International Journal of Progressive Sciences and Technologies (IJPSAT)
ISSN: 2509-0119.

https://ijpsat.org/
Vol. 55 No. 2 February 2026, pp. 569-582

Optimization Of Wastewater Treatment Through Multi-Agent Simulation Using Sugarcane Bagasse Cellulose

Miranto R. Randriamaherison[1], Marie Hanitriniaina Ratsimba[1,2], Falihery Rajoelison[2], Damien Ali Hamada Fakra [2,4], Rijalalaina Rakotosaona[1,2], Mino Patricia Randrianarison[2,3] , Mirana Razafimahefa[2]

[1] Doctoral Schools of Science and Engineering and Innovation, University of Antananarivo, Madagascar
[2] Laboratory for Research in Materials, Processes, and Civil Engineering LRMPGC, Antananarivo Polytechnic School, University of Antananarivo, Madagascar
[3] Doctoral School of Engineering and Geosciences, University of Antananarivo, Madagascar
[4]Faculty of Science and Technology, University of Lorraine, France
Corresponding author: Miranto R. Randriamaherison. E-mail: miranto.randriamaherion@gmail.com

Abstract – The uncontrolled release of untreated domestic wastewater continues to pose a significant public health and environmental challenge in Madagascar. Among the pollutants, anionic surfactants from household detergents are particularly concerning due to their persistence and poor removal by conventional low-cost treatment methods. Sulfo-acetylated cellulose, derived from sugarcane bagasse, has emerged as a promising and locally available biosorbent for addressing this issue. Laboratory experiments demonstrate a maximum adsorption capacity of 154.18 mg/g for anionic surfactants. Moreover, for detergent concentrations up to 0.3% (m/V), the treated water meets key World Health Organization (WHO) physico-chemical standards, including pH, conductivity, total dissolved solids (TDS), salinity, and oxidation-reduction potential (ORP). This study presents an agent-based model (ABM) developed using GAMA (v.1.9.3), designed to scale laboratory findings toward practical, compact treatment units. The model evaluates the influence of adsorbent bed thickness (10, 20, and 30 mm) and initial detergent concentrations ranging from 0.1% to 0.6%, while predicting the temporal evolution of treated water quality. After calibration with experimental data, the simulation successfully reproduces key trends: increased adsorption capacity (qe, mg/g) with greater bed thickness and pollutant load, rapid breakthrough beyond 0.3% detergent concentration, and sustained WHO-compliant water quality for beds of at least 20 mm thickness.

Keywords: Agent-based modelling; GAMA; Sulfo-acetylated cellulose; Sugarcane bagasse; Adsorption; Domestic wastewater treatment; Process optimization.

International Journal of Progressive Sciences and Technologies (IJPSAT)
ISSN: 2509-0119.

https://ijpsat.org/
Vol. 55 No. 2 February 2026, pp. 569-582

I. INTRODUCTION

Context and problem statement

The management of domestic wastewater in developing countries remains a major challenge, particularly in Madagascar, where a large proportion of the population lacks adequate sanitation infrastructure. The “Health and Pollution” action plan for Madagascar stresses that many infectious diseases and a significant fraction of mortality in sub-Saharan Africa are directly linked to inadequate management of water and wastewater [1]. In this context, nearly 80% of Malagasy households discharge their wastewater directly into the environment without prior treatment, generating both a substantial public health burden and the degradation of aquatic and terrestrial environments.

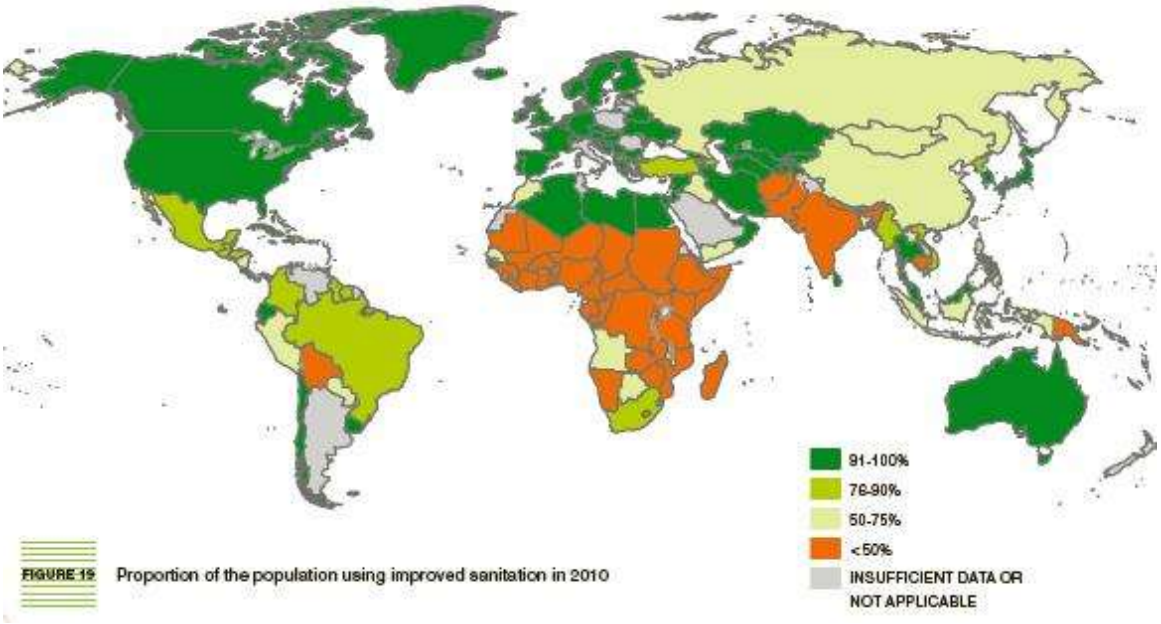

Fig. 1- Percentage of the population with access to improved sanitation in 2010 (Source: Progress on Drinking Water and Sanitation, 2012 Update Report, JMP) [2]

Among domestic pollutants, anionic surfactants originating from household detergents are especially important (Randriamaherison et al., 2025). They are only weakly removed by conventional low-cost systems (simple sedimentation, rudimentary pits, sand filters), even though WHO guidelines require compliance with recommended values for several physico-chemical parameters (pH, electrical conductivity, TDS, salinity, ORP) in order to limit health risks associated with consumption or contact with such waters [3]. The search for simple, robust, low-cost treatment processes adapted to low-resource settings therefore remains a priority.

