

Supporting Material

Developing machine learning algorithms to predict the dissolution of zinc oxide nanoparticles in aqueous environment

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Table S1: Formalisation of categorical inputs for application of one hot coding

Inputs	Categories
NOM types	1. DOC 2. SRHA 3. SRFA 4. TOC
Salt types	1. Monovalent (Na^+ , Cl^- , HCO_3^- , K^+ , NH_4^+ , NO_3^-) 2. Divalent (Ca^{2+} , SO_4^{2-} , Mg^{2+} , SO_4^{2-}) 3. Both (Na^+ , Cl^- , HCO_3^- , Ca^{2+} , SO_4^{2-} , Mg^{2+} , SO_4^{2-} , K^+)
Coating	1. Coatings (dodecyltrichlorosilane, and 3-aminopropyltrimethoxysilane, Citrate, Gelatin, PVP and Chitosan, PAA, HMP, cationic 3-aminopropyl triethoxysilane, PEG, PVA- PVP) 2. Non-coating
Coating types	1. Bare 2. Electrostatic e.g. Citrate, 3. Steric e.g. PEG, PVA, PVP
Shapes	1. Spherical 2. Non-spherical

TOC; Total dissolved carbon, DOC; dissolved organic carbon, SRHA; Suwannee River Humic acid, SRFA; Suwannee River Fulvic Acids, Polyvinylpyrrolidone (PVP), PEG: Polyethylene glycol, PVA: Polyvinyl alcohol. PAA: Polyacrylic acid-stabilized HMP: Sodiumhexametaphosphate-stabilized

Table S2: Literature studies on the dissolution of nZnO in aquatic systems

<i>Physicochemical, exposure medium, and experimental parameters</i>	<i>Reference</i>
6 nm and spherical, 20 nm and spherical, 71 nm and irregular, Hexagonal wurtzite, non-coated. Purified water: pH 7–9, Conc. (50–100 mg/ℓ). Time (0-200 mins). Ionic strength = 0.1 M, buffer concentration of 0.02M (KCl or KNO ₃)	(David et al., 2012)
5 nm, coating type: PVP. Purified water: pH 4 and 7.4, Conc. (0.01366 mg/ℓ), Time (24 hours).	(Briffa et al., 2018)
PEG, PVA- PVP coated nZnO, and bare nZnO were 58 ± 6.3, 60 ± 1.9, 52 ± 2.3 and 69 ± 1.2 nm respectively. Platelets. Purified water: pH 7, 1 mM NaHCO ₃ . SRHA (0, 5, 20 and 80 mg/ ℓ). Conc. (20 mg/ℓ), time (1 to 72 hours)	(Kizhakkumpat et al., 2021)
28±11 nm, 38m ² /g, cationic 3-aminopropyl triethoxysilane, wurtzite-like crystal structure. Purified water: pH 8.5-8.6. 0.1 M KCl SRHA, SRFA (1 to 40 mg/ℓ). Time (0-1 hour). Conc. (75 Mm/20 mM). 25 °C	(Jiang et al., 2015)
20 ± 5 nm, 15.0 ± 0.87 mv, 50 ± 10 m ² / g, non-coated. Natural water, pH, IS (mM), DOC (mg C/ℓ), Conductivity mS/cm Davis medium: 7.2, 0.04, 495, 3.47 Luria-Bertani medium: 7.0, 0.198, 6216, 21.8. Conc. (50 and 100) mg/ℓ, time (50 hours)	(Mei Li et al., 2011)
20 nm, non-coated. Purified water: pH 6.0, 7.0, 8.0, 9.0, TOC and NP-9 stock solutions were 537.3 ± 4.2 and 616.8 ± 5.8 mg/ℓ, respectively. Time (0-24 hours). Conc. (50 mg/ℓ).	(Li et al., 2017)
7, 17, 24, 15, 47, and 130 nm, wurtzite crystal structure and spherical. Non-coated. Purified water: pH = 7.5, 0 – 500 mM) (NaCl), Citric acid (0, 5, 10, 50, 100 mM). Time (24 hours), nTiO ₂ (500 mg/ℓ).	(Rupasinghe, 2011)
7, 17, 24, 15, 47, and 130 nm, wurtzite crystal structure for the ZnO. Spherical in shape and non-coated. Purified water: pH 7.5, Citric acid (0, 5, 10, 25, 50 mM). Time (24 hours), nTiO ₂ (500 mg/ℓ).	(Mudunkotuwa et al., 2012)
4.5 and 27 nm, coated, Citrate, Gelatin, PVP and Chitosan, Purified water: pH 7.6 and 6.1, IS: 0.029 M. (Ca ²⁺ , Mg ²⁺ , Na ⁺ , K ⁺ , NH ₄ ⁺ , NO ₃ ⁻ , SO ₄ ²⁻ , HCO ₃ ⁻), DOM (0, 1, 2, 4, 6 and 10 mg/ℓ). Time (5, 10, and 19 days). Conc. (1.0 mg/ℓ) in the dark at 23°C.	(Odzak et al., 2014)

