Data in Brief 63 (2025) 112125

Contents lists available at ScienceDirect

Data in Brief

journal homepage: www.elsevier.com/locate/dib

Data Article

Data from high-temperature and high-pressure carbon dioxide sequestration experiments limited to 24 hours, performed on Platinum Group Metals mine tailings from the South African Bushveld Igneous Complex

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ARTICLE INFO

Article history:
Received 13 June 2025
Revised 24 September 2025
Accepted 26 September 2025
Available online 11 October 2025

Dataset link: Experimental carbon dioxide sequestration in Bushveld Igneous Complex mine tailings at high temperatures and pressures (Original data)

Keywords:
Carbon dioxide removal
PGM tailings
Mineral carbonation
Supercritical reaction

ABSTRACT

Mine tailings derived from mafic-ultramafic rock formations may offer promising potential for mineral carbon dioxide (CO_2) sequestration. This dataset evaluates the suitability of South African tailings, produced during Platinum Group Metals (PGM) extraction at the Two Rivers mine, for CO_2 mineralisation under supercritical conditions in a batch reactor. These tailings are typically enriched in oxides such as MgO (12 %), Fe_2O_3 (22 %), and CaO (2 %), which can provide the necessary alkalinity for carbonate formation. They also contain significant amounts of Al_2O_3 (11 %), SiO_2 (18 %), and Cr_2O_3 (34 %), which may influence reaction pathways. Reactivity with CO_2 was investigated under supercritical conditions (200 °C, 160 bar) in a saline aqueous solution for various reaction times ranging from 2 h to 24 h. The geochemical and physicochemical properties of the fresh tailings were

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DOI of original article: 10.1016/j.wasman.2016.02.021

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https://doi.org/10.1016/j.dib.2025.112125

determined using X-ray fluorescence (XRF) and X-ray diffraction (XRD). Post-reaction tailings were further analysed using scanning electron microscopy (SEM), Carbon and Sulphur (C&S) analysis, and particle size distribution (PSD) analysis.

Specifications Table

Subject	Earth & Environmental Sciences
Specific subject area	Carbon Capture and Storage Technology
Type of data	Table, Image, Figure
Data collection	The mine tailings were analysed using various instruments. The chemical composition was obtained using X-ray Fluorescence (ARL Perform'X Sequential Spectrometer) via the fusion method, and the data set was processed using Quantas software. The mineralogy was determined by X-ray Diffraction (Panalytical X'Pert Pro diffractometer, cobalt source). Mineral phase identification and quantification were completed using the X'Pert Highscore, Rietveld and AutoQuan software. The mineral morphology was determined using Scanning Electron Microscopy (JOEL JSM-6300) after the carbon-coated samples (Emitech K550X). Carbon and sulphur content were determined using an elemental analyser (Eltra CS 800). Particle size distribution was determined using laser diffraction (Malvern Mastersizer, 2000.
Data source location	Grab samples of ~200 kg of tailings were collected from a tailing storage facility (TSF) at the Two Rivers Mine (GPS coordinates 24°57′03.0 "S, 30°06′20.1′'E " E), which is located 4 km away from the main mine shaft. The mining operation is in the southern sector of the eastern limb of the Bushveld Igneous Complex (BIC), which straddles the current boundary of the Limpopo and Mpumalanga provinces of South Africa. Experimental and analytical work was completed at the Council for Geoscience (CGS), Pretoria,and the Stoneman Laboratory, University of Pretoria, South Africa.
Data accessibility	Repository name: UP Research Data Data identification number: doi.org/10.25403/UPresearchdata.29192204 Direct URL to data: https://doi.org/10.25403/UPresearchdata.29192204
Related research article	Mohamed, S., van der Merwe, E. M., Altermann, W., & Doucet, F. J. (2016). Process development for elemental recovery from PGM tailings by thermochemical treatment: Preliminary major element extraction studies using ammonium sulphate as extracting agent. Waste Management, 50, 334–345. doi: 10.1016/j.wasman.2016.02.021