Valorization of sugarcane bagasse

In this perspective, the valorization of agro-industrial residues such as sugarcane bagasse appears as a promising option. Bagasse, an abundant by-product of the sugar industry, consists of a mixture of cellulose, hemicellulose and lignin that can be transformed into low-cost bio-based materials for effluent treatment. Numerous studies have shown that bagasse, either raw or chemically modified, can serve as an efficient biosorbent for the removal of various pollutants (heavy metals, dyes, pesticides, organic compounds) from wastewater [4], [5]. For instance, bagasse pulp has been used for the sorption of textile dyes, achieving significant reductions in colour and TDS after adsorption [6], [7]. Other work has demonstrated that chemical modification of bagasse (alkaline activation, grafting of functional groups, conversion into biochar) greatly enhances its adsorption capacity for pollutants such as

International Journal of Progressive Sciences and Technologies (IJPSAT)
ISSN: 2509-0119.

https://ijpsat.org/
Vol. 55 No. 2 February 2026, pp. 569-582

heavy metals and dyes [8], [9]. More recently, sulfonated biosorbents derived from bagasse have been developed to increase the density of acidic sites (–SO_3H) and optimize the adsorption of cationic dyes, achieving high capacities in aqueous systems. These studies confirm the potential of bagasse as a platform for adsorbent materials, particularly when the cellulosic fraction is extracted and functionalized to increase specific surface area and active-site density [5]. He presents study is positioned within this dual context and extends previous work on the valorization of sulfo-acetylated cellulose derived from sugarcane bagasse for the adsorption of anionic surfactants from domestic wastewater (Randriamaherison et al., 2025).

Innovation of the agent-based model and positioning of the study

In parallel with developments in biosorbents, a large number of studies rely on classical mathematical models (Langmuir and Freundlich isotherms, pseudo-first- and pseudo-second-order kinetics) and, more recently, on artificial intelligence approaches (artificial neural networks, meta-models) to describe adsorption and optimize operating conditions [10], [11]. These models are largely macroscopic: they provide a good description of the global relationship between concentration, contact time and adsorption capacity, but they offer limited insight into spatial heterogeneities within the adsorbent bed and the progressive saturation of different layers.Agent-based modelling (ABM), initially developed for complex systems in which global behaviours emerge from local interactions [12], [13] , has begun to be applied to certain water treatment processes, in particular for modelling activated sludge or biofilms (for example, to simulate microbial communities in wastewater treatment plants). However, the application of ABM to adsorption processes on bio-based materials remains very scarce.The interest of the approach adopted here is twofold. First, it makes it possible to evaluate system performance before building a physical infrastructure, thereby reducing experimental costs. Second, it can be adapted to local specificities. The model thus provides a framework for designing decentralized treatment solutions that are easily deployable and adapted to low-resource regions.The originality of this work lies specifically in the coupling between : a local, low-cost, functionalized adsorbent material sulfo-acetylated cellulose derived from sugarcane bagasse whose performance with respect to anionic surfactants has been quantified experimentally; and an agent-based simulation model implemented in the GAMA platform (v1.9.3), which transposes laboratory findings to a compact treatment module, explicitly represents the spatial heterogeneity of the adsorption bed, and anticipates breakthrough as a function of household usage scenarios.Unlike most studies that focus either on the preparation and testing of new biosorbents or on purely global adsorption models, this research proposes an integrated “material and ABM simulation” framework specifically oriented toward anionic surfactants in domestic wastewater and WHO water-quality requirements.

Research objectives

The overall objective of this study is to propose a numerical simulation method capable of predicting the performance of domestic wastewater treatment by adsorption on sulfo-acetylated cellulose derived from sugarcane bagasse, as a function of key operational parameters. More specifically, the study aims to :

- Model, using an agent-based model, the adsorption of anionic surfactants in a decentralized treatment module at the household scale, using experimental data on maximum adsorption capacity (q_e, mg/g) and physico-chemical water quality (pH, conductivity, TDS, salinity, ORP) as input.
- Assess the influence of adsorbent bed thickness (10, 20 and 30 mm) and initial detergent concentration (0.1% – 0.6% m/V) on q_e and on the compliance of treated water with the main WHO recommendations.
- Estimate the useful lifetime of the adsorbent bed before saturation, defined as the point at which the treated water no longer simultaneously satisfies the targeted physico-chemical criteria, for pollutant loads representative of Malagasy domestic discharges.
- Provide sizing elements for replaceable or regenerable biosourced adsorption cartridges, in order to guide the design of low-cost, decentralized treatment units adapted to low-resource contexts.

International Journal of Progressive Sciences and Technologies (IJPSAT)
ISSN: 2509-0119.

https://ijpsat.org/
Vol. 55 No. 2 February 2026, pp. 569-582

II. MODELLING METHODOLOGY AND NUMERICAL PROTOCOL

1. Overall framework and rationale for the approach

The methodology is based on the construction of an agent-based model implemented in the GAMA platform (version 1.9.3), with the aim of transferring the adsorption performance observed in the laboratory to a compact domestic wastewater treatment module. The system considered is an adsorption bed made of sulfo-acetylated cellulose obtained from sugarcane bagasse, through which a flow of domestic wastewater containing anionic surfactants passes. Experimental results (adsorption capacity q_e, together with the evolution of pH, conductivity, TDS, salinity, specific gravity and ORP) are used to parameterize and calibrate the model.

The model is documented using the ODD protocol (Overview, Design concepts, Details), which is widely recommended for individual-based models, in order to ensure transparency and reproducibility [13]. An agent-based approach is preferred here because it allows explicit representation of spatial heterogeneity within the adsorbent bed and of the progressive saturation of different layers, rather than reducing the system to purely global variables. The numerical simulation links bed configuration (10, 20 or 30 mm), initial detergent concentration (0.1%–0.6% m/V) and flow conditions to adsorption performance and treated water quality, in line with WHO criteria for drinking water.

2. Structure of the agent-based model

The system is represented by a regular 10 × 10 grid, corresponding to a two-dimensional cross-section of the adsorption bed. This grid forms the environment in which two main types of entities interact: Adsorbent cells, representing elementary volumes of sulfo-acetylated cellulose, each characterized by an initial adsorption capacity (mg of pollutant per g of material) and a remaining capacity that decreases as local adsorption events occur. Pollutant agents, representing packets of anionic surfactants, which move from the inlet to the outlet of the grid.

