This dataset is related to the research article in Chemosphere, entitled ‘The limited facilitating effect of dissolved organic matter extracted from organic wastes on the transport of titanium dioxide nanoparticles in acidic saturated porous media’ [1]. The data summarised the characterization of dissolved organic matter (DOM) extracted from organic wastes and their effects on the transport of titanium dioxide nanoparticles (TiO$_2$ NPs) in acidic saturated porous media in the presence of monovalent electrolyte. Three types of dissolved organic matter were extracted from organic materials, including swine manure, sludge, and sediment, using deionized water, and were characterized with UV–Vis, FTIR and elementary analysis. The adsorption of DOM onto TiO$_2$ NPs was evaluated in the presence of NaCl, and zeta potentials of TiO$_2$ NPs were also determined. Breakthrough column experiments were conducted to quantify the effects of the extracted DOM on the transport behaviours of TiO$_2$ NPs in acidic porous media.
compared with humic acid. Moreover, the interaction energy between nanoparticles and between nanoparticles and quartz media was calculated according to the classical DLVO theory. The dataset could be used as a reference for the evaluation and prediction of the environmental fate and subsequent risk of engineered nanomaterials.

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1. Data

The current dataset contains 2 tables and 7 figures. Elementary compositions (C, H, O, N, S and H/C) and ash contents of the extracted DOM and HA are given in Table 1. Fig. 1 shows the UV–Vis absorbance spectra of the extracted DOM and HA at wavelength of 190–800 nm. The tested concentrations were 46.9, 43.3, 42.9, and 18.8 mg/L for swine manure-derived DOM (SWDOM), sludge-derived DOM
(SLDOM) and sediment-derived DOM (SEDOM) and HA respectively. All DOM concentrations in this study are reported as the dissolved TOC concentrations and not the total mass concentrations. FTIR spectra of the extracted DOM and HA at wavenumbers range of 400–4000 cm⁻¹ and the assignment of absorption bands in FTIR spectra are shown in Fig. 2 and Table 2 respectively. Fig. 3 shows the adsorption of the DOM onto TiO₂ NPs in the presence of 1, 10 and 20 mmol/L NaCl for the extracted DOM and 5, 10 and 25 mmol/L NaCl for HA. Fig. 4 shows the zeta potentials of TiO₂ NPs in the presence of DOM and NaCl. Fig. 5 represents the calculated DLVO interaction energy between TiO₂ NPs and quartz sand under varying NaCl concentrations in the presence of SWDOM (a), SLDOM (b) and SEDOM (c) and 2 mg/L HA (d). Fig. 6 shows the breakthrough curves of TiO₂ NPs in acidic porous media at different NaCl concentrations in the presence of SWDOM (a), SLDOM (b), SEDOM (c), and HA (d). All raw data for the 7 figures are provided as Supplementary material.

2. Experimental design, materials, and methods

2.1. Materials

The nanoparticles, quartz sand and HA used in this study were identical to those used in our previous work [1,2]. TiO₂ NPs were purchased from Shanghai Aladdin Reagent Co., Ltd. They were spherical with a nominal size of 30 ± 10 nm and a specific surface area of 80.8 m²/g. The crystalline composition was determined to be a pure anatase phase, and the point of zero charge was 6.2 in deionized water (18.2 MΩ cm). TiO₂ NPs were used as received in all experiments. Stocking suspension of TiO₂ NPs was prepared by adding 250 mg TiO₂ NPs to 1.0 L deionized water. The suspension was sonicated for 30 min (500 W, 40 kHz) with vigorous stirring at room temperature (25 ± 4 °C) and stored no longer than 2 d at 4 ± 4 °C. Quartz sand (40–70 mesh) with an average diameter of approximately 350 μm was purchased from Sinopharm Chemical Reagent Co., Ltd. The sand was purified according to the method of Litton and Olson [3]. Surface impurities were removed by soaking in 12 mol/L HCl for 24 h followed by rinsing with deionized water until the pH of the rinse solution matched that of the deionized water. The sand was then baked in a furnace (FB1400, Thermo Scientific, USA) at 120 °C for 1 h and the at 800 °C for 5 h. HA was obtained from Sigma-Aldrich Chemical Co., Ltd. Stocking solution of HA was prepared at 1 g/L in deionized water with a small amount of NaOH as hydrotropic agent, and was stored no longer than 2 d at 4 °C. Other analytical grade chemicals used in this study were purchased from Sinopharm Chemical Regent Co., Ltd.