1. Value of the Data

- Data [1] on the geochemical and physical characteristics of specific mine waste materials are necessary for future carbon capture, utilisation, and storage (CCUS) research or future mine waste beneficiation research using similar materials.
- The data from the carbon mineralisation experiments may be used to optimise similar experiments that explore carbonation using mine waste materials or to compare the carbonation potential of various mine tailings from the South African Platinum Group Metal (PGM) industry or other mining sectors.
- Using the data from this study, the efficiencies of this type of mineral carbonation method can be compared to other methods in greenhouse gas removal and storage studies.
- Potential beneficiaries of these data include geologists interested in the Bushveld Igneous Complex, as well as scientists working on mineral carbonation (CO_2 mineral sequestration), mine tailings, and high-pressure supercritical CO_2 reactions.

2. Background

The data-gathering efforts were motivated by an interest in characterising and understanding tailings' reactivity with CO_2 under supercritical conditions, providing data to inform future Carbon Capture, Utilisation, and Storage (CCUS) research and mine waste beneficiation [2]. Thus, further enhancing the understanding of the potential of South African Platinum Group Metal (PGM) mine tailings for mineral carbon dioxide sequestration, building upon the work of other researchers [3] who are working on carbon dioxide removal (CDR) methods as part of a worldwide effort to reduce and limit the increase of greenhouse gases [4].

Originating from mafic-ultramafic rock formations found in a world-class layered intrusion [5], these tailings contain elements like magnesium, iron, and calcium oxides [6], essential for carbonate formation, alongside other major elements. To assess reactivity, tailings were subjected to supercritical conditions (200 °C, 160 bar) in a saline solution, with varying reaction times. The geochemical and physicochemical properties of treated tailings were analysed using XRF, XRD, and SEM, and the reacted counterparts were analysed for carbon/sulphur and PSD. The resulting data will enable the optimisation of similar carbonation experiments, comparison of carbonation potential across mine tailings, and evaluation of this method's efficiency against other greenhouse gas removal strategies. This data contributes to understanding and potentially utilising mine waste for effective CO_2 sequestration.

3. Data Description

The data set (Table 1) described in this article is related to the sampling campaign that occurred in three different locations along the strike of the eastern limb of the BIC (Fig. 1a) and the subsequent experimental work on said materials, described later. This was part of a Univer-