Each time step corresponds to one flow cycle through the cartridge. At every step, pollutant agents move towards the outlet following a global flow direction, perturbed by stochastic noise to reflect heterogeneities in porosity and flow paths. When a pollutant agent enters a cell that still has residual capacity, an adsorption event may occur with a probability that depends on the local remaining capacity, local pollutant concentration and bed thickness. If adsorption occurs, the agent changes state (captured) and the cell's remaining capacity is reduced; otherwise, the agent continues downstream. Agents reaching the outlet without being captured are counted as residual pollution in the treated water.

Global parameters of the aqueous phase (pH, conductivity, TDS, salinity, specific gravity and ORP) are updated at each time step in a "collector" representing the treated water, based on the number of non-captured agents and empirical relationships or fitted functions derived from experimental data.

From a conceptual point of view, global system behaviour (pollutant removal efficiency, cumulative adsorption capacity, useful bed life) emerges from local interactions between pollutant agents and adsorbent cells. The pollutant agents themselves do not adapt their behaviour, but the adsorbent "adapts" indirectly through the progressive depletion of its remaining capacity. This structure makes it possible to represent differences in saturation between upstream and downstream zones of the bed: the first layers saturate more rapidly for thin beds or high pollutant loads, while increasing bed thickness (30 mm) delays pollutant breakthrough at the outlet.

3. Numerical protocol and simulation workflow

Each simulation starts with an initialization phase in which the experimental scenario and inlet conditions are set. An initial detergent concentration is chosen among the laboratory values (0.1%, 0.2%, 0.3% or 0.6% m/V), together with a bed thickness (10, 20 or 30 mm). These choices determine the mass of sulfo-acetylated cellulose present in the system and the corresponding theoretical global adsorption capacity. The number of pollutant agents released at the inlet is proportional to the initial concentration, and each adsorbent cell receives an initial capacity proportional to the mass of material it represents. The inlet water quality parameters are set to their pre-adsorption values.

International Journal of Progressive Sciences and Technologies (IJPSAT)
ISSN: 2509-0119.

https://ijpsat.org/
Vol. 55 No. 2 February 2026, pp. 569-582

The core of the numerical protocol is a time loop in which pollutant–adsorbent interactions occur. At each time step: Pollutant agents move across the grid according to the global flow direction plus a stochastic component. When a pollutant agent enters an adsorbent cell with remaining capacity, an adsorption attempt occurs with a probability that depends on local conditions (remaining capacity, pollutant load, bed thickness). Captured agents are removed from the mobile phase and the local capacity of the cell is decreased; non-captured agents continue to move downstream. Agents that exit the grid without being adsorbed are counted in the treated water.

Throughout the simulation, the total amount of adsorbed pollutant is recorded and converted into cumulative adsorption capacity q_e (mg/g) by dividing by the total active adsorbent mass. The relationship between adsorbed quantity and residual concentration in solution is based on the Freundlich isotherm fitted to the experimental data :

$$q = K.C^{\frac{1}{n}}$$

q : the amount of pollutant adsorbed per unit mass of adsorbent (mg/g).

C : the equilibrium pollutant concentration in the liquid phase (mg/L).

K : the Freundlich constant related to adsorbent–adsorbate affinity (–).

n : an empirical exponent that reflects adsorption intensity and surface heterogeneity (–).

This ensures consistency between the local adsorption dynamics in the model and the experimental laboratory results. In parallel, the number of non-captured pollutant agents at each time step is used to update global water-quality parameters (pH, EC, TDS, salinity, specific gravity, ORP) using proportional relationships or fitted functions derived from measurements.

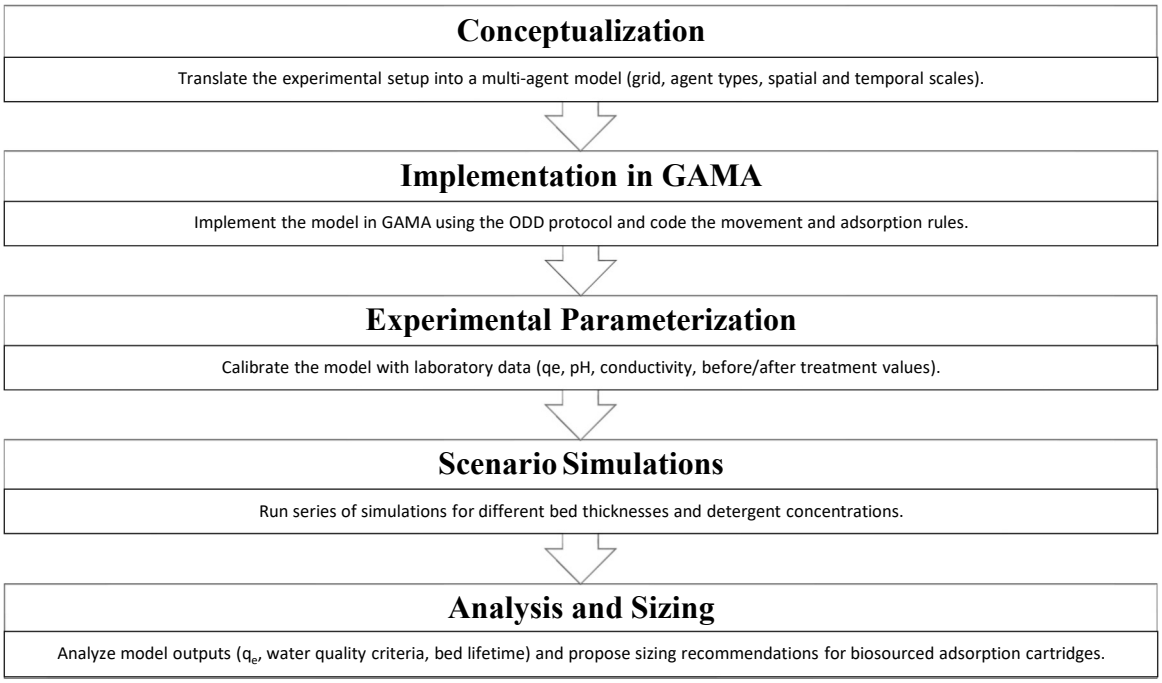

Fig. 2- Schematic representation of the agent-based adsorption modelling process: use of experimental data (Freundlich isotherm) for parameterization, implementation in GAMA, calibration/validation phase and scenario exploration.