2.2. Extraction of DOM

DOM derived from three natural organic materials were extracted by deionized water using certain dry solid/water ratios of 1:20, 1:20 and 1:10 for swine manure, sludge and sediment respectively in a rotating shaker at 180 rpm at 25 °C for 12 h. The suspensions were centrifuged at 3500×g (3 K 15, Sigma Laborcentrifugen) for 30 min and then filtered through a 0.45 μm cellulose acetate filter membrane. The filtrates were referred to as swine manure-derived DOM (SWDOM), sludge-derived DOM (SLDOM) and sediment-derived DOM (SEDOM). The extracted DOM solutions were stored no longer than 2 d at 4 °C.

2.3. Preparation of TiO₂ NPs suspensions

Immediately prior to each experiments, aqueous TiO₂ NPs suspensions containing a final TiO₂ NPs concentration of 50 mg/L were prepared by diluting the stocking suspension in 8 mg/L extracted DOM or 2 mg/L HA solution at the desired NaCl concentrations (1, 10 and 20 mmol/L for the extracted DOM batches and 5, 10 and 25 mmol/L for HA batch), and were adjusted to pH 4.0 with 0.1 mol/L HCl. The mixtures were sonicated for 4 min at 25 °C to obtain homogeneous suspensions. The zeta potentials of the TiO₂ NPs suspensions were determined using a Zeta potential analysis (Zetasier Nano ZS90, Malvern Instruments, UK).
2.4. Adsorption of DOM onto TiO2 NPs

After 24 h, the suspended nanoparticles in TiO2 NPs suspension prepared above were pelleted by sequential centrifugation [4]. Briefly, 10 mL suspension was added to Teflon centrifuge tubes and centrifuged for 20 minutes at 9400×g. Then 8 mL of supernatant was carefully withdrawn from each

| Sample | C (mass %) | H | O | N | S | Ash | H/C |
|--------|------------|---|---|---|---|-----|-----|
| SWDOM  | 26.06      | 3.14 | 23.44 | 4.41 | 3.68 | 39.28 | 1.45 |
| SLDOM  | 24.87      | 3.85 | 20.54 | 3.33 | 3.37 | 44.04 | 1.86 |
| SEDOM  | 19.02      | 2.36 | 14.98 | 2.26 | 2.67 | 58.71 | 1.49 |
| HA     | 40.41      | 3.67 | 48.71 | 3.03 | 1.51 | 2.67  | 1.09 |

Table 1
Elemental compositions of the extracted DOM and HA.

![Absorbance spectra](image1)

**Fig. 1.** UV–Vis absorbance spectra of the extracted DOM and HA.

![FTIR spectra](image2)

**Fig. 2.** FTIR spectra of the extracted DOM and HA.
tube and transferred into another clean centrifuge tube for centrifugation. This procedure was repeated 3 times until the TiO2 NPs were completely removed from the solution. The DOM concentration in the supernatant was measured as TOC on a TOC analyzer (TOC-VCPN, Shimadzu, Japan). The adsorbed DOM was then determined by the difference between the initial and final DOM concentrations in the aqueous phase. Control experiments with TiO2 NPs-free solutions showed no variations in DOM

| Wavenumber (cm⁻¹) | Assignment                                      |
|-------------------|--------------------------------------------------|
| 3500–3400         | OH-stretching vibration of phenol, hydroxyl and carboxyl groups |
| 3000–2800         | Asymmetrical stretching vibration of C–H in aliphatics       |
| 1650–1600         | Aromatic C–C stretching vibration and C–O stretching vibration of conjugated carbonyl groups |
| 1450–1400         | Stretching vibration of C–H in aliphatics, asymmetrical stretching vibration of carboxyl, and deformation vibration of C–OH |
| 1260–1000         | Aliphatic C–OH stretching vibration                |
| 870–640           | Bending vibration of unsaturated band and benzene ring |

Fig. 3. Adsorption of DOM onto TiO2 NPs in presence of NaCl.

Fig. 4. Zeta potential of TiO2 NPs in the presence of NaCl.
concentrations before and after the centrifugation processes in the range of DOM concentrations tested.

2.5. Column transport experiments

Schematic of transport experiments setup is shown in Fig. 8. Glass columns (2.5 cm in diameter and 10 cm in length) were packed uniformly with the purified quartz sand. The resulting porosity of the porous medium was gravimetrically measured to be 0.42–0.47. Once packed, the column was preconditioned with at least 10 pore volumes (PVs) of TiO2 NPs-free background solution with the desired DOM and NaCl concentration. Then, 3 PVs of TiO2 NPs suspensions (50 mg/L) with the same background chemistry were introduced into the column, followed by a nanoparticle-free background solution. The Darcy velocity was maintained at 0.35–0.38 cm/min for all experiments. The influent suspension was vigorously sonicated at room temperature to maintain consistent TiO2 NPs dispersion throughout the experiment. Column effluent was collected using a fraction collector (BS-110A, Huxi Analytical Instrument Factory Co., Ltd., China). The concentrations of TiO2 NPs in the influent ($C_0$) and effluent ($C$) were determined spectrophotometrically at a wavelength of 343 nm. All transport experiments were conducted in duplicate with a deviation less than 3%; therefore, only one representative breakthrough curve for each experiment was shown in the results.