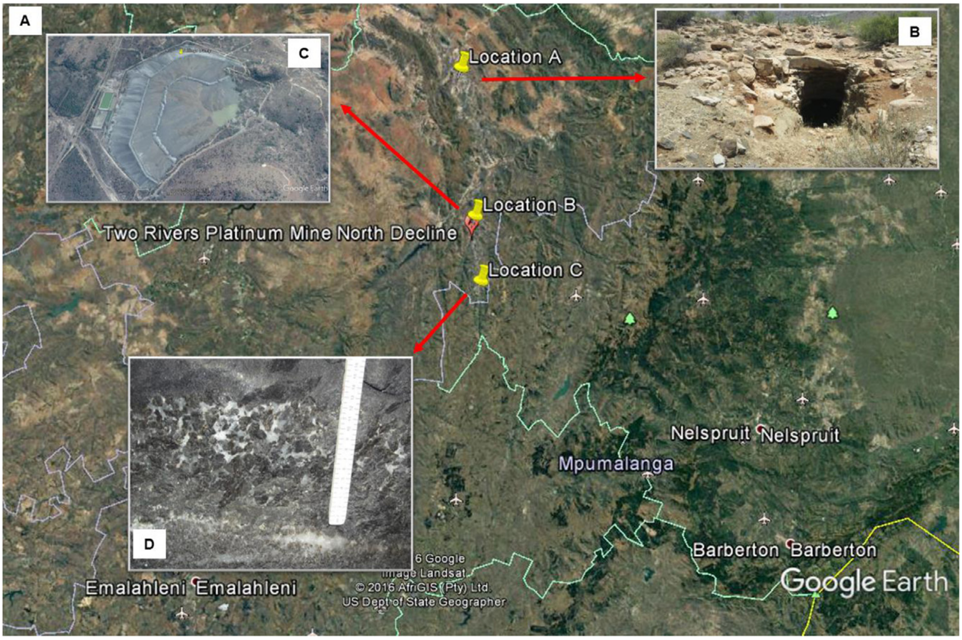

Fig. 1. Image shows (a) a satellite image of the Eastern BIC limb and the associated images of the sampling sites; Image (b) shows an old exploration dig from which the first pyroxenite bulk rock sample was retrieved; (c) the Two Rivers mine's processing plant where the tailings storage facility from which the tailings were collected; and (d) is underground Booysendal mining stooping face from which the second pyroxenite bulk rock was obtained.

Table 1
Content of the related dataset of mine tailings and reacted mine tailings in this study.

Table	Title	Parameter Content
0	Description	Summary and general description of all the experimental outputs and analytical techniques used in the study.
1	Bulk chemical analyses of the mine tailings (MT) sample, which was split into triplicate sub-samples, were measured for major elements in weight percentage (wt. %) and analysed using XRF.	Major oxides: SiO_2, TiO_2, Al_2O_3, Cr_2O_3, MgO, Fe_2O_3, CaO, MnO, P_2O_5, Na_2O, K_2O
2	The mineralogical composition (normalised to 100 %) of the pristine bulk MT sample was analysed with a silica standard to account for possible structureless phases.	Mineral phases (%): Chromite ($FeCr_2O_4$), enstatite ($MgSiO_3$), plagioclase ($CaAl_2Si_2O_8$), hornblende ($(Ca,Na)_2(Mg,Fe,Al)_5(Al,Si)8O_{22}(OH, F)_2$), diopside ($(CaMg)SiO_3$), unknown amorphous phases.
3	Carbon and Sulphur analyses result (%) of pre- and post-experiment MT sub-samples. The post-experiment results are segmented into 2, 4, 8 and 24 hours, each with triplicate experiment results.	Elemental concentration: C (%) and S (%)
4	Summary table that recalculates and compares the mean carbon changes in initial and final measurements. And the difference is recalculated as the CO_2 equivalent wt. % gained/loss or net carbon equivalent (NCE)	Elemental and molecular concentration: C (%) and CO_2e (wt. %)
5	Particle size distribution of untreated (MT) and treated (RMT) samples.	Volume (%) and Particle Size (µm)

sity of Pretoria CCUS research project commissioned in 2012, wherein both the tailings produced from mining the Merensky and underlying UG2 reefs, as well as the associated dominant hanging and footwall host rocks (pyroxenites), were collected. The samples of PGM tailings, which are the focus of this publication, were obtained from the Two Rivers platinum mine from one of its tailing storage facilities (Fig. 1c) with coordinate numbers 24° 57′ 03.0′’S and 30° 06′ 20.1′’E. The TSF is situated 4 km away from the main shaft, which is located in the southern sector of the eastern limb of the BIC and is close to the current boundary between the Limpopo and Mpumalanga provinces in South Africa. A grab-sampling technique was used, where ~200 kg of tailings material was collected randomly from the surface of the TSF. The bulk rock materials collected from the same region were used in a related experiment [7] that investigated the reactivity of the dominant target mineral phases found in the tailings – pyroxene and plagioclase.

The bulk geochemistry of the untreated tailings (with sample ID of MT - ‘mine tailings’) is detailed in Supplementary Tables 1 and 2. The effects of milling the untreated samples are shown through SEM imaging (Fig. 3). The experimental setup consisted of the proprietary batch reactor displayed in Fig. 3, and the experimental setup/procedure is described later. The C and S analyser results are shown in Supplementary Table 3, followed by Supplementary Table 4, which summarises the total CO_2 wt. % recalculated from the average carbon measured from the reacted mine tailings (RMT). Supplementary Table 5 compares the particle size volume distribution between the untreated (MT) and the experimentally treated (RMT) samples.

