Imperial College London

Department of Earth Science and Engineering

MSc in Applying Computer Science and Engineering

Independent Research Project

Project Plan

Predicting Removal of Arsenic from Sorbents

by

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1. Introduction

Although excessive arsenic content in drinking water can cause various diseases such as bladder, kidney, and lung cancers in the human body, the arsenic treatment plants developed in South Asia cannot effectively remove excessive concentrations of arsenic in drinking water. According to the paper [1], a study in northern India found that only 34 of the 200 arsenic treatment plants were in regular operation after a decade, and only 1 of the 34 arsenic treatment plants met the UN-set minimum criteria for arsenic in drinkable water (10 $\mu g \ L^{-1}$).

The difficulty in removing arsenic from drinking water is because As(III) exists in the form of H_3AsO_3 and is released under hypoxic conditions. Furthermore, due to the neutral charge of As(III), traditional adsorption methods cannot remove As(III) in water [2]. Therefore, As(III) can only be removed by adsorption after chemical methods such as oxidation after pretreatment.

When optimizing a water treatment plant to remove arsenic, As(III) can be treated with conventional oxidizing reagents such as chlorine and permanganate. However, they are costly and tend to form toxic by-products such as Cl_2 [3].

Therefore oxidation can be carried out using TiO_2 can reduce the production of toxic by-products [4]. In addition, Fe_2O_3 is used to adsorb arsenic oxide based on the photocatalytic action of TiO_2 to oxidize As(III) to As(V), which is then adsorbed onto Fe_2O_3 [5,6].

The project aims to determine the minimum absorber concentration required for an arsenic treatment plant to address the high cost of the absorber. The cost of replacing the sorbent medium is an essential factor in the purification of arsenic in drinking water, maximizing the arsenic concentration on the sorbent at a lower price. And the overall workflow of the project is shown in Figure 1. The objectives need to be achieved :

1. Determine the adsorption isotherms and kinetic entry parameters of the TiO2-Fe2O3 adsorption simulation system
2. Developing an As(III) adsorption kinetic model capable of observing changes in adsorbent and adsorbent concentration.
3. investigating the changes in As(III) at different concentrations for both batch and continuous flow treatment models.
4. using the model to simulate and determine a household The most economical solution for a year of clean water demand.
5. Produce a user-interactive interface allowing a more intuitive display of the minimum sorbent dosage.
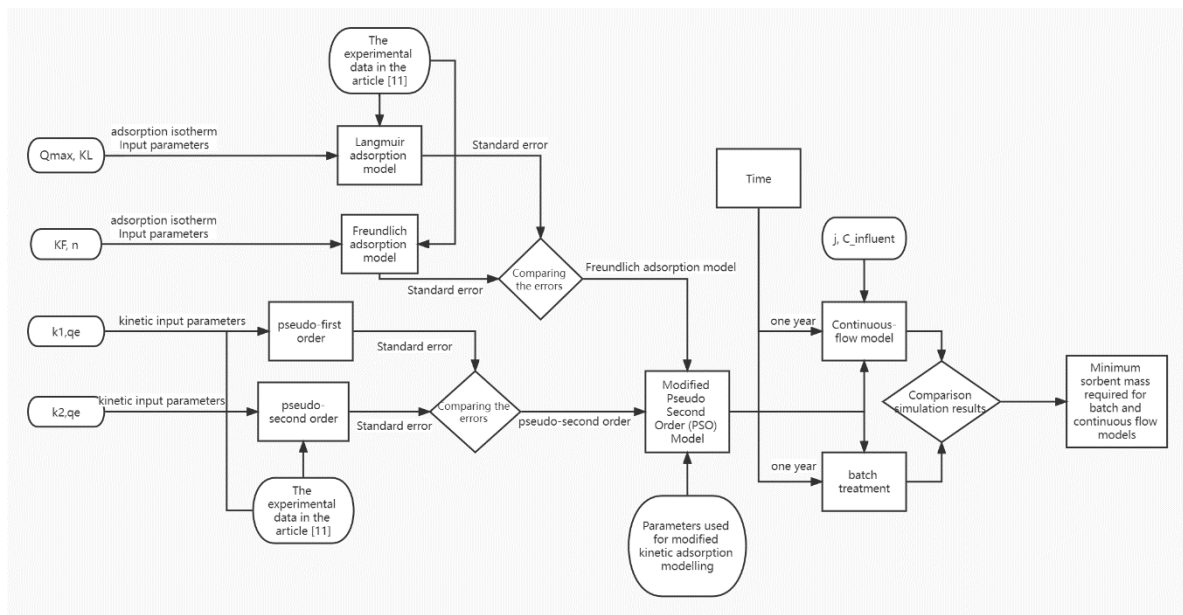
Figure 1:The main workflow of the project

