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Digital Twin Modeling and Control of an MBBR for COD and H_2S Removal in Petroleum Produced Water

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Abstract

Produced water is the largest by-product of oil and gas production and can carry a complex mixture of dissolved organic, hydrocarbon, salt, metallic and sulfide components, the composition of which is highly variable depending on various reservoir and field factors. This work focuses on the engineering design and model-based development of a Moving Bed Biofilm Reactor (MBBR) digital-twin for reduction of the organic pollutant loading, namely chemical oxygen demand (COD) and dissolved H 2 S, from high-salinity produced water reflecting conditions typical of the Libyan oilfield. A baseline design flow of 100,000 bbl/day and a 12-hour liquid hydraulic retention time (HRT) were selected as the basis for design. The biological component was composed of halotolerant heterotrophic bacteria (Halomonas, Bacillus, Marinococcus) and sulfide-oxidising functional groups (Halothiobacillus, Thiohalophilus). The cyber-physical simulator based on the Unity computing engine, incorporates hydraulic mass balances, Explicit Euler numerical integration, proportional/deadband control of process variables, an emergency-shutdown control schema, Monod-type biological kinetics, phenomenological pH/DO /salinity response functions, attached-biomass decay/detachment, and a simplified diffusion-effectiveness term. In the simulation, under the nominal optimal environmental conditions used for the simulation, final predicted removal efficiencies for COD and H2S were 90% and 82% respectively.

Keywords: Moving Bed Biofilm Reactor (MBBR) COD Removal; Halophilic Bacteria; Bioreactor Design; Digital Twin; Process Simulation

1. Introduction

Produced water is a voluminous by-product of oil and gas production and is expected to become an increasingly significant water stream in mature fields. Composition of produced water can vary significantly with reservoir geology, production history, water cut and operating characteristics. In water-injection schemes, treated produced water can be used to sustain reservoir pressure and lessen needs for freshwater make-up, but treatment objectives are site-specific and tailored to formation suitability, reinjection objectives and regulations.



Figure 1: Field observations of raw produced water storage facilities in central Libyan oilfields.

In case of reuse or reinjection, feed treatment is usually applied to free and dispersed oil, suspended solids, biodegradable and non-biodegradable organics, sulfide and other potential corrosive, plugging, toxic or formation damaging substances. Accordingly, the necessary sequence of treatment is generally a mixture of physical, chemical and/or biological processes rather than a single unit operation [1].

Produced water contains soluble and dispersed hydrocarbons, organic acids, salts, metals, biocides, CO_2, and sulfides. The ranges of these contaminants vary greatly from one field to another, making it necessary to characterize each site independently in order to select appropriate biological parameters [1].

It is thus important to connect changes in water chemistry to the biological kinetics, biofilm attachment, hydraulic operation, and controls. Digital twin technology provides a means for merging mechanistic/reduced-order models of process operations with dynamic control and sensor data, such that different scenarios and system faults can be assessed prior to implementation [2].

1.1Produced-Water Treatment and MBBR Evidence

MBBR technology retains active microorganisms on mobile carriers, allowing biomass retention to become less dependent on liquid HRT than in suspended-growth systems. General MBBR studies identify carrier surface area, filling fraction, loading, aeration, hydrodynamics, and biofilm detachment as key performance variables [3]. More specifically, saline produced-water studies have demonstrated that MBBR performance remains feasible under elevated TDS, but the attainable removal rate is condition-dependent and should not be represented by a single universal HRT value [4].

An increase in the concentration of salt acts to restrict the growth of microorganisms that are not adapted, due to osmotic shock. Halophiles and halotolerants use various physiological processes that ensure the proper functioning of macromolecules and help balance water content in cells. They involve adaptation via ion and the presence of compatible solutes like ectoine and betaine [5]. Accordingly, the present study treats salinity tolerance values as model inputs rather than universal properties of an entire genus.

The process of biodegradation of hydrocarbons in a saline medium is likewise strain-dependent. Halophilic microorganisms have the ability to oxidize organics produced by the decomposition of petroleum; however, the amount of available substrate is dependent on the composition of the hydrocarbon, emulsion formation, presence of oxygen, and pre-treatment. The MBBR technology is beneficial as it enables the attachment of biomass in the liquid phase even with short HRT [6].

EPS also play a role in cell adhesion and biofilm formation. EPS on the carrier surfaces in the MBBR system have the potential of retaining the biomass and forming diffusion gradients between the bulk liquid and the biofilm. This is the reason behind the biological justification of including the biomass and diffusion terms in the reduced order model [5].

One key aspect of biochemistry that must be considered in sulfide removal is acid-base speciation. Sulfide is present in solution mainly as H_2S and HS^- within the pH range applicable for wastewater treatment, and the proportion differs greatly with pH value. One commonly adopted first dissociation pK_a value is 7.0 at ambient temperature. As a result, pH not only affects microorganism growth but also the chemical species of sulfide in solution [7]. Under aerobic biological oxidation, sulfide can be converted to elemental sulfur and/or sulfate depending on oxygen availability and operating conditions, so the model interprets sulfide removal as a biological oxidation pathway rather than assuming one fixed sulfur product [8].