4. Experimental Design, Materials and Methods

4.1. Experimental design

All direct carbonation experiments were performed in a 600 mL Hastelloy C-276 (i.e., nickel-chromium-molybdenum alloy) Parr 4568 Series Mini Bench Top Reactor (Parr Instrument Co., Illinois, USA) fitted with a pressure gauge and a heating furnace and connected to a Parr 4857 controller (Fig. 2). The reactor is characterised by a maximum operating temperature and pres-

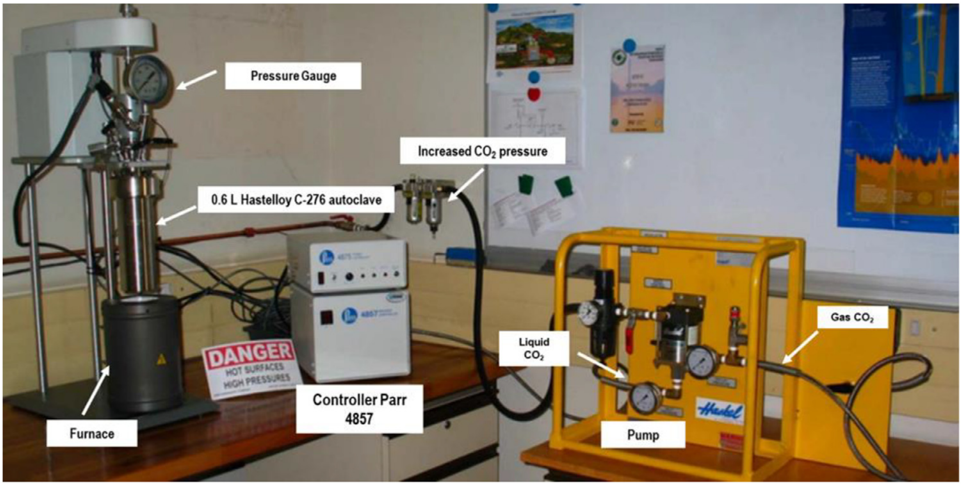

Fig. 2. Photograph of the Parr reactor setup at the Council for Geoscience.

sure of 350 °C and 200 bar, respectively. The slurry was then charged to the reactor. All triplicate experiments were performed at 200 °C and 160 bars over 2, 4, 8 and 24 h. The high pressure was maintained by pumping ~55 bar liquid CO_2 using an MS-36 Series liquid booster pump (Haskel International, Inc., USA) throughout the experiments. The slurry was continuously agitated at 1700 rpm during the reaction using a gas entrainment impeller connected to a Parr magnetic drive.

After the experiment, the reactor was cooled below 40 °C before degassing and opened to recover the suspension. The slurry was centrifuged at 2500 rpm for 5 min to separate the solid particles from the liquid fraction. After removing the clear supernatant, the solid residue was washed three times with ultrapure water to remove excess $NaHCO_3$ and NaCl. The rinsed solids were dried in a dry air oven at 40 °C for 3 days to remove free moisture. Dried samples were thoroughly homogenised using a mortar and pestle and subsequently subjected to analysis. This experimental design was adapted from research [8,9,10] that conducted supercritical batch reaction experiments on silicate materials.

4.2. Materials

The slurry contained 20.00 g of the milled tailings sample, 10.75 g of sodium bicarbonate, $NaHCO_3$, and 11.69 g of sodium chloride, NaCl, (ACS, Reag. pH Eur grade, 99.5 %, Merck, South Africa), which were accurately weighed and added to 200 mL ultrapure water (electrical conductivity < 1 µS cm^{-1}), resulting in a 1 M saline solution containing 0.64 M $NaHCO_3$. Milling of the tailings was conducted to both internally homogenise the sample and reduce potential selective reactivity because of phase-dependent grain size distribution, which was observed by both [6,10]. When comparing the samples under a scanning electron microprobe (JEOL 5800 LV, 20 kV) set at 90 times magnification, there was a distinct morphological difference between the ‘pristine’ tailings (Fig. 3A) and the milled tailings (Fig. 3B).

