A revised pseudo-second order kinetic model for adsorption, sensitive to changes in adsorbate and adsorbent concentrations

Supplementary Information

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# Data sets

Table S: Data sets collected, and the experimental conditions varied across each data set. C0 is the initial adsorbate concentration (mg L-1), Cs is the adsorbent concentration (g L-1) and r is particle radius (nm, μm or mm).

| Sorbate | Sorbent | Which experiments was the data used for? | Reference |
| --- | --- | --- | --- |
| Cd(II) | graphene oxide-Fe3O4-C3N3S3 | Influence of early data availability on the calculation of initial rates | 1 |
| Reactive yellow | Activated carbon | Initial rates | 2 |
| Antibiotics | Activated carbon | Initial rates | 3 |
| Methylene blue | Polymer-grafted magnetic microspheres | Initial rates | 4 |
| Pyridine | Polystyrene | Initial rates | 5 |
| Congo red | Shiitake mushroom | Initial rates | 6 |
| As(V) | Lanthanum-modified ceramics | Initial rates | 7 |
| Pb(II) | Algae biomass | Initial rates | 8 |
| PO43- | Fe3O4-SiO2 | Initial rates | 9 |
| Cr(III) | Kaolin | Initial rates | 10 |
| Pb(II) | Sulphuric acid treated acorn waste | Initial rates | 11 |
| Zn(II) | Regenerated cellulose | Initial rates | 12 |
| Tetracycline | Biochar | Initial rates | 13 |
| Methyl orange | Coal-kaolinite composite | Initial rates | 14 |
| As(V) | Fe2O3 | Initial adsorbate concentration, C0 | 15 |
| As(V) | Laterite | C0 | 16 |
| As(III) | Hydrous ferric oxide | C0 | 17 |
| HPO42- | Iron hydroxide | C0 | 18 |
| Cr(VI) | Activated carbon | C0 | 19 |
| Cu(II) | Soil | C0 | 20 |
| Pb(II) | Soil | C0 | 20 |
| Hg(II) | Raw activated sludge | C0 | 21 |
| Rose Bengal dye | ZnCl2-activated carbon | C0 | 22 |
| Cr(VI) | Fe2O3 | Adsorbent concentration, Cs | 23 |
| Cr(VI) | Mg-Al-CO3 | Cs | 24 |
| Cr(VI) | Chitin | Cs | 25 |
| Cu(II) | Fe2O3 | Cs | 26 |
| Zn(II) | Fe2O3 | Cs | 26 |
| Hg(II) | Lessonia nigrescens (kelp) | Cs | 27 |
| Hg(II) | Lessonia trabeculata (kelp) | Cs | 27 |
| Methylene blue | Raffia fibres | Cs | 28 |
| As(V) | Fe2O3 | particle size, r | 15 |
| As(V) | Fe2O3 | r | 29 |
| As(V) | Fe2O3 | r | 30 |
| As(V) | Fe2O3 | r | 31 |
| As(V) | Fe2O3 | r | 32 |
| As(V) | Fe2O3 | r | 33 |
| As(V) | Fe3O4 | r | 31 |
| As(V) | Fe3O4 | r | 34 |
| As(V) | Fe3O4 | r | 35 |
| As(V) | Fe3O4 | r | 36 |
| As(V) | Fe3O4 | r | 37 |
| As(V) | Fe3O4 | r | 34 |
| As(V) | FeOOH | r | 38 |
| As(V) | FeOOH | r | 31 |
| As(V) | FeOOH | r | 39 |
| As(V) | FeOOH | r | 40 |
| As(V) | FeOOH | r | 41 |
| As(III) | Fe2O3 | r | 30 |
| As(III) | Fe2O3 | r | 31 |
| As(III) | Fe2O3 | r | 32 |
| As(III) | Fe2O3 | r | 33 |
| As(III) | Fe3O4 | r | 31 |
| As(III) | Fe3O4 | r | 34 |
| As(III) | Fe3O4 | r | 36 |
| As(V) | Al2O3 | r | 42 |
| As(V) | Al2O3 | r | 43 |
| As(V) | Al2O3 | r | 44 |
| As(V) | Al2O3 | r | 45 |
| As(III) | Al2O3 | r | 46 |
| As(III) | Al2O3 | r | 42 |
| As(III) | Al2O3 | r | 45 |

# Comparison of mathematical techniques for the calculation of initial rates

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Figure S: The influence of the availability of early kinetic data on the calculation of initial rates using three mathematical approaches. Experiments from the literature were analysed (N=14), recalculating the initial rate as early data was consecutively removed, using three approaches: the initial slope approach (open diamonds), linearised PSO kinetics (red squares) and non-linear PSO kinetics (blue circles).

# Determining the order of reaction

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| --- | --- |
| (a) | (b) |

Figure S: Legend for the different adsorbate-adsorbent combinations presented in (a) Figure 2a and 3a, and (b) Figure 2b and 3b of the main text respectively.

# Application study 1



Figure S: Application study 1: Stick plot highlighting the relative error of qt calculated via the original PSO model and the rPSO (6 literature sources, 22 experiments and 198 data points). The average value and its standard deviation is indicated by μ±σ. Literature sources are denoted as As(III)/HFO 17 (dark blue squares), As(V)/Fe2O3 15 (light blue circles), HPO42-/iron hydroxide 18 (dark green diamonds), Cr(VI)/Fe2O3 23 (light green triangles), Cr(VI)/Mg-Al-CO3 24 (orange squares), and Cd(II)/Fe2O3 26 (red circles).

# Application study 2

|  |  |
| --- | --- |
| (a) | (b) |

Figure S: (a) The influence of particle radius (r) on the equilibrium adsorption capacity (qe) for the adsorption of inorganic As(V) and As(III) onto iron oxide adsorbents (red and orange filled shapes respectively) and inorganic As(V) and As(III) onto alumina adsorbents (dark blue open squares and light blue open circles respectively). Values of qe were determined by fitting the original PSO kinetic model. (b) Values of initial adsorbate concentration (C0) for the same experiments.

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Figure S: Legend indicating the different adsorbate-adsorbent systems presented in Application study 2.

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