2.6. Derjaguin–Landau–Verwey–Overbeek (DLVO) theory

DLVO theory was applied to evaluate the role of electrostatic and van der Waals interactions on the interaction between the nanoparticles and the nanoparticle-quartz surfaces.

$$\Phi_{Total}(h) = \Phi_{elW}(h) + \Phi_{dl}(h)$$

(1)

![Fig. 5. Calculated DLVO interaction energy between TiO2 NPs under varying NaCl concentrations in the presence of SWDOM (a), SLDOM (b), SEDOM (c) and HA (d).](image-url)
DLVO interaction energies between TiO2 NPs were calculated assuming sphere-sphere geometry by utilizing the following equations [5]:

\[
\Phi_{vdW}(h) = -\frac{A_{101}a_p}{12h(1+14h/\lambda)}
\]  

\[
\Phi_{dl}(h) = 2\pi\varepsilon_0\varepsilon_r a_p \psi^2_p \ln[1 + \exp(-kh)]
\]  

Interaction profiles for nanoparticles and quartz sand particles were developed assuming sphere-plate geometry and the following equations were used for calculation [5]:

\[
\Phi_{vdW}(h) = -\frac{A_{102}a_p}{6h(1+14h/\lambda)}
\]  

\[
\Phi_{dl}(h) = \pi\varepsilon_0\varepsilon_r a_p \left\{ 2\psi_p\psi_c \ln\left[ \frac{1 + \exp(-kh)}{1 - \exp(-kh)} \right] + \left( \psi_p^2 + \psi_c^2 \right) \ln[1 - \exp(-2kh)] \right\}
\]  

In DLVO interaction energy profiles, positive interaction energy values represent repulsive condition whereas negative interaction energy values correspond to attraction.

Fig. 6. Breakthrough curves for TiO2 NPs at different NaCl concentrations in the presence of SWDOM (a), SLDOM (b), SEDOM (c), and HA (d).
When DLVO interaction energy between TiO$_2$ NPs is calculated, $a_p$ is the radius of the initial TiO$_2$ NPs, 30 nm, and in the case of the energy between TiO$_2$ NPs and quartz surface, the radius of an equivalent sphere for the nanoparticle aggregates which were measured by DLS has been used as the nanoparticle radius ($a_p$). $h$ denotes the (minimum) surface-to-surface separation distance between the spheres (for sphere–sphere geometry) or between a sphere and a plate (for sphere–plate geometry). A

**Fig. 7.** Calculated DLVO interaction energy between TiO$_2$ NPs and quartz sand under varying NaCl concentrations in the presence of SWDOM (a), SLDOM (b), SEDOM (c) and HA (d).

**Fig. 8.** Schematic of transport experiments setup.
characteristic wavelength ($\lambda$) of 100 nm was assumed in the calculations. Permittivity of free space ($\varepsilon_0$) and dielectric constant ($\varepsilon_r$) of water are $8.854 \times 10^{-12}$ C/V/m and 81.5 respectively, $\kappa$ is the inverse Debye length (m$^{-1}$) which was estimated for each electrolyte solution using eq. (6), and $\psi_p$ and $\psi_c$ are the surface potentials of TiO$_2$ NPs and quartz collector (V), respectively. For the calculation of interaction profiles, zeta potentials of TiO$_2$ NPs and quartz were measured under different chemical conditions and these values were used instead of surface potentials. The Hamaker constant for TiO$_2$ NPs–water–TiO$_2$ NPs interaction system ($A_{101}$) used was $3.7 \times 10^{-20}$ J [6] and for TiO$_2$ NPs–water–quartz system ($A_{102}$) $1 \times 10^{-20}$ J was used [7].

$$\kappa = \left(\frac{10^3 e^2 N_A (2I)}{\varepsilon_0 \varepsilon_r kT}\right)^{1/2}$$ (6)

where $e$ is the electron charge, $1.60 \times 10^{-19}$ C, $N_A$ is Avogadro’s constant, $6.02 \times 10^{23}$ mol$^{-1}$, and $I$ is the ionic strength of the solution.

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Conflict of 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.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.dib.2019.105021.

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