International Journal of Progressive Sciences and Technologies (IJPSAT)
ISSN: 2509-0119.

https://ijpsat.org/
Vol. 55 No. 2 February 2026, pp. 569-582

4. Calibration, validation and use of the model

Model calibration consists in adjusting the parameters governing local adsorption probability so that, for each experimental combination (bed thickness 10, 20 or 30 mm and detergent concentration between 0.1% and 0.6%), simulated adsorption capacities q_e match laboratory values as closely as possible. For each scenario, several stochastic repetitions are run using different random seeds, allowing the calculation of goodness-of-fit indicators such as root-mean-square error, mean relative error and the slope of the regression line between simulated and measured q_e Calibration is considered satisfactory when the regression slope is close to unity, the intercept is small and the overall error remains below a pre-defined threshold.

Validation is based on a joint comparison of several types of results: cumulative adsorption capacity q_e, reduction in residual surfactant concentration in the effluent and changes in treated water physico-chemical parameters. Simulations are deemed credible when they reproduce the main experimental trends: improved pollutant removal with increasing bed thickness, decreased effectiveness as initial detergent concentration rises, and convergence of treated water parameters towards WHO-recommended ranges in the most favourable scenarios.

Once calibrated and validated, the model is used as a scenario-exploration tool to investigate configurations that were not tested in the laboratory or to extrapolate the operational lifetime of the cartridge under realistic domestic usage conditions. Simulation series make it possible to estimate, for each (bed thickness, pollutant load) pair, the number of flow cycles beyond which the treated water no longer simultaneously meets the selected criteria (for example, conductivity and TDS below guideline values, ORP within an acceptable range). These results provide design and decision-support elements for low-cost, decentralized treatment modules based on sulfo-acetylated cellulose derived from sugarcane bagasse.

5. Experimental and simulated data set

The data set used for calibration and validation combines experimental measurements and simulation outputs.

On the experimental side, a total of 60 data points were obtained from adsorption tests carried out for three biosorbent bed thicknesses (10, 20 and 30 mm), with 20 experimental conditions per thickness. For each condition, the following variables were measured: initial detergent concentration (C_0), residual equilibrium concentration (C_e), solution volume V, biosorbent mass m, contact time and, when available, some physico-chemical parameters (pH, conductivity, turbidity) before and after treatment. The equilibrium adsorption capacity q_e was calculated systematically as :

$$q_e = \frac{(C_0 - C_e)V}{m}$$

where q_e is the amount of detergent adsorbed per unit mass of cellulose (mg/g), C_0 is the initial detergent concentration (mg/L), C_e is the equilibrium concentration (mg/L), V is the solution volume (L), and m is the mass of cellulose (g).

The simulated data set consists of 600 runs of the agent-based model, corresponding to 10 independent repetitions for each of the 60 experimental conditions (combinations of bed thickness and detergent concentration). For each scenario, the model records the temporal evolution of detergent concentration in the aqueous phase, the number of adsorption events per biosorbent particle and the simulated equilibrium adsorption capacity.

III. RESULTS

The results are presented in three steps. First, the spatial distribution of pollutant capture within the adsorption bed is analysed using visual outputs from the agent-based model, which highlight the progression of the saturation front. Second, the quantitative agreement between simulated and measured adsorption capacities is examined to assess the quality of model calibration. Third, simulated water-quality parameters are compared with experimental measurements and WHO guideline values, in order to discuss the relevance of the process at the household scale and to position its performance relative to other bagasse-based biosorbents.

International Journal of Progressive Sciences and Technologies (IJPSAT)
ISSN: 2509-0119.

https://ijpsat.org/
Vol. 55 No. 2 February 2026, pp. 569-582

1. Spatial distribution of pollutant capture

Visual outputs from the agent-based simulations show that pollutant capture does not occur uniformly throughout the adsorption bed. Instead, a progressive saturation front develops. At the beginning of a simulation, the upstream zone of the fluid matrix is densely populated with pollutant agents, and nearly all adsorbent cells still possess a large residual capacity. As time steps progress, the concentration of pollutant agents decreases markedly in the first layers of the bed, which saturate first, while deeper layers remain partially available.

For thin beds (10 mm), this saturation front quickly traverses the entire adsorbent zone, resulting in a rapid rise in outlet pollutant concentration. Conversely, for 20 mm and especially 30 mm thickness, the active capture zone extends over a longer distance and the saturation front moves more slowly downstream, delaying pollutant breakthrough at the module outlet. This spatial dynamic is consistent with experimental adsorption results obtained for sulfo-acetylated bagasse cellulose and with findings reported for other agro-industrial biosorbents, where increasing adsorbent thickness or mass stabilizes removal performance over time [4], [14].

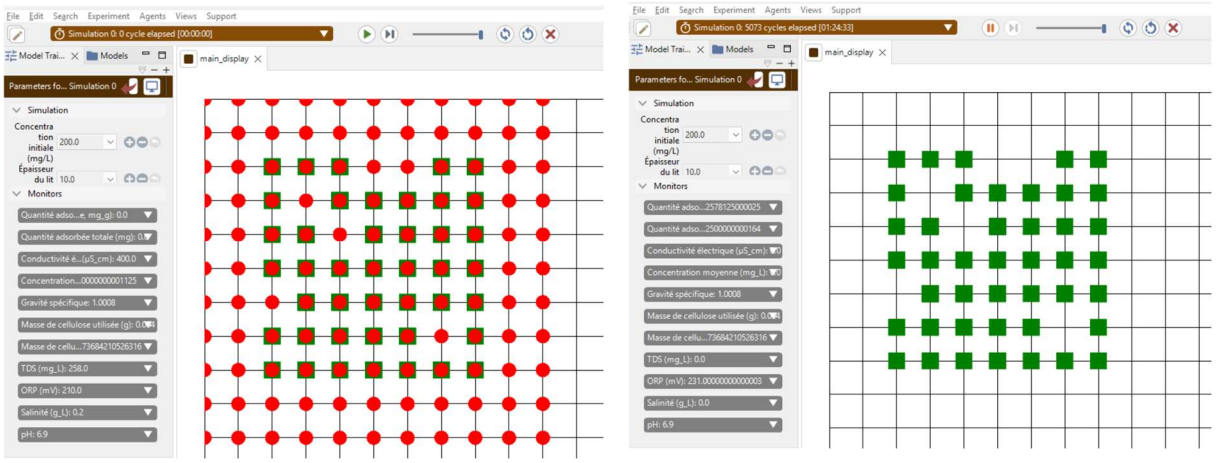

Fig. 3 – Screenshot of the GAMA simulation showing the spatial distribution of pollutant agents (in red) within the sulfo-acetylated cellulose adsorption bed (in green) for different bed thicknesses (10, 20, 30 mm) and a given initial concentration.

