Influence of titanium dioxide nanoparticles on metallic trace elements behaviour in soils

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Introduction

Titanium dioxide nanoparticles (n-TiO_2) are among the most extensively engineered nanomaterials (ENMs) produced worldwide due to their innovative properties for various applications in many fields[1]. Their tremendous various applications have led to their widespread distribution in the environment including urban and industrial waste waters, which are treated in wastewater treatment plants (WWTPs). Sewage sludges coming from these WWTPs contain ENMs and are often used as amendment onto agricultural soils, thus unintentionally leading to an accumulation of these nanomaterials including n-TiO_2 into soils.

Objective

The objective of this study is to get a better insight into the influence of n-TiO_2 presence (rutile, 60 nm) on metallic trace elements (MTE; Cu) retention onto soils and transfer to the aquifers and surface waters, for a better prediction of their mobility and fate in agricultural soils.
In this way, Cu adsorption experiments are conducted on soil individual phases (e.g., goethite) by investigating the effect of several parameters (pH, ionic strength, n-TiO_2 and MTE concentrations). The modelling of experimental data using an integrated multi-surface approach enable to describe and predict the behaviour of MTE in soils considering the presence of n-TiO_2 .

Experimental methods

[Cu^{2+}] =10 µmol.L^{-1}

[Goethite] = 5 g.L^{-1}

[n-TiO_2] = 100 mg.L^{-1}

pH adjusted 3-8 → Suspension → Shaking 20h → Filtrates → ICP-OES analysis

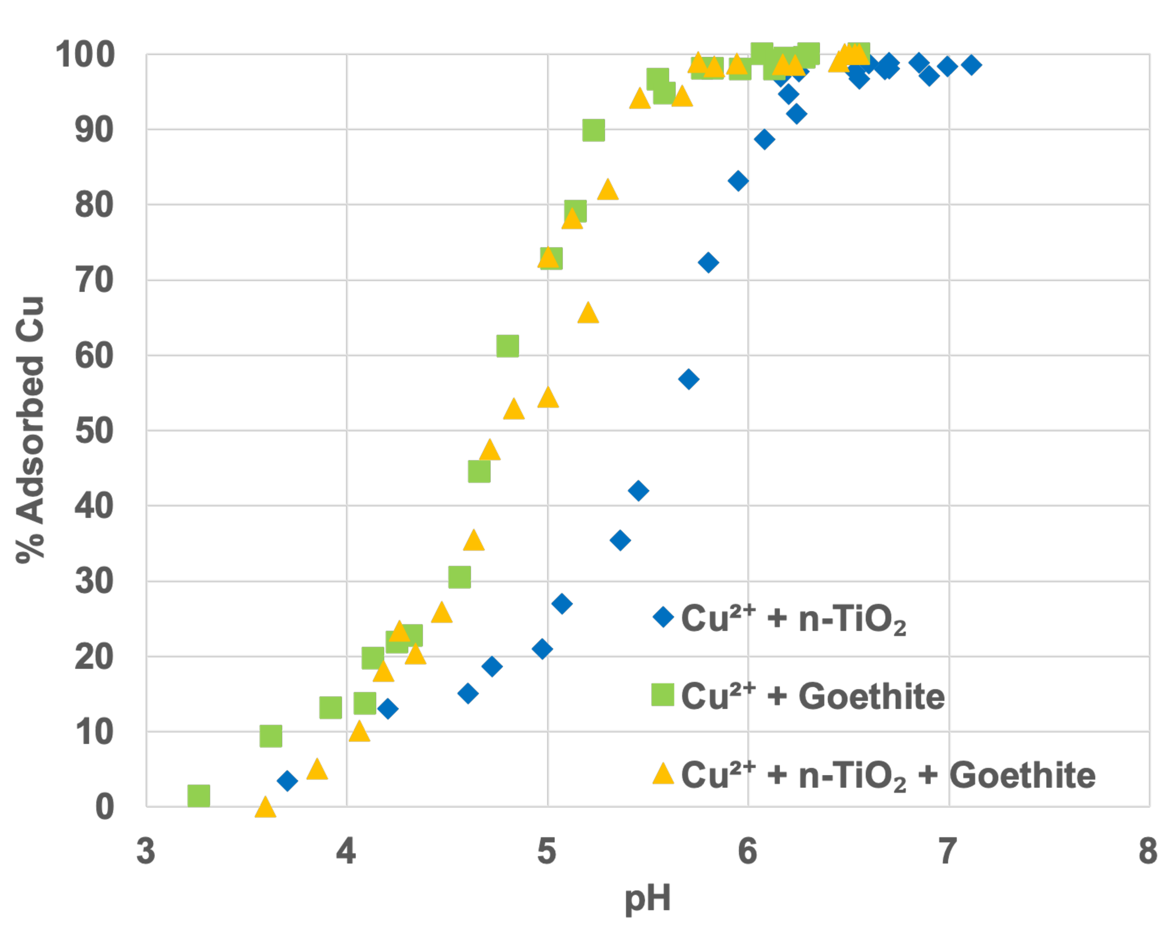
20° C

Filtration 0.45 µm

Acidified with HNO_3

Results

Experimental results



Cu^{2+} adsorption onto n-TiO_2, goethite, and goethite + n-TiO_2 as a function of pH

Modelling parameters

For n-TiO_2

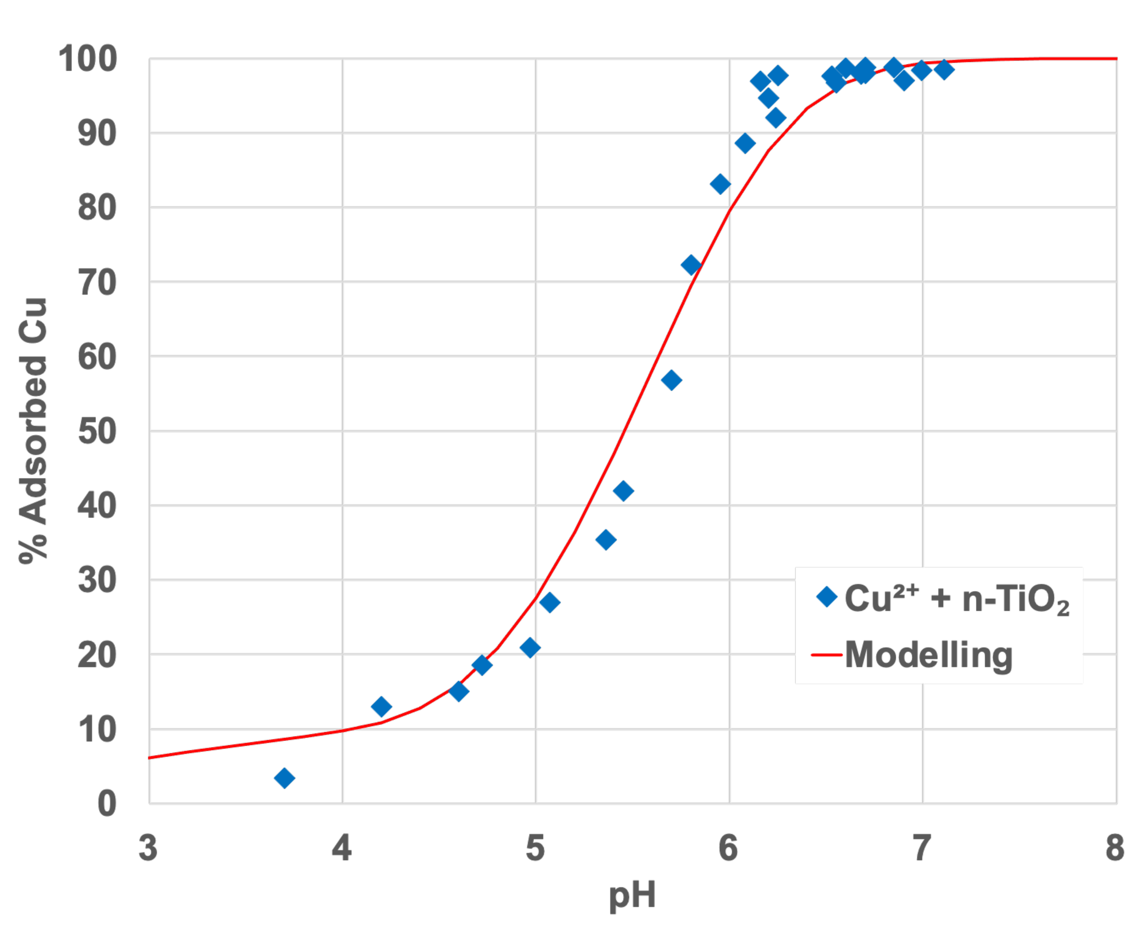
✓ Diffuse double layer (DDL) surface complexation model adapted from Dzombak et Morel[2]
Adjusted model parameters :
- specific surface area = 80 $m^2.g^{-1}$
- site density (one surface site) = 2.5 site.nm^{-2}
- protonation constants (2pK):
  - log K_1 = 3.2
  - log K_2 = -9
- Cu adsorption constants:
  - log K $TiOCu^+$ = 7
  - log K TiOCuOH = 16