4.3. Methods of data acquisition

Several instruments were used to collect bulk geochemical data; the materials had to be analysed thoroughly before and after the experiments to observe and quantify the changes.

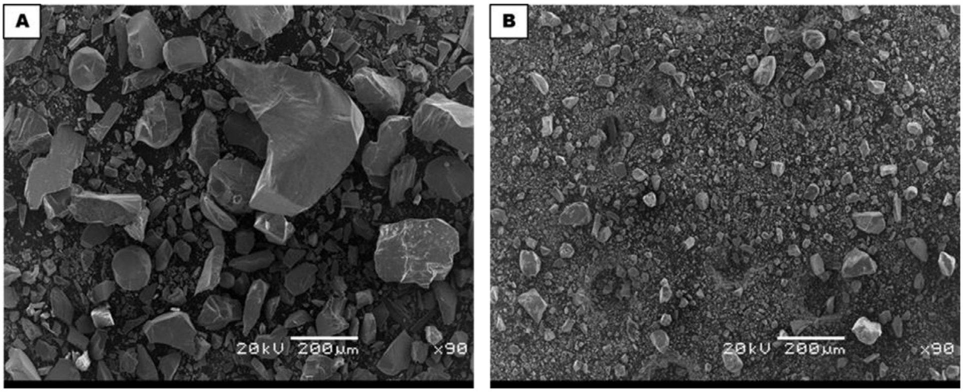

Fig. 3. A comparison of the SEM micrographs of (a) unprocessed and (b) milled MT.

4.3.1. X-ray fluorescence (XRF)

The bulk chemical composition data of the tailings were obtained using an ARL Perform'X Sequential X-ray fluorescence (XRF) spectrometer and the Quantas^{TM} software for data analysis. Before the measurements, the samples were roasted at 1000 °C until the sample had a constant mass, and the difference between the initial and final mass was calculated to determine each sample's loss on ignition (LOI). For the fused disk, 1 g of the roasted sample was carefully weighed and thoroughly mixed with 6 g of flux consisting of lithium tetraborate ($Li_2B_4O_7$) in a platinum-gold crucible, then fused at 1050 °C to form a stable glass disk. The disk was then analysed to determine the elemental composition of the sample.

4.3.2. X-ray diffraction (XRD)

To quantitatively determine the mineralogical phase distribution of the tailings, the samples were analysed using a Panalytical X'Pert Pro Powder diffractometer with an X'Celerator detector and Co cathode. - Measurements were conducted over a 2θ interval of 5 – 90°, with a step size of 0.08° 2θ and a counting time of 9.53 s per step, using a rotating sample.

The samples were micronised, dried, and mounted on a standard Panalytical backloading sample holder, which allows for a nearly random distribution of the particles. The mineralogy was determined by selecting the best–fitting pattern from the Inorganic Crystal Structure Database (ICSD) for the measured diffraction pattern using X'Pert Highscore plus software. The relative phase amounts (weight of crystalline portion) were estimated using the Rietveld method and AutoQuan software. To quantitatively determine the amorphous content in the tailings, a silica (SiO_2) standard (Sigma-Aldrich, 99 % purity) made up 20 % of the mass of the total sample before analysis. Given the results from the C&S analysis, the post-experiment materials were not analysed using XRD due to the tools' limitation in detecting small amounts of amorphous carbonates or trace crystalline phases in samples with complex mineralogical compositions.