- 4, 15 and 241 nm, 105 ± 13 m²/g, wurtzite structure, non-coated. Purified water: pH 1.0, 3.0 6.0, 9.0, and 11. IS= 0, 0.02 M (NaCl), Humic acid (100 mg/ℓ). Time (24 hours). Conc. (0.100 and 1000 mg/ℓ). (Bian et al., 2011)
- 20 ± 5 nm, 7, 15.0 ± 0.87 mv, 50 ± 10 , m²/g, non-coated (Li et al., 2013)
 Natural water: pH, IS (mM), DOC (mg C/ℓ),
 Tap water: 7.5, 4.0, 6.8
 West Lake: 7.8, 4.3, 12.6
 Xixi river: 7.5, 5.7, 5.3
 Qiantang river: 7.9, 7.5, 6.1
 Conc. (0-50 mg/ℓ).
- Uncoated ZnO-NPs (20 nm), dodecyltrichlorosilane-coated ZnO-NPs (23 ± 1 nm) and 3-aminopropyltrimethoxysilane ZnO-NPs (24 ± 1 nm). Purified water: pH 7 or 8 5, IS= 0.1 mM (NaCl), Time (0-96 hours). Conc. (0.1, 0.5, 1, 3, 5, 10, 30, 50, 80 or 100 mg/ℓ). 25 ± 1 °C (Yung et al., 2017)
- PAA-nZnO:20 nm, HMP-nZnO: (40 nm), Purified water: Merdzan et al., 2014
 pH 7.0, I= 0.01M, Time (24 h), Conc. (5.0 mg/ℓ).
- 50 nm and < 100 nm hexagonal wurtzite structure. Non-coated. Purified water: pH =1, 6, 7 and 9), I= (3 mM and 5 mM) (NaCl). Time (24 hours). Conc. (100 mg/ℓ). (Velintine et al., 2017)
- 18.3 nm, non-coated. Purified water: pH 8.5, IS = 5.6 mM, TOC = 219 mg/ℓ, conductivity = 318 μs/cm. Time (0-72 hours), Conc. (0.1 and 1 mg/ℓ). (Minghua Li et al., 2011)
- 35 nm, non-coated. (Gagné et al., 2019)
 Natural water: pH, TOC (mg C/ℓ), IS (mg/ℓ), Conductivity (μS/cm)
 Laboratory: 8.0, 2.1, <1, 310
 Brown: 7.1, 6.5, 5, 82.5
 Green: 8.1, 2.9, 13, 277
 Time (1, 48, and 96 hours). Conc. (10 mg/Lmg/ℓ).

70 nm, non-coated. (Blinova et al., 2010)
Natural water: water type, pH, DOC (mg C/ℓ), IS; Ca²⁺-Cl⁻, SO₄²⁻ (mg/ℓ)
River 1: 8.2, 13.3, 122 15.4, 96.1
River2: 8.2, 13.2, 124, 17, 69.1
River 3: 7.9, 25.9, 106, 4.6, 55.6
River 4: 8.1, 29.2, 111, 13.5, 76.1
River 5: 7.5, 34.5, 82.0, 9.2, 20.9
River 6: 8.1, 31.5, 58.0, 7.7, 14.9
Conc. (0.001, 0.01, 0.1, 1, 10 mg/ℓ). Time (24 hours).

14.9 ± 4.5 nm, non-coated. (Du et al., 2019)
Natural water: pH 8.12, IS= 1.02 mg /ℓ (Nitrate), DOC (0.65 mM), Conc. (10, 100, 1000 mg/ℓ). Time (0, and 1 hour).

< 130 nm, non-coated (Odzak et al., 2017)
Natural water: pH, IS (mM), DOC (mg C/ℓ), Conductivity mS/cm
Lake Greifen Maur: 8.1, 6.4, 3.1, and 404
River Rhine Eglisau: 8.2, 5.3, 1.9 and 318
Lake Lucerne Kastanienbaum: 8.2, 3.4, 1.1, and 202
Lake Gruere Saignelegier: 6.5, 1.4, 21.7 and 96
Lake Cristallina Alps Ticino: 6.4, <0.3, 1.0, and 7.0
Rainwater Dübendorf: 4.8, <0.3, 0.9 and 15.5
Time (0, 1, 3, and 8 days). (22.5 ± 0.1 °C) Conc. (50 mM).