2. Agreement between simulations and experiments

The adsorption capacities simulated by the agent-based model were systematically compared with laboratory measurements for all tested scenarios (bed thicknesses of 10, 20 and 30 mm; detergent concentrations from 0.1% to 0.6% m/V). Table 1 reports, for each (thickness, concentration) pair, the corresponding (q_e,sim, q_e,exp) values in mg/g. Figure 3 provides a synthetic representation in the form of a scatterplot, with q_e,sim on the x-axis and q_e,exp on the y-axis, together with the equality line q_e,sim = q_e,exp.

The dispersion of points around the equality line is generally low, indicating good agreement between simulation and experiment. For most cases particularly for low to moderate concentrations (0.1% - 0.3% m/V) and bed thicknesses of 20 and 30 mm points cluster near the diagonal, showing that the model correctly reproduces the increase in adsorption capacity as the available adsorbent mass increases. The largest discrepancies are observed for the highest load (0.6%) and the thinnest bed (10 mm), where some points deviate more noticeably from the equality line. This behaviour reflects the faster saturation of upstream layers under these extreme conditions, as well as the enhanced sensitivity of adsorption dynamics to local parameter choices (capture probability, initial pollutant distribution).

Overall, the near-linear relationship between q_e,sim and q_e,exp, with a slope close to unity and a small intercept, confirms that the probabilistic representation of local adsorption, derived from the Freundlich isotherm fitted to laboratory data, is sufficient to reproduce the main observed patterns. The performance is comparable to that obtained in advanced modelling studies using, for example, neural networks or hybrid models for pollutant adsorption in solution, while offering a more intuitive spatio-temporal

interpretation thanks to the agent-based approach. In this sense, the model is not only a tool for reproducing measurements, but also a platform for virtually exploring scenarios that were not tested experimentally (changes in flow rate, series of use cycles, multiple cartridges in series, etc.).

Tab. 1- Experimental and simulated adsorption capacities q_e (mg/g) for each combination of bed thickness (10, 20, 30 mm) and detergent concentration (0.1%–0.6% m/V). These data form the basis of the scatterplot in Figure 3.

Epaisseur (mm)	Concentration (%)	qe_simulé (mg/g)	qe_mesuré (mg/g)
10	0.10	11.00	10.50
10	0.20	19.00	21.52
10	0.30	31.00	34.39
10	0.40	44.00	47.00
10	0.50	58.00	61.00
10	0.60	65.00	72.19
20	0.10	17.00	20.35
20	0.20	34.00	39.60
20	0.30	51.00	57.56
20	0.40	73.00	78.00
20	0.50	77.00	79.00
20	0.60	81.00	89.62
30	0.10	25.00	27.20
30	0.20	49.00	54.45
30	0.30	75.00	83.46
30	0.40	107.00	112.00
30	0.50	133.00	133.00
30	0.60	139.00	154.18

International Journal of Progressive Sciences and Technologies (IJPSAT)
ISSN: 2509-0119.

https://ijpsat.org/
Vol. 55 No. 2 February 2026, pp. 569-582

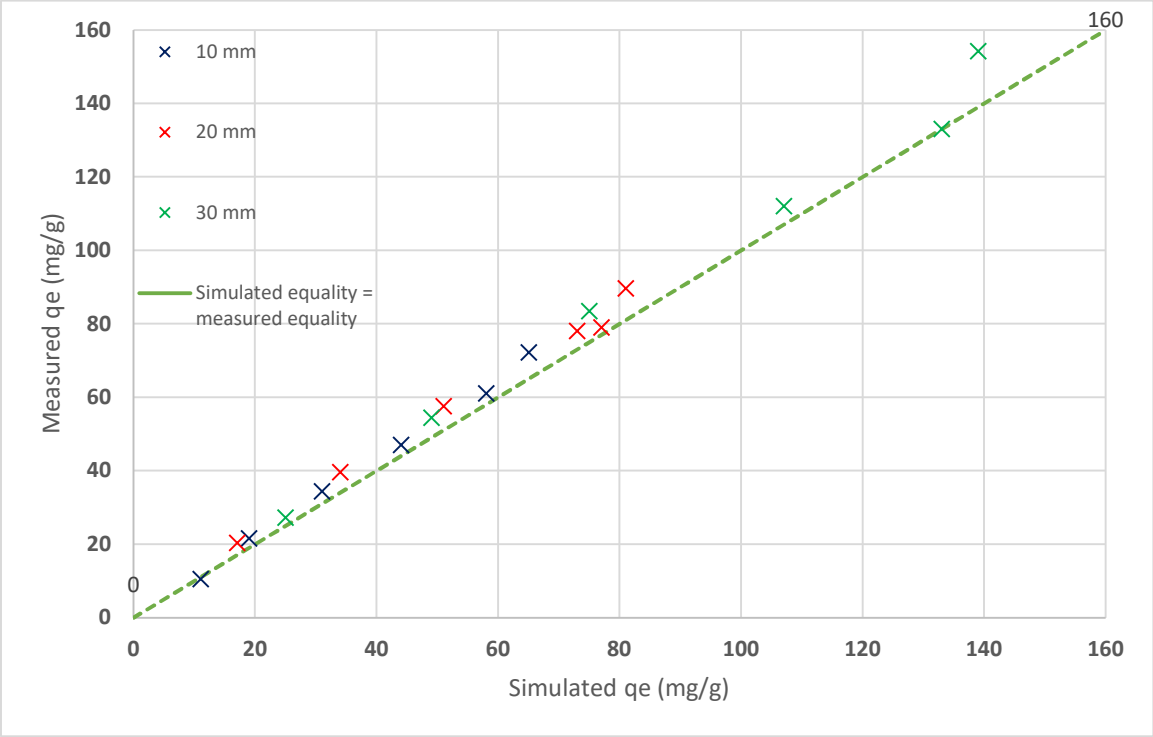

Fig. 4 – Comparison between simulated and experimental equilibrium adsorption capacities q_e for different bed thicknesses (10, 20, 30 mm) and detergent concentrations (0.1% – 0.6% m/V). Points represent the (q_e,sim, q_e,exp) pairs in Table 1; the dashed line represents the equality q_e,sim = q_e,exp.

3. Simulated physico-chemical quality of the treated water

Tables 2 (experimental results) and 3 (simulation results) summarize the evolution of water physico-chemical quality before and after adsorption for the different combinations of bed thickness and detergent concentration. For each scenario, pH, electrical conductivity (EC), TDS, salinity, specific gravity (S.G.) and ORP are reported, allowing direct comparison between laboratory measurements and model outputs.

