in the embryos exposed to the distillate (scoliosis, and pericardial and yolk sac edemas) were absent.

3.2.6. *The expression of zebrafish biotransformation, oxidative stress, and endocrine disruption-related genes after exposure to post-treated water*

Fig. 7 presents the relative expression results of the targeted genes in *D. rerio* after 7 days of exposure. The results of the Mann-Whitney U non-parametric statistical test, used to assess significant differences between the control and the post-treated water.

3.2.7. *Endocrine Disruption-Related Genes*

The relative expression of Aromatase A (*cyp19a1a)* and Aromatase B (*cyp19a1b*) (Figs. 7a and 7b) exhibited minimal changes in expression levels, with no statistically significant differences between treated and control groups. Both gene products exhibited minimal changes in expression levels, with no statistically significant differences between treated and control groups ($P > 0.05$). Considering the critical role of Aromatase A and Aromatase B in converting androgens to bioactive estrogens [53,54], this suggests that post-treated water did not trigger any significant response in terms of abnormal androgen generation. Similarly, while it appeared that *Vtg1* normalized expression levels (3.23) were elevated in the treated PW group (Fig. 7c), the ANOVA results revealed no significant differences in expression levels compared to the control group ($P > 0.05$). Androgen Receptor (*ar*) showed relative expression values close to 1.0 (Fig. 7k), indicating no significant response to post-treated water exposure. The lack of altered expression for *ar* suggests that the receptor expression was not directly impacted, which further supports the findings seen in *cyp19a1a* and *cyp19a1b*.

3.2.8. *Biotransformation-related genes*

Cytochrome P450 1 A (*cyp1a*) and Cytochrome P450 1B1 (*cyp1b1*) similarly showed no significant differences in expression. The lack of