2. Literature Review

The concentration of the adsorbent and the environment will have a particular impact on the project's parameters. According to the article's description [6], under the condition of a high concentration of adsorbent, the reaction rate is limited by photon supply and light scattering effects. The article [7] concluded that the reaction rate decreases with increasing adsorbent concentration. The description of [6] is also confirmed. However, as described in the article [11], low adsorption capacity is due to inadequate concentration of adsorbent and shortened filter life. Therefore in [8], the authors consider the sturdiness and stability of the adsorbent material to be an essential technical factor in the purification of drinking water.

From [9], which can be known that most of the current drinking water purification schemes choose between batch treatment and continuous flow treatment. Although the articles [10] found that most home-scale drinking water purification schemes use continuous flow columnar arrangement treatment, the study found that continuous flow treatment improved the degradation efficiency by 110%. However, according to the research of Dichiara et al. in the article [9], The paper concludes that the degradation efficiency of batch treatment is better than that of continuous flow treatment, given the complexity of the design and the difficulty of controlling the constant process. In the article [12], by comparing the removal of arsenic from drinking water by different concentrations of adsorbents, Lekic et al. found that a continuous flow column was more efficient than batch processing, but unlike the previous article, Lekic et al. believe that the reason for the phenomenon is in the process of filtering

The adsorption isotherm model for this project is based on the equations in the Langmuir and Freundlich article [13]. Whereas in [13], adsorption kinetics are modelled through pseudo-first and pseudo-second-order rate equations. Based on the adsorption capacity. Kinetic parameters and the data are given in the paper [11]. The standard errors between the models and data were calculated, and the adsorption kinetic model with the minor error was selected. Afterwards, the adsorption isotherm and kinetic models were combined into a modified pseudo-second-order (PSO) model for batch and continuous flow modelling design.

3. Description of Problem and Objectives

There are currently two ways to purify arsenic: batch treatment and continuous flow treatment. The principle of batch processing is to divide untreated water into multiple volumes and process them in sequence within a particular time until they meet safety standards. Furthermore, in continuous-flow treatment, influent water is continuously pumped into the reaction vessel and outflow water that meets safety standards.

Under the same adsorption isotherm parameters, the isotherm was modelled by the Langmuir and Freundlich equations, and the standard error was compared to determine the adsorption isotherm model.

For the Langmuir model, adsorption occurs through forming an adsorption monolayer on a homogeneous solid surface. The model is represented by the function (1).

$$q_e = \frac{Q_{max} \, K_L \, C_e}{1 + K_L \, C_e} \tag{1}$$

C_e is the concentration of As(III) in solution at equilibrium (mg L^{-1}), q_e is the concentration of As(III) in the adsorbent when the reaction reaches equilibrium (mg g^{-1}), Q_{max} is the maximum adsorption capacity (mg g^{-1}) and K$_L$ is the Langmuir constant (L mg^{-1}) [13].