The experimental data show that introducing a 10 mm sulfo-acetylated cellulose bed already produces a noticeable decrease in conductivity and TDS compared with the raw effluent, with further improvement when the bed thickness is increased to 20 and then 30 mm. Changes in pH remain modest and within the range compatible with WHO recommendations for drinking water, while ORP values tend to move towards less reducing conditions compared to the initial effluent. These trends are consistent with the conclusions of recent reviews, which highlight that biosorbent-based adsorption processes can improve several water-quality parameters simultaneously while remaining compatible with simple infrastructure and limited operating costs [15].

Below, Table 2 presents the experimental results; Table 3 gives the corresponding simulated values (numbers kept identical to your original data, headings translated).

International Journal of Progressive Sciences and Technologies (IJPSAT)
ISSN: 2509-0119.

https://ijpsat.org/
Vol. 55 No. 2 February 2026, pp. 569-582

Tab.2 – Experimental physico-chemical parameters before and after adsorption for different combinations of detergent concentration and bed thickness, with WHO guideline values and measurement uncertainties.

Detergent concentration (%)	Sulfo-acetylated cellulose bed thickness (mm)	pH	EC (µS/cm)	TDS (mg/L)	Sel (g/L)	S.G	ORP (mV)
0.1	0	6.9	400	258	0.2	1.0008	210
	10	6.90	397	258	0.19	1.0007	207
	20	6.93	387	250	0.18	1.0006	198
	30	6.95	375	241	0.17	1.0005	191
0.2	0	6.8	700	465	0.4	1.001	190
	10	6.80	690	463	0.39	1.001	183
	20	6.85	663	439	0.37	1.0009	172
	30	6.88	633	414	0.34	1.0008	161
0.3	0	6.7	1000	635	0.7	1.002	160
	10	6.70	978	632	0.59	1.0014	158
	20	6.75	928	603	0.55	1.0012	148
	30	6.78	862	576	0.52	1.0011	141
0.6	0	6.5	1650	1040	1.4	1.004	110
	10	6.51	1570	1042	1.38	1.003	118
	20	6.57	1481	972	1.29	1.0025	109
	30	6.63	1402	919	1.19	1.0023	102
WHO drinking-water guidelines (for reference)		6.5 - 8.5	< 1500	< 1000	< 0.25	1	200 - 400
Measurement uncertainty		±0.05 à ±0.1	±2% à ±5%	±2% à ±5%	±0.01	±0.0005 à ±0.001	±5 à ±10

Tab.3 – Simulated physico-chemical parameters (GAMA agent-based model) for the same scenarios as in Table 2, with the same variables and uncertainty ranges.

Detergent concentration (%)	Sulfo-acetylated cellulose bed thickness (mm)	pH	EC (µS/cm)	TDS (mg/L)	Sel (g/L)	S.G	ORP (mV)
0.1	0	6.9	400	258	0.2	1.0008	210
	10	6.92	390	250	0.18	1.0006	195
	20	6.95	370	235	0.17	1.0005	220
	30	6.98	360	225	0.16	1.0005	230
0.2	0	6.8	700	465	0.4	1.001	190
	10	6.82	680	450	0.38	1.001	185
	20	6.88	640	420	0.3	1.0008	210
	30	6.92	600	390	0.25	1.0007	225
0.3	0	6.7	1000	635	0.7	1.002	160

International Journal of Progressive Sciences and Technologies (IJPSAT)
ISSN: 2509-0119.

https://ijpsat.org/
Vol. 55 No. 2 February 2026, pp. 569-582

Detergent concentration (%)	Sulfo-acetylated cellulose bed thickness (mm)	pH	EC (µS/cm)	TDS (mg/L)	Sel (g/L)	S.G	ORP (mV)
	10	6.72	960	610	0.55	1.0013	170
	20	6.8	900	560	0.24	1.0011	210
	30	6.85	840	520	0.23	1.001	230
0.6	0	6.5	1650	1040	1.4	1.004	110
	10	6.55	1600	1100	1.4	1.0035	105
	20	6.6	1580	1080	1.35	1.003	100
	30	6.65	1520	1000	1.2	1.0028	95
WHO drinking-water guidelines (for reference)		6.5 - 8.5	< 1500	< 1000	< 0.25	1	200 - 400
Measurement uncertainty		±0.05 à ±0.1	±2% à ±5%	±2% à ±5%	±0.01	±0.0005 à ±0.001	±5 à ±10

The comparison between Tables 2 and 3 shows that the model reproduces not only overall adsorption capacity but also the magnitudes and trends of physico-chemical parameters. For low to moderate detergent concentrations (0.1%–0.3%), differences between experimental and simulated EC, TDS and salinity remain within ranges compatible with measurement uncertainties, confirming the relevance of coupling the adsorption sub-model with the water-quality sub-model. For the highest load (0.6%), simulations indicate that, although removal remains significant for a 30 mm bed, some parameters (especially EC and TDS) struggle to stay below target values. This is consistent with other studies on anionic surfactants such as SDS, where even optimized materials are strongly challenged under high pollutant loads [15]. Overall, the good agreement strengthens the case for sulfo-acetylated sugarcane bagasse cellulose as a competitive biosorbent for domestic anionic surfactant removal, in line with performances reported for other modified or sulfonated bagasse materials [4], [14].

IV. DISCUSSION

The results first confirm that sulfo-acetylated cellulose derived from sugarcane bagasse is an efficient and locally available biosorbent for reducing anionic surfactants in domestic wastewater. Laboratory measurements, combined with their numerical reproduction by the agent-based model, show that for low to moderate detergent concentrations (0.1%–0.3% m/V), the adsorbent substantially reduces residual pollution while keeping physico-chemical parameters such as pH, conductivity, TDS, salinity, specific gravity and ORP within ranges compatible with WHO recommendations for water intended for human use [3]. These performances are consistent with earlier work on bagasse valorization as a low-cost adsorbent for various pollutants [4], [5], and highlight the added value of sulfo-acetylation for targeting household anionic surfactants.

The main contribution of this study, however, lies in the coupling between experimental characterization and agent-based numerical simulation. While many studies focus on the calibration of macroscopic adsorption models such as Langmuir and Freundlich isotherms or on AI-based optimization using neural networks [10], the approach proposed here emphasizes the spatio-temporal dynamics of pollutant capture within the adsorbent bed. The explicit representation of pollutant agents and adsorbent cells under GAMA, documented via the ODD protocol [12], [13], [16], makes it possible to visualize the progression of the saturation front and clearly show that upstream layers saturate faster than downstream layers, especially in thin beds or under high pollutant loads. The model thus complements global q_e measurements by illustrating how bed structure and cartridge thickness jointly control adsorption effectiveness and useful lifetime.