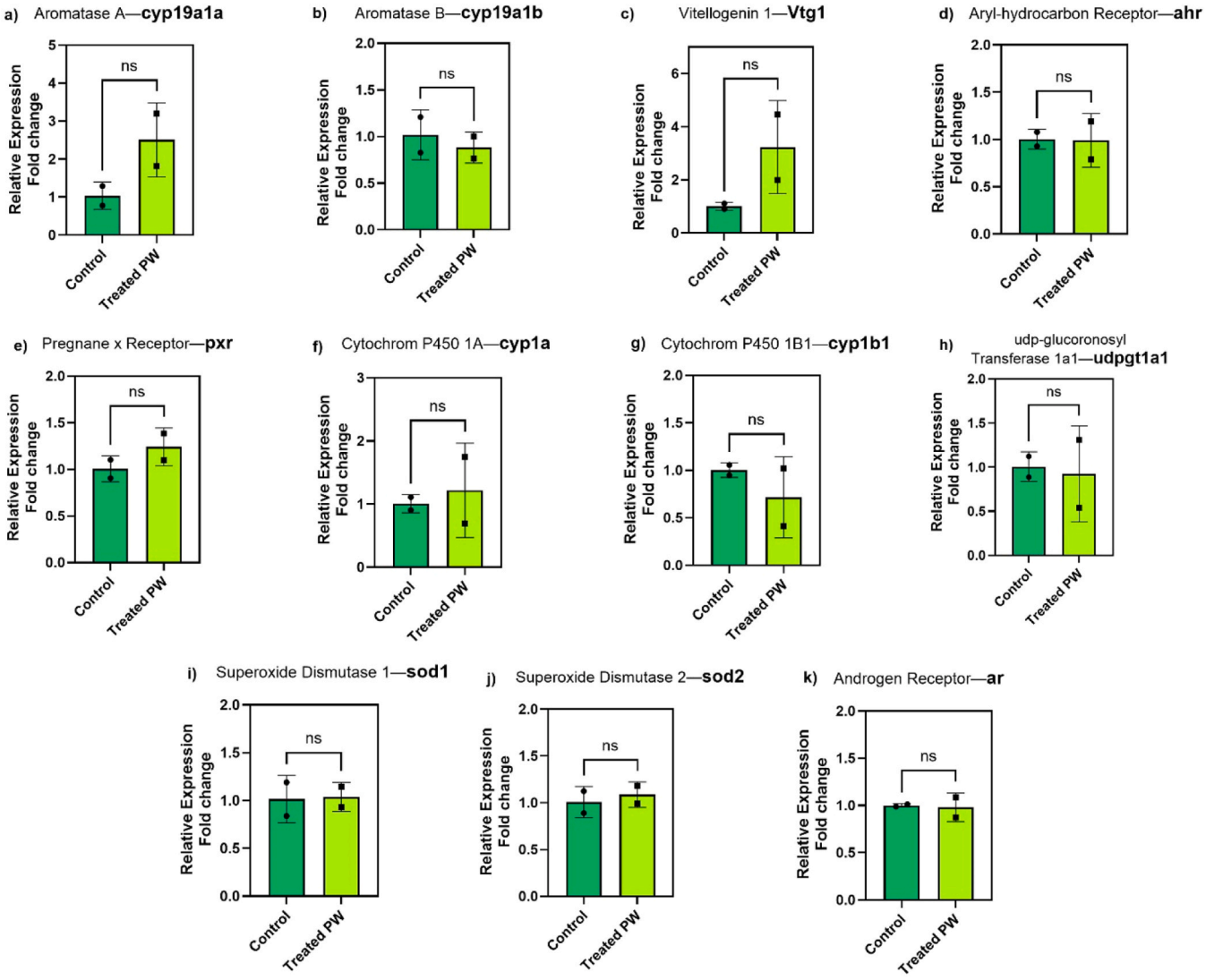

Fig. 7. Gene expression in zebrafish embryos after 7 days of semi-renewal exposure to post-treated water treated with GAC and zeolite. Ten embryos were exposed per treatment, with larvae pooled in groups of five for RNA extraction, cDNA synthesis, and qPCR analysis. No significant difference was observed between the control and post-treated PW groups (Mann-Whitney test, $P > 0.05$).

induction for these phase I metabolism genes suggests that polycyclic aromatic hydrocarbons (PAHs) or other potential inducers of these enzymes were effectively removed during the treatment process [55–57]. Pregnane X receptor (*pxr*) and aryl-hydrocarbon receptor (*ahr*) also showed no significant changes in relative expression compared to controls, with fold changes close to 1.0. The *pxr* and *ahr* genes are critical in the regulation of xenobiotic metabolism, and their unchanged expression implies that post-treated effluent did not induce a significant metabolic response in zebrafish embryos, pointing to minimal activation of detoxification pathways typically triggered by exposure to environmental contaminants [53,58] UDP-glucuronosyltransferase 1A1 (*udpgt1a1*), a phase II detoxification enzyme, also showed no significant change in expression, remaining around 1.0 fold compared to the MHRW control. This further indicates that there was no activation of glucuronidation pathways, reinforcing the conclusion that post-treated water did not significantly trigger detoxification responses [59].

3.2.9. *Oxidative stress-related genes*

Superoxide Dismutase 1 (*sod1*) and Superoxide Dismutase 2 (*sod2*) are genes encoding enzymes that play a crucial role in detoxifying reactive oxygen species (ROS). Both genes exhibited minimal variation in expression between treated and control groups, with relative expression levels staying below 1.5-fold. Specifically, *sod1* had a fold change close to 1.0, while *sod2* exhibited a minor increase to around 1.5-fold but was not statistically significant ($P > 0.05$). This suggests that final post-treated water did not induce oxidative stress in zebrafish embryos, which is a positive indicator of effluent safety [60,61].

Due to the limited RNA amount per embryo, pooled larvae were used to evaluate the alterations in gene expression. For a more comprehensive investigation, a future study is needed to examine individual embryos/larvae with a larger sample size. Furthermore, embryos/larvae could be collected at different developmental stages for the gene expression and enzyme activity study after exposure.

3.3. *Integrating chemical characterization with WET assay outcomes*

Across all trophic levels tested, adverse responses in aquatic organisms aligned closely with changes in water quality. For raw PW, severe adverse effects were observed at concentrations as low as 6%, including complete mortality of C. *dubia* and *D. rerio* embryos, suggesting the presence of multiple stressors at high levels. The extremely high salinity (TDS ≈ 172,000 mg/L) and elevated major ion concentrations (Na^+, Cl^-,