The Freundlich adsorption model represents the multilayer adsorption of an adsorbent on a solid surface and is represented by the function (2).

$$q_e = K_F C_e^{1/n} \tag{2}$$

K$_F$ (mg g^{-1} (mg L^{-1}) $^{-1/n}$) is the Freundlich constant, and n is experimentally determined constants [13].
Primary and secondary reaction kinetics are the kinetics of chemical reactions in which reactants are converted directly into products in one step. In addition, other types of reactions that may also conform to primary or secondary reaction kinetics are called pseudo-first and second reaction kinetics.
The kinetic adsorption model was designed to study the removal rate of As(III) from drinking

water at initial adsorbate (C_0) and adsorbent (C_s) concentrations. The kinetic adsorption model was determined by establishing pseudo-first-order (PFO) (shown in Function (3)) and pseudo-second-order (PSO) (shown in Function (4)) kinetic models to observe changes in the concentration of As(III) in the adsorbent and compared by the standard error.

$$\frac{dq}{dt} = k_1 \left(q_e - q_t \right) \tag{3}$$

$$\frac{dq}{dt} = k_2 \left(q_e - q_t \right)^2 \tag{4}$$

q_e is the concentration of As(III) in the adsorbent when the reaction reaches equilibrium (mg g^{-1}), q_t is the quantity of arsenic adsorbed at time t (mg g^{-1}), k_2 is the pseudo-second-order rate constant (g mg^{-1} min^{-1}) and k_1 is the pseudo-second-order rate constant (g mg^{-1} min^{-1}) [13].

Combining predictive models of adsorption isotherms and adsorption kinetics to form an improved pseudo-second-order model for predictive modelling (shown in Function (5)). Furthermore, comparing the two modelling methods of batch and continuous treatment, the best solution, and suitable adsorbent concentration is found.

$$\frac{dq}{dt} = k_2 \left(K_F C_t^{1/n} - q_t \right)^2 \tag{5}$$

C_t is the concentration of aqueous As(III) at time t (mg L^{-1}).

Function (6) shows the equation for the reactor design model for batch treatment.

$$\frac{dC}{dt} = C_s k' C_t \left(1 - \frac{q_e}{q_t} \right)^2 \tag{6}$$

Where k' is the rate constant (L g^{-1} min^{-1}), C_s is sorbent   concentrations

Function (7) shows the equation for the reactor design model for continuous flow, which differs from the batch treatment in that the continuous flow reactor considers the inflow and outflow of As(III) during the continuous reaction.

$$\frac{dC}{dt} = j C_{\text{influent}} - C_t C_s k' \left(1 - \frac{q_e}{q_t} \right)^2 - j C_t \tag{7}$$

where j is the reactor turnover rate (min⁻¹) and $C_{influent}$ is the inflow As(III) concentration (mg L⁻¹) [13].

4. Progress to Date and Future Plan

The planning of the project has become the focus of the current project. Table 1 shows the basic plan data for the future of the project.

Table 1: Key dates and scheduled tasks

Dates	Task
1 Jun – 9 Jun	1. Literature reading 2. reading the background thesis on sorbents in water remediation 3. Set up a workflow 4. Outline the project proposal
10 Jun – 16 Jun	Experimental data from papers on adsorbent properties are obtained to test the correctness of the batch treatment and continuous models.
17 Jun – 24 Jun	Adsorption isotherm modelling code for Langmuir and Freundlich equations
24 Jun – 1 Jul	Project plan writing
2 Jul – 29 Jul	1. Pseudo-first-order and pseudo-second-order adsorption kinetic modelling codes 2. Batch , continuous flow model codes 3. User interface code (The specific workflow for the tasks are consistent with Figure 1)
1 Aug – 10 Aug	Presentation Course
12 Aug – 30 Aug	1. Identify characterization papers that have experimental data 2. Apply a model to simulate clean water for the home needs over a 365 days period

5. References

[1] Kumar, Abhishek, et al. "Assessment of Arsenic Removal Units in Arsenic-Prone Rural Area in Uttar Pradesh, India." *Journal of The Institution of Engineers (India): Series A*, vol. 100, no. 2, 2019, pp. 253–259., https://doi.org/10.1007/s40030-018-0349-9.