From a methodological standpoint, the workflow used in this study experimental tests, model parameterization, calibration, validation and scenario exploration provide a coherent framework for using agent-based simulation in wastewater treatment. Experimental tests first provide the baseline data (adsorption capacities, physico-chemical parameters before and after treatment)

International Journal of Progressive Sciences and Technologies (IJPSAT)
ISSN: 2509-0119.

https://ijpsat.org/
Vol. 55 No. 2 February 2026, pp. 569-582

needed to fit the Freundlich isotherm and assign local adsorption capacities [17]. These same data are then used to calibrate adsorption probabilities in the model so that it reproduces measured q_e values and trends for the different combinations of bed thickness and detergent concentration. Once calibrated, the simulation becomes an extension of laboratory experiments, enabling the virtual testing of conditions that would be costly or difficult to reproduce experimentally for instance, thousands of flow cycles, variable flow rates or multiple cartridges in series. The discussion of results is therefore grounded in a clear loop: laboratory data feed the model; the model reproduces and explains observations; and simulation opens up new design scenarios.

Operationally, the simulations show that there is a trade-off between admissible pollutant load and cartridge thickness. For detergent concentrations representative of typical household discharges (≤ 0.3% m/V), bed thicknesses between 20 and 30 mm appear realistic: they provide high removal rates, stabilize water-quality parameters over a significant number of cycles and keep material requirements and head losses at reasonable levels. These findings are consistent with recent studies on adsorption technologies for wastewater treatment, which highlight that biosorbents derived from agro-industrial residues can achieve performances comparable to commercial materials, provided they are properly sized and used in compatible load ranges [16], [4]. In contrast, when detergent concentration reaches 0.6%, saturation occurs much faster, even for a 30 mm bed, pointing to the limits of the process for extreme loads and suggesting the need for combined strategies (pre-dilution, pre-treatment, multiple adsorption stages in series).

It is also important to acknowledge the limitations of the proposed model. From a physico-chemical perspective, the current formulation focuses on a dominant pollutant group (anionic surfactants) and assumes that competition from other species present in domestic wastewater remains limited. In reality, domestic effluents contain complex mixtures of ions, organic matter and suspended solids, which may compete for adsorption sites or alter bed structure through clogging. Recent studies on SDS adsorption show that the presence of dissolved ions and organic matter can influence the effective capacity of adsorbent materials [15]. Moreover, the model does not yet explicitly account for phenomena such as adsorbent loss, structural degradation, biofilm formation or adsorbent regeneration, all of which may be critical for long-term cartridge performance under real-world operating conditions. These simplifications do not invalidate the model but underline that its predictions should be interpreted as cautious estimates, valid within a well-defined framework.

Finally, this study opens several avenues for further research and application. Scientifically, extending the model to pollutant mixtures, more complex bed geometries or multi-stage devices would allow a more detailed characterization of the limits of sulfo-acetylated cellulose and comparisons with other biosorbents derived from bagasse or lignocellulosic residues [18], [4], [5]. Operationally, integrating such cartridges into compact, low-energy treatment modules co-designed with local communities could significantly reduce domestic pollutant loads before they are released into the environment, in synergy with other decentralized sanitation solutions. In this perspective, the combination of bagasse valorization, agent-based modelling and consideration of local constraints appears as a promising pathway to progressively improving access to safer water in developing countries.

V. CONCLUSION

This study has shown that sulfo-acetylated cellulose derived from sugarcane bagasse is a local, low-cost and effective biosorbent for removing anionic surfactants from domestic wastewater. Experimental tests highlighted a maximum adsorption capacity of about 154.18 mg/g for anionic surfactants, while keeping physico-chemical parameters such as pH, conductivity, TDS, salinity, specific gravity and ORP within ranges compatible with WHO guidelines for safe domestic water, particularly for detergent concentrations ≤ 0.3% (m/V) [3]. These findings are consistent with previous work on bagasse valorization as a low-cost adsorbent [4], [5], and show that sulfo-acetylation further targets the specific family of household anionic surfactants.

Beyond these experimental performances, the key contribution of this work lies in the coupling between laboratory characterization and agent-based simulation implemented in GAMA. The methodology follows a structured sequence: acquisition of experimental data, formulation of an appropriate Freundlich isotherm, setting local adsorption capacities, calibration and validation of the model, and finally numerical exploration of use scenarios. This process makes it possible to move from a purely macroscopic view centred on global q_e values to a dynamic, spatially explicit representation of the saturation front progressing through the adsorbent bed [17], [12], [13], [19]. The simulation thus offers a robust interpretive framework to understand how bed structure and cartridge thickness jointly determine adsorption efficiency, useful lifetime and stability of water-quality parameters [10].

Experimental and numerical results converge in recommending, at the operational level, sulfo-acetylated cellulose cartridges with thicknesses between 20 and 30 mm for treating diluted household effluents with typical detergent concentrations ≤ 0.3% (m/V). Within this range, the treated water remains compatible with common domestic use criteria and surfactant removal remains high over a significant number of cycles. These results are in line with recent studies on adsorption technologies based on agro-industrial residues, which show that appropriately sized biosorbents can reach performances close to some commercial materials while remaining compatible with low-resource contexts [16], [4]. Conversely, for 0.6% detergent concentration, bed saturation is significantly faster even at 30 mm thickness, highlighting process limitations under extreme loads and supporting the use of combined strategies such as pre-dilution, pre-treatment or multi-stage adsorption.

The study nonetheless has several limitations that point to future research needs. From a physico-chemical standpoint, the model focuses on anionic surfactants and assumes that competition with other solutes or suspended matter is secondary, whereas real domestic wastewater contains complex mixtures of ions, organic matter and particles that can affect effective adsorption capacity [15]. Likewise, key long-term processes such as clogging, mechanical degradation of the bed, biofilm growth and regeneration cycles are not yet represented. These simplifications do not undermine the main conclusions but imply that predictions of lifetime and performance should be treated as estimates within a defined domain of validity and complemented by field studies.