Ca^{2+}, Mg^{2+}) likely contribute to the severe adverse responses observed. Osmotic imbalance alone can disrupt membrane integrity, ion regulation, and metabolic function in freshwater organisms [62–65]. The impacts of salinity were rapid and severe, with *C. dubia* neonates dying within minutes and zebrafish embryos floating in raw PW due to its high density. Beyond salinity, the chemical and toxicological characterization indicates additional stressors, including ammonia (TAN = 139 mg/L), aluminum (1.8 mg/L), and acetic acid (112 mg/L). Unionized ammonia (NH_3) is well established as a potent toxicant to fish embryos and invertebrates, causing neurotoxicity, mitochondrial dysfunction, and disruption of oxidative phosphorylation [66,67]. Elevated aluminum concentrations, as detected in the raw PW, can impair osmoregulation in sensitive species and compromise respiratory function [68]. Although aluminum bioavailability is strongly controlled by pH and hardness, adverse effects have been reported at comparable concentrations [68]. While its specific contribution cannot be isolated in this matrix due to co-occurring stressors, aluminum should be considered a relevant water-quality target in PW treatment evaluations. Raw PW contained monoaromatic hydrocarbons (benzene, toluene, xylenes), phenolic compounds, and other VOCs and SVOCs. Although all the detected organic compounds have concentrations a few orders of magnitude below acute toxicity thresholds (EC_{50} or LC_{50}), potential cummulative and synergistic effects cannot be ignored. Many hydrophobic organics can partition into biological membranes, producing narcosis-type toxicity and developmental perturbations [69]. Acetic acid may contribute to the toxicity of raw PW, as its concentration (112 mg/L) exceeded the EC_{50}/LC_{50} values for Daphnia and *D. rerio* (Table S10).

MVR distillation removed > 99.9% of dissolved solids and substantially reduced bulk organic parameters, metals, and other analytes, including radionuclides; however, adverse effects persisted across all species, particularly at 100% concentration. These results indicate that while salinity reduction improved overall water quality, additional stressors remained in the PW. This improvement was evident in all WET tests, where dose-response assessments showed reduced adverse effects at concentrations ≤ 50% (Fig. 5 and Table 4). Although linking individual stressor concentrations directly to the observed adverse effects is beyond the scope of this study, compounds such as ammonia and VFAs likely played significant roles in the observed toxicity. Ammonia was present at 21 mg/L TAN, a level exceeding reported EC_{50}/LC_{50} values for *C. dubia* and *D. rerio*, and is therefore a plausible primary stressor. This interpretation is supported by Redman et al. [70], who identified ammonia as the dominant contributor to toxicity in treated PW. In addition, caproic acid (86.5 mg/L), propionic acid (123 mg/L), and valeric acid (198 mg/L) exceeded toxicity thresholds (Table S10) and likely contributed to the severe responses observed at full-strength distillate. In parallel, chemical analysis revealed that several hydrophilic VOCs (e.g., acetone, 2-propanol, 2-butanone, methyl acetate) exhibited limited removal or net increases during distillation. Although these compounds are individually less toxic than hydrophobic monoaromatics, their combined presence at elevated concentrations may contribute to chemical stress. Among the detected SVOCs, methylphenol and phenol were the most abundant compounds in the distillate and could be considered potential stressors. However, their measured concentrations remained approximately 3–10-fold below reported EC_{50}/LC_{50} values and about twofold below the NOECs for the tested aquatic organisms. All other detected SVOCs were present at concentrations 40–1000 times lower than their respective toxicity thresholds. Ammonia and monoaromatic hydrocarbons have been reported to interfere with ion channel regulation and embryonic cardiogenesis [71,72]. Given their simultaneous presence in PW distillates and the cardiotoxicity (reduced heart rate and pericardial edema) observed in the present study, future work should use toxicity identification evaluation (TIE) to determine which constituents or fractions drive these cardiac responses.

The complete mitigation of adverse effects following GAC and zeolite treatment co-occurred with near-complete removal of residual ammonia (TAN < 0.05 mg/L), VOCs, SVOCs, dioxins/furans, and hydrocarbons. The post-treated water exhibited NOEC values of ≥ 100% across trophic levels, with complete survival of invertebrates and fish embryos, normal algal growth, and no evidence of cardiac or developmental abnormalities or altered gene expression. These results demonstrate that targeted post-treatment to address residual organics and ammonia is effective, as evidenced by both targeted chemical characterization and comprehensive toxicological evaluations. Importantly, although PFAS were detected at ng/L levels in the post-treated effluent, these levels are orders of magnitude below proposed aquatic life AWQC and acute toxicity thresholds for zebrafish embryos and invertebrates[52].

It is important to note that the toxicological responses observed in both raw PW and distillate may be partly attributable to constituents not captured by the targeted analyte list. Although this study applied broad-spectrum targeted chemical analyses, comprehensive identification and quantification of organic constituents in PW remain challenging due to the presence of unknown, non-target, and potential transformation products. A comprehensive assessment of toxic effluents containing residual organics, therefore, requires advanced non-target analytical approaches. These methods can help characterize stressors that may be recalcitrant to treatment. When combined with quantitative structure–activity relationship (QSAR) models, they can provide insights beyond those obtainable from WET testing alone, including screening-level evaluations of bioaccumulation and biomagnification potential. Moreover, treated PW is a complex mixture, and toxicity can be modified by mixture interactions (additive, synergistic, antagonistic) and water chemistry that affects bioavailability (e.g., dissolved constituents, hardness, alkalinity). Therefore, hazard identification for treated PW remains challenging. WET tests are designed to measure the combined toxic effects of all constituents present in an effluent; reductions in PW effluent toxicity after treatment should be interpreted as reduced mixture hazard rather than definitive removal of a single toxicant. In addition, long-term exposure studies using both aquatic organisms and mammalian models are warranted to further improve our understanding of the safety of treated PW for both direct and indirect receptors.