[2] Singh, Rachana, et al. "Arsenic Contamination, Consequences and Remediation Techniques: A Review." *Ecotoxicology and Environmental Safety*, vol. 112, 2015, pp. 247–270.,https://doi.org/10.1016/j.ecoenv.2014.10.009.

[3] Sharma, Virender K., and Mary Sohn. "Aquatic Arsenic: Toxicity, Speciation, Transformations, and Remediation." *Environment International*, vol. 35, no. 4, 2009, pp. 743–759., https://doi.org/10.1016/j.envint.2009.01.005.

[4] J. Gamage and Z. Zhang, "Applications of photocatalytic disinfection," *International Journal of Photoenergy*, vol. 2010, pp. 1–11, 2010.

[5] Z Zhou, Wei, et al. "Mesoporous Tio2/α-FE2O3: Bifunctional Composites   for Effective Elimination of Arsenite Contamination through Simultaneous Photocatalytic Oxidation and Adsorption." *The Journal of Physical Chemistry C*, vol. 112, no. 49, 2008, pp. 19584–19589., https://doi.org/10.1021/jp806594m.

[6] Colombo, Enrico, and Muthupandian Ashokkumar. "Comparison of the Photocatalytic Efficiencies of Continuous Stirred Tank Reactor (CSTR) and Batch Systems Using a Dispersed Micron Sized Photocatalyst." *RSC Adv.*, vol. 7, no. 76, 2017, pp. 48222–48229., https://doi.org/10.1039/c7ra09753k.

[7] Yu, Lian, et al. "Arsenite Removal from Aqueous Solutions by γ-fe2o3–tio2 Magnetic Nanoparticles through Simultaneous Photocatalytic Oxidation and Adsorption." *Journal of Hazardous Materials*, vol. 246-247, 2013, pp. 10–17., https://doi.org/10.1016/j.jhazmat.2012.12.007.

[8] German, Michael S., et al. "Evidence of Economically Sustainable   Village-Scale Microenterprises for Arsenic Remediation in Developing Countries." *Environmental Science & Technology*, vol. 53, no. 3, 2019, pp. 1078–1086., https://doi.org/10.1021/acs.est.8b02523.

[9] Dichiara, Anthony B., et al. "On the Choice of Batch or Fixed Bed   Adsorption Processes for Wastewater Treatment." *Industrial & Engineering Chemistry Research*, vol. 54, no. 34, 2015, pp. 8579–8586., https://doi.org/10.1021/acs.iecr.5b02350.

[10]   Bhardwaj, Anuja, et al. "Status of Arsenic Remediation in India."   *Advances in Water Purification Techniques*, 2019, pp. 219–258., https://doi.org/10.1016/b978-0-12-814790-0.00009-0.

[11]   Bullen, Jay C., et al. "On the Application of Photocatalyst-Sorbent Composite Materials for Arsenic(III) Remediation: Insights from Kinetic Adsorption Modelling." *Journal of Environmental Chemical Engineering*, vol. 8, no. 5, 2020, p. 104033., https://doi.org/10.1016/j.jece.2020.104033.

[12]   Lekić, Branislava M., et al. "Arsenic Removal from Water UsingIndustrial by-Products." *Journal of Chemistry*, vol. 2013, 2013, pp. 1–9., https://doi.org/10.1155/2013/121024.

[13]   Ayawei, Nimibofa, et al. "Modelling and Interpretation of Adsorption   Isotherms." *Journal of Chemistry*, vol. 2017, 2017, pp. 1–11., https://doi.org/10.1155/2017/3039817.

[14]   Hu, Wei, et al. "Evaluation of Parameter Uncertainties in Nonlinear   Regression Using Microsoft Excel Spreadsheet." *Environmental Systems Research*, vol. 4, no. 1, 2015, https://doi.org/10.1186/s40068-015-0031-4.