Looking ahead, there are many research and application perspectives. On the scientific side, extending the model to pollutant mixtures, more complex bed structures or multi-stage devices would allow systematic comparison between sulfo-acetylated cellulose and other biosorbents derived from bagasse or different lignocellulosic wastes, building on already well-documented pretreatment and functionalization strategies [18], [4], [5]. On the operational side, embedding such cartridges in compact, low-energy modules co-designed with local communities could significantly reduce the pollutant load of domestic discharges before environmental release, supplementing other decentralized sanitation options. In this perspective, the combined use of an under-utilized agricultural resource, agent-based modelling and local constraint analysis emerges as a promising route to progressively improving access to safer water in developing countries.

ACKNOWLEDGEMENTS

The authors gratefully acknowledge the Molo graphite mine laboratory in Fotadrevo, which hosted the first phase of this study (January 2024 – January 2025), and the pesticide control laboratory in Antananarivo, where the second phase was conducted (from February 2025). Their logistical support, the quality of their facilities and the availability of their staff were essential for the treatment, characterization and analysis of samples under optimal conditions, fully aligned with the requirements of this research.

REFERENCES

[1] INDRI. Madagascar Health and Pollution Action Plan: Accelerating the Implementation of Actions to Reduce Pollution-Related Illness. INDRI Publications, 2023.

[2] UNICEF & World Health Organization. Progress on Drinking Water and Sanitation: 2012 Update. WHO Press, Geneva, 2012.

[3] World Health Organization. Guidelines for Drinking-water Quality. 4th Edition, 1st–2nd Addenda. WHO Press, Geneva, 2022.

[4] Sarker, T.C., Azam, S.M.G.G., El-Gawad, A.M.A., Gaglione, S.A., & Bonanomi, G. Sugarcane bagasse: a potential low-cost biosorbent for the removal of hazardous materials. Clean Technologies and Environmental Policy, 19(2), 2343–2362, 2017.

[5] Melesse, G.T., Hone, F.G., & Mekonnen, M.A. Extraction of cellulose from sugarcane bagasse: optimization and characterization. International Journal of Polymer Science, 2022, Article ID 6502760, 1–13.

[6] Elshabrawy, S.O., Elhussieny, A., Taha, M.M., Pal, K., & Fahim, I.S. Wastewater treatment via sugarcane bagasse pulp. International Journal of Environmental Science and Technology, 20(10), 12405–12416, 2023.

[7] Chaudhari, M. Sugarcane bagasse as a biosorbent for removal of dyes. International Journal of Pharmacy and Pharmaceutical Research, 27(3), 388–412, 2023.

[8] Khan, I., Ali, A., Naz, A., Baig, Z.T., Shah, W., Rahman, Z.U., Shah, T.A., Attia, K.A., Mohammed, A.A., & Hafez, Y.M. Removal of Cr(VI) from wastewater using acrylonitrile grafted cellulose extracted from sugarcane bagasse. Molecules, 29(10), 2207, 2024.

[9] Zafeer, M.K., Menezes, R.A., Venkatachalam, H., & Bhat, K.S. Sugarcane bagasse-based biochar and its potential applications: a review. Emergent Materials, 7(1), 133–161, 2024.

[10] Fiyadh, S.S., Alardhi, S.M., Al Omar, M.A., Al-Anazy, M.M., & Al-Fatesh, A.S. A comprehensive review on modelling the adsorption process for heavy metal removal from wastewater using artificial neural network technique. Heliyon, 9(4), e15455, 2023.

[11] Nighojkar, A., et al. Application of neural network in metal adsorption using biomaterials: a review. Environmental Science: Advances, 2(1), 11–38, 2022.

[12] Ferber, J. Les systèmes multi-agents : vers une intelligence collective. InterEditions, 1995.

[13] Grimm, V., Berger, U., Bastiansen, F., Eliassen, S., Ginot, V., et al. A standard protocol for describing individual-based and agent-based models. Ecological Modelling, 198(1–2), 115–126, 2006.

[14] Oliveira, A.C., Lins, P.M.P., Amaral, M.C.S., & da Silva, F.V. Use of surfactant-modified adsorbents in the removal of pollutants from water: a review. Journal of Environmental Chemical Engineering, 11(10), 109678, 2023.

[15] Hu, Q., & Hao, L. Adsorption technologies in wastewater treatment processes. Water, 17(15), 2335, 2025.

[16] Taillandier, P., Gaudou, B., Grignard, A., Huynh, N.Q., Lhommet, H., Chapuis, K., & Drogoul, A. Building, composing and experimenting complex spatial models with the GAMA platform. GeoInformatica, 23(1), 243–269, 2019.

[17] Freundlich, H.M.F. Über die Adsorption in Lösungen. Zeitschrift für Physikalische Chemie, 57, 385–470, 1906.

[18] Bhandari, P.S., & Gogate, P.R. Adsorptive removal of sodium dodecyl sulfate from aqueous solutions using low-cost adsorbents and activated carbon: kinetics and equilibrium studies. Desalination and Water Treatment, 165, 111–123, 2019.

[19] Kumar, P., Barrett, D.M., Delwiche, M.J., & Stroeve, P. Methods for pretreatment of lignocellulosic biomass for efficient hydrolysis and biofuel production. Industrial & Engineering Chemistry Research, 48(8), 3713–3729, 2009.

ILLUSTRATION TABLES

Fig. 1- Percentage of the population with access to improved sanitation in 2010 (Source: Progress on Drinking Water and Sanitation, 2012 Update Report, JMP).

Fig. 2-Schematic representation of the agent-based adsorption modelling process: use of experimental data (Freundlich isotherm) for parameterization, implementation in GAMA, calibration/validation phase and scenario exploration.

Fig. 3- Screenshot of the GAMA simulation showing the spatial distribution of pollutant agents within the sulfo-acetylated cellulose adsorption bed for different bed thicknesses (10, 20, 30 mm) and a given initial concentration.

Fig. 4- Comparison between simulated and experimental equilibrium adsorption capacities q_e for different bed thicknesses (10, 20, 30 mm) and detergent concentrations (0.1%–0.6% m/V), with the reference line $q_{e,sim} = q_{e,exp}$.

Tab. 1- Experimental and simulated equilibrium adsorption capacities q_e (mg/g) for each combination of bed thickness (10, 20, 30 mm) and detergent concentration (0.1%–0.6% m/V), used for the comparison in Figure 3.

Tab. 2- Experimental physico-chemical parameters after adsorption (pH, EC, TDS, salinity, specific gravity S.G., ORP) for each scenario, with comparison to WHO guideline values.

Tab. 3- Physico-chemical parameters simulated by the GAMA agent-based model (pH, EC, TDS, salinity, S.G., ORP) for the same scenarios as Table 2, including the measurement uncertainties adopted.