Non-coated crystallized with wurzite structure. The shape of nZnO-(137.9 nm) was irregular, and nZnO-2 (19.2 nm) was spherical. Purified water: pH (6.0 and 9.0), SRHA (1 and 5 mg/ℓ). Conc. (20 mg/ℓ), Time (0.5 hours). (Han et al., 2014)

20 nm, spherical, non-coated. Purified water: pH (4–10), IS (0.005–0.1 M), SRFA (0–60 mg/ℓ), Time (24 hours). Conc. (1.0–30.0 mg/ℓ). (Domingos et al., 2013)

30-30 nm, non-coated, spherical, 25.7 ± 0.3 mV. River water: pH = 7.9, IS = 0.008 M, DOC (35.37 mg/ℓ) Time (24, 48, and 72 hours). Conc. (70 ug/ ℓ). (Londono et al., 2017)

15 nm, 240 m²/g, non-coated. Purified water: pH =2-10, IS = 0.001 M (NaCl), HA (3, 4, 5, 7 and 10 mg/ℓ). Time (0-70 hours), Conc. (50 mg/ℓ). (Jiang et al., 2012)

52 nm, 19± 3 m²/g, non-coated. (Majedi et al., 2014a)
water: pH, IS (mM), TOC (mg /ℓ),
Very soft water: 6.4-6.8, 0.572, 2
Moderately hard water; 7.4-7.8, 4.58, 2
Very hard water; 8.0-8.4,18.34, 2

Conc. (20 mg/ℓ). Time (0 - 180 hours)

41± 8 nm, 26± 3 m²/g, non-coated (Majedi et al., 2014b)

Purified water: pH 6, 7.5, and 9.0, IS (2 mM KCl), 50 mM CaCl₂, 10 Mm NaNO₃, HA (5 mg/ℓ), Oxalic acid (2 mg/ℓ), Citric acid (20 mg/ ℓ). Time (0-50 hours). Conc. (100 mg/ℓ).

20±5 nm (99.5), non-coated, 50 m²/g. (Zhang et al., 2016)

Natural waters: pH, IS (mM), TOC (mg /ℓ),

Pond: 7.06, 6.88, 15.4

countryside river; 7.30, 3.19, 23.3

Dongjiang river: 7.19, 5.19, 7.74

Taihu lake; 7.17, 7.99, 15.1

Conc. (100 mg/ℓ). Time (0.5 hours).

10-15 nm, non-coated. (Muna et al., 2018)

Natural waters: pH, IS (mM), TOC (mg C/ℓ), IS (Cl, SO⁴⁻, Ca²⁺, Mg²⁺, Na⁺ mg/ℓ),

lake water: 8.3, 5.1, 3.4, 22, 44, 4.6, 2.7

Tap water; 8.2, 10, 11, 29, 66, 7.8, 6.7

Time (0, 48, and 144 hours). Conc. (10 mg/ℓ).

<50 nm, crystalline structure, hexagonal, 12.5 m²/g, not (Khan et al., 2019)

coated Natural waters: pH= 6.95, IS = 0.002 mM, conductivity (82.4 us cm⁻¹). Time (0.55 -10 days). Conc. (10 mg/ℓ).

40 to 50 nm, 57 m²/g, non-coated. (Liu et al., 2018)

Natural water: pH, IS (mM) TOC (mg C/ℓ),

Lake water: 7.31 ± 0.43, 6.11 ± 0.42, 11.28 ±0.93

Tap water; 7.52 ± 0.37, 4.15 ± 0.36, 6.65±0.48

Rainwater; 7.66 ± 0.32, 3.66 ± 0.23 21.26 ±1.83

Pool water; 7.96 ±0.24, 6.96 ±0.52, 15.64 ±1.40

Conc. (100 mg/ℓ). Time (2, 20, 40, 60, 80, 100 hours).

*The freshwater used (TOC and DOC) and synthetic medium were based on (SRHA and SRFA as surrogates for natural organic matter (NOM). PVP, PEG, PVA, PAA, HMP

S1. Pre-cleaning

Environmental indicators are mainly quantified using diverse units. To provide uniformity, the units were harmonised to the single standard metric system, e.g. conversion from mol/l to mg/l for NOM. The Deybe-Huckel expression in Equation 1 was used to compute ionic strength from the concentration of ions (Na^+ , Cl^- , HCO_3^- , Ca^{2+} , SO_4^{2-} , Mg^{2+} , SO_4^{2-} , K^+):

$$I = 0.5 \sum_i^n c_i z_i^2 \quad (1)$$

Where I is the ionic strength, n is the total number of ionic species, i represents the specific ionic speciation, c_i is the molarity of the ionic species, and z_i is the charge on the ionic species (French et al., 2009).

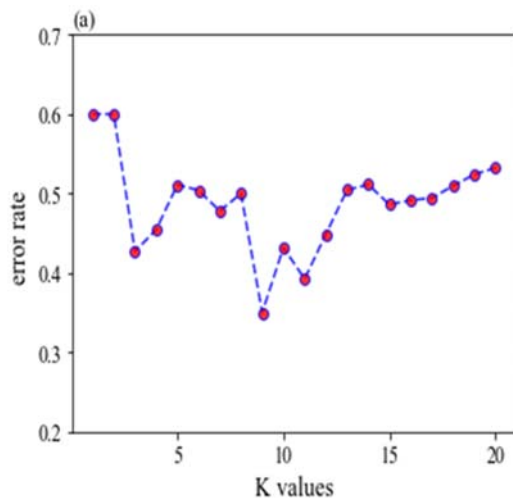


Figure S1. (a) k values in KNN

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