4.3.3. Scanning electron microscopy (SEM)

To observe the samples' morphology using scanning electron microscopy (SEM), the powder samples were mounted on a sticky-plastic substrate and coated with a thin carbon layer to prevent charge build-up. They were then analysed using a JOEL JSM-6300 instrument coupled with a Bruker^{TM} X-Flash EDX-detector (energy resolution of 125 eV); the machine processed the raw data using the software program Quantax 200 by Bruker^{TM}.

4.3.4. Total inorganic carbon and sulphur analysis (C&S)

The tailings' total inorganic carbon and sulphur were determined using the Eltra CS 800 Double Dual Range system. A minimum of about 50 mg (milled to an average of <75 µm) of the sample was required. The sample was incinerated under a stream of oxygen, resulting in the digestion of all carbon (organic and inorganic) to form CO_2 as “waste”. The produced gas molecules were then detected and measured using four infrared absorption detectors.

4.3.5. Particle size distribution (PSD)

The particle sizing analysis was carried out to confirm the effects of the batch reaction experiment on changes in the net particle size distribution. The PSD for the pre- and post-experiment tailings fractions were obtained using laser diffraction with a Malvern Mastersizer 2000 equipped with a Hydro 2000 G dispersion unit. Duplicate analysis was performed on the sub-samples, dispersed in water at ambient temperature and pressure conditions. The analysis was conducted under the following conditions: obscuration set between 10 % and 20 %, stirring speed at 650 rpm, pump speed at 1650 rpm, and ultrasonic treatment at 20 %. The results were recorded as particle volume percentages and averaged for the overall particle size distribution.

Limitations

During the experimental phase of this study, the laboratory was often affected by intermittent country-wide electrical power outages (referred to as ‘load shedding’), which made operating the instrument difficult since there was no heat or rotary capacity. This meant some experimental runs had to be abandoned altogether, and longer experiment durations (above 24 h) could not be explored. In addition, some measurement techniques, i.e., water analyses via inductively coupled plasma atomic emission spectroscopy (ICP-OES), also could not be utilised due to electrical instability since such instruments were sensitive to power surges. The water samples were subsequently never retroactively measured due to sample integrity concerns. Consequently, a decision was taken during the lead author’s MSc studies to conduct longer experiments at Martin Luther University of Halle-Wittenberg targeting the concentrate pyroxene and plagioclase minerals [7], which are the main phases that host Mg and Ca cations found in these tailings.

Ethics Statement

The authors confirm they have read and followed the ethical requirements for publication in Data in Brief. They confirm that the current work does not involve human subjects, animal experiments, or any data collected from social media platforms.

Credit Author Statement

Zakhele Nkosi: Investigation, Writing - Original Draft, Data Curation, Project administration, Funding acquisition. **Wladyslaw Altermann:** Conceptualisation, Supervision, Resource, Funding acquisition, Writing - Review & Editing. **Frederic Doucet:** Conceptualisation, Supervision, Resource, Writing - Review & Editing. **Sameera Mohamed:** Investigation, Conceptualisation, and Methodology. **Karabo Phala:** Investigation, Conceptualisation and Methodology. **Christoph Gauert**: Review & Editing, Funding acquisition

Data Availability

- Experimental carbon dioxide sequestration in Bushveld Igneous Complex mine tailings at high temperatures and pressures (Original data) (UP Research Data).

Acknowledgements

This work is based on the research supported by CIMERA (DST-NRF Centre of Excellence for Integrated Mineral and Energy Resources Analysis) [Grant no: 91487] and the National Research Fund through the DAAD-NRF scholarship programme. The authors thank the Council for Geoscience for providing supervisory assistance, insight, expertise and access to valuable resources that made this research possible. The National Research Foundation's (DAAD-NRF) financial assistance towards this research is hereby acknowledged. Opinions expressed and conclusions arrived at are those of the author and are not necessarily to be attributed to the DAAD-NRF [Grant No.: 88119].

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Supplementary Materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.dib.2025.112125.

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