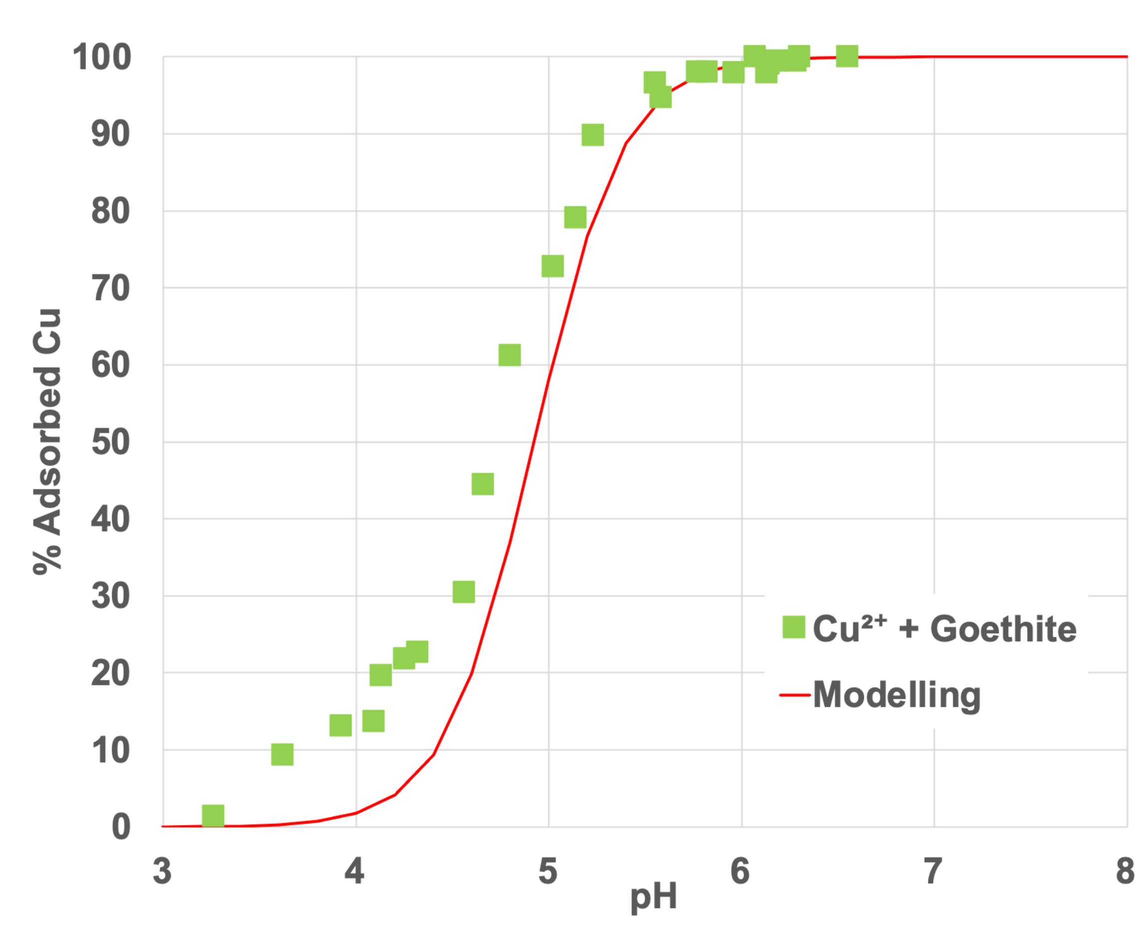
For goethite

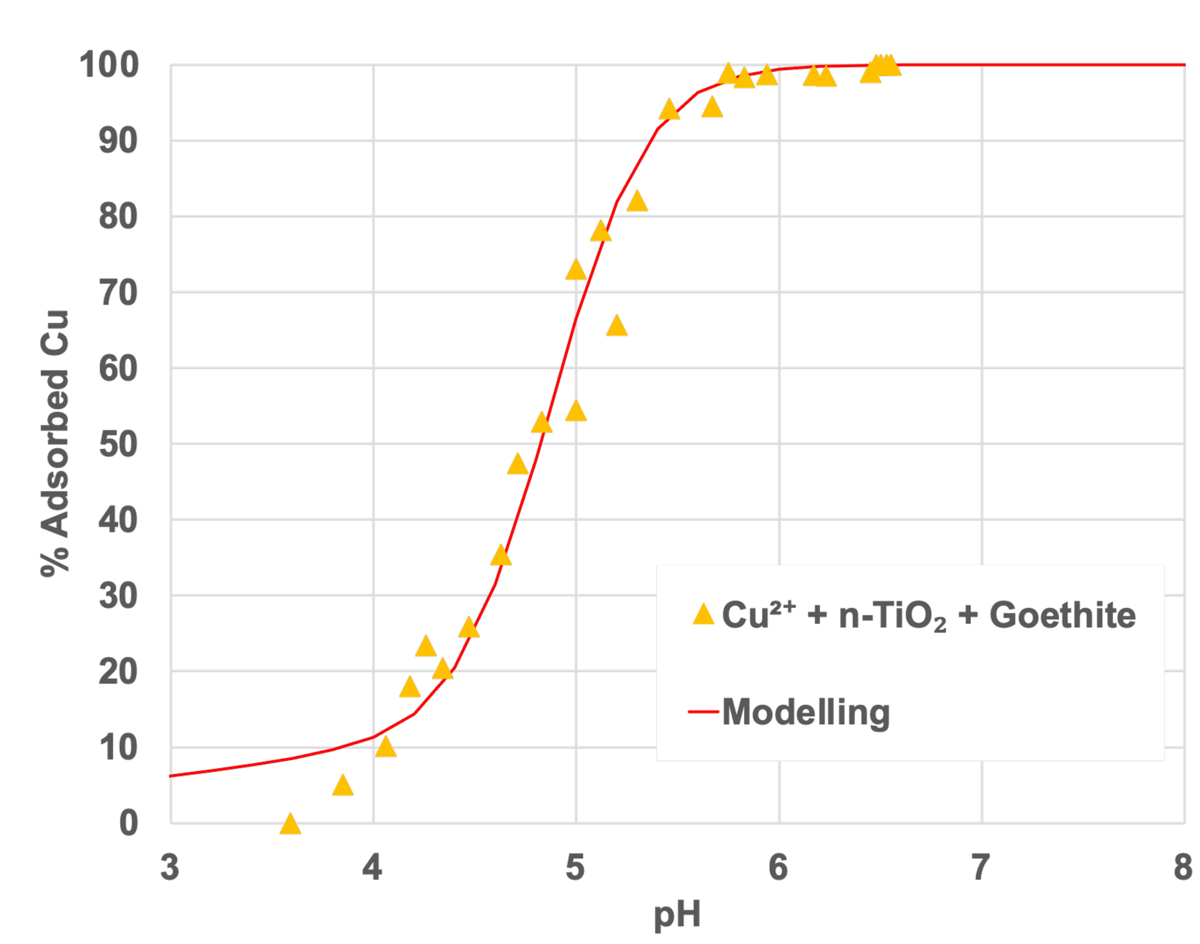
✓ CD-MUSIC model[3]
Model parameters from Weng et *al*.[4]:
- specific surface area = 94 $m^2.g^{-1}$
- site density (two surface site):
  - $FeOH^{-0.5}$ = 3.45 site.nm^{-2}
  - $Fe_3O^{-0.5}$ = 2.7 site.nm^{-2}
- protonation constants for both sites (1pK):
  - log K = 9.3
- Cu adsorption constants:
  - log K -$(FeOH)_2Cu^{+1}$ = 9.18
  - log K -$(FeOH)_2CuOH^0$ = 3.60
  - log K -$(FeOH)_2Cu_2(OH)_2^{+1}$ = 3.65
  - log K -$(FeOH)_2Cu_2(OH)_3^0$ = -3.10

✓ The model calculations were carried out using the computer program ECOSAT[5].

Modelling results







Cu adsorption data and modelling onto n-TiO_2, goethite, and goethite + n-TiO_2 as a function of pH

Conclusion

In the studied experimental conditions (environmentally relevant) there is no influence of the n-TiO_2 presence on Cu^{2+} adsorption onto goethite.
The proposed model enabled to predict the proportions of adsorbed Cu with a relatively good agreement to the experimental data. It will be confirmed regarding other experimental conditions. This approach will be applied to other soil phases and MTEs at different conditions.

References

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