4. Conclusions

This study provides a comprehensive chemical and toxicological characterization of raw, distilled, and post-treated PW from the Permian Basin. The analysis profiled over 400 target analytes, including volatile and semivolatile organics, metals, radionuclides, and other priority pollutants. In addition to standardized WET tests, the study assessed developmental and cardiovascular endpoints and expression of 12 genes linked to endocrine disruption, biotransformation, and oxidative stress in zebrafish embryos. MVR distillation achieved desalination of hypersaline PW but is insufficient by itself to produce a chemically safe effluent. Relying on TOC and TPH alone to assess organic removal performance can undermine PW treatment evaluations. Reductions in TOC and TPH were not aligned with trends observed for individual VOCs, SVOCs and other organics. VOC and SVOC carryover did not exhibit a systematic dependence on vapor pressure. Despite lower volatility compared to VOCs, most SVOCs either increased or showed limited reductions after distillation. Data suggest that solubility, hydrophobicity, molecular weight, and process-driven mechanisms may exert a stronger influence. Distillation and post-treatment was associated with the emergence of new compounds, including furans, VFAs, and PFAS. Addressing these issues is essential to ensure consistent water quality suitable for reuse. The toxicological characterization was consistent with the chemical characterization findings. Raw PW induced serious adverse effects across all tested species. Although water quality improved following MVR distillation, these toxic effects persisted, notably causing severe morphological and cardiac abnormalities in zebrafish embryos. Post-treatment with GAC and zeolite reduced most identified PW constituents to below the analytical method detection

limits. As demonstrated by the toxicological assessment, the integrated treatment train reduced PW constituents to non-toxic levels. Adverse effects were fully mitigated across all tested organisms, with no developmental, cardiac, or gene-expression alterations observed in zebrafish embryos. This study demonstrates that the integration of advanced treatment processes can address the complex matrix of PW from the Permian Basin and produce purified water potentially suitable for surface water discharge.

Environmental Implication

The reuse of treated produced water (PW) through advanced treatment processes offers a strategic solution to alleviate water scarcity while addressing environmental challenges in oil- and gas-producing regions. Highly saline PW from the Permian Basin was desalinated using mechanical vapor recompression, followed by granular activated carbon and zeolite adsorption. However, a limited understanding of environmental and public health risks remains a key barrier to reuse. This study addresses this knowledge gap by quantifying more than 400 analytes and performing whole effluent toxicity testing across four trophic levels, incorporating zebrafish embryo development and gene expression assays to detect early-life and sublethal effects that are overlooked by conventional toxicological methods.

CRediT authorship contribution statement

Yeinner Tarazona: Writing – review & editing, Writing – original draft, Visualization, Validation, Investigation, Formal analysis, Data curation. **Joseph Alexander:** Writing – review & editing, Validation, Investigation, Formal analysis, Conceptualization. **Mike Hightower:** Resources, Project administration, Investigation, Funding acquisition, Conceptualization. **Himali M.K. Delanka-Pedige:** Project administration, Investigation, Data curation. **Huiyao Wang:** Writing – review & editing, Supervision, Investigation, Funding acquisition, Conceptualization. **Pei Xu:** Writing – review & editing, Supervision, Resources, Project administration, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization. **Yanyan Zhang:** Writing – review & editing, Visualization, Validation, Supervision, Resources, Investigation, Funding acquisition, Conceptualization.

Declaration of Competing Interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Pei Xu, Huiyao Wang and Yanyan Zhang reports financial support was provided by U.S. Bureau of Reclamation. Pei Xu, Huiyao Wang and Yanyan Zhang reports was provided by New Mexico Higher Education Department. Pei Xu, Mike Hightower, Huiyao Wang and Yanyan Zhang reports was provided by New Mexico Produced Water Research Consortium. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Statement

This work has received approval for research ethics from the Institutional Animal Care and Use Committee (IACUC) at New Mexico State University, and a proof/certificate of approval is available upon request.

Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.jhazmat.2026.142274.

Data availability

Data will be made available on request.

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