1.2 Digital-Twin Modeling and Process Control

The modern wastewater engineering digital twins make increasing use of the integration of process models, sensor data, control schemes, and scenario analysis in a continually refreshed virtual copy of the treatment process. This is consistent with the chosen architecture where hydraulic balances, kinetics of biochemistry, biofilm states, sensors, actuators, and emergency supervision rules are all modeled in the same environment. The current Unity-based model can be considered an engineering digital twin of the reduced order type, not a plant copy that has been calibrated, since it awaits experiments and hardware-in-the-loop validations [2].

This study aims to develop a simulation-supported MBBR design for high-salinity produced water, with emphasis on the coupling between biochemical activity, biofilm behavior, hydraulic conditions, and process control. The specific objectives are to:

1. Characterize the pollutant load typical of Libyan produced water.
2. Design an MBBR reactor employing a salinity-tolerant bacterial consortium.
3. Develop a dynamic cyber-physical simulator integrating algorithmic process control.
4. Assess the simulated treated-water quality against applicable site-specific discharge or reinjection criteria, without assuming that one numerical standard applies to all Libyan oilfields.

2. Materials and Methods

2.1 Produced Water Characteristics

The produced water from oil wells of Libya may contain extremely high salt concentration and large variability of salts, organics, and metals in the water stream. According to Aghow and Idris (2025), for three Sirte Basin fields, the TDS was found to range between 40,000 and 160,000 mg/L and large variations in chloride, sulfate, and other elements; these data are presented in Table 1 below. These data are specific for individual fields and cannot be generalized to the entire produced water from Libya. The high COD/BOD ratio may suggest that the organic compounds present are more resistant to degradation (Metcalf & Eddy, 2014).

Parameter	Unit	Zaltan	Al-Lahib	Al-Jabal
TDS	ppm	40,000	160,000	96,000
Chloride	mg/L	6,658	26,658	15,991
Sulfate	mg/L	133	143	153

Table 1. Representative chemical characteristics of produced water from Sirte Basin oilfields.

2.2 Pre-Treatment Train

Raw produced water typically needs to shield the biological treatment stage from excess levels of oil, solid materials, contaminants and saltiness. It is thus recommended that solids and free-oil removal processes take place prior to equalizing the flow to the MBBR. The design process will involve sequential treatment using sand filtration, gravity separation, coalescing, hydrocycloning, and flow equalization; effectiveness of individual components should be determined based on specific site data [1].

2.3 Microbial Consortium Selection

The biological model considers two functional groups instead of considering all members of a genus to be physiologically similar. Halomonas, Bacillus, and Marinococcus are considered to be halotolerant heterotrophs that can contribute to COD degradation within the aggregate, while Halothiobacillus and Thiohalophilus can be considered to exhibit sulfur oxidation. “Halophilic SOB” is a classification used as a functional group and not as a taxon name. Salinity, temperature, pH, and oxygen requirements of the bacteria vary among the strains. Therefore, the numerical values given in Table 2 can only be considered simulation screening limits taken from halophile/wastewater literature. The specific strain or enrichment used in a real reactor needs to be determined experimentally [9].

Genus/Consortium	Target	T (°C)	pH	TDS (ppm)	DO (mg/L)	Primary Role
Halomonas	COD	25–40	6.5 – 8.5	30,000–300,000+	2.0–6.0	Biodegrades aliphatic hydrocarbons/volatiles under salinity stress
Bacillus	COD	20–45	6.5 – 8.5	5,000–100,000	2.0–6.0	Secretes extracellular enzymes to break down complex polymers

Marinococcus	COD	25–40	7.0 – 8.5	30,000–250,000	2.0–6.0	Rapid mineralization of simple organics in hypersaline media
Halothiobacillus	H_2S	20–35	6.0 – 8.0	10,000–120,000	1.5–6.0	Autotrophic oxidation of sulfide/H_2S to sulfate
Thiohalophilus	H_2S	20–35	6.5 – 7.8	30,000–200,000	1.0–5.0	Chemolithotrophic sulfide oxidation, saline near-neutral media

Table 2. Optimal operational ranges and metabolic roles of the selected microbial consortium.

2.4 Bioreactor Design Basis

2.4.1 Carrier Selection and Fill Ratio

The selection criteria for the mobile carrier is a high surface area that will help maintain active biofilm. The design fill fraction for the mobile carriers is chosen to be 50%. From MBBR literature, carrier characteristics and fill fractions have been found to be essential design parameters, but their specific values depend upon various factors [3]. The carrier area and fill fraction should therefore be confirmed against the exact commercial media selected for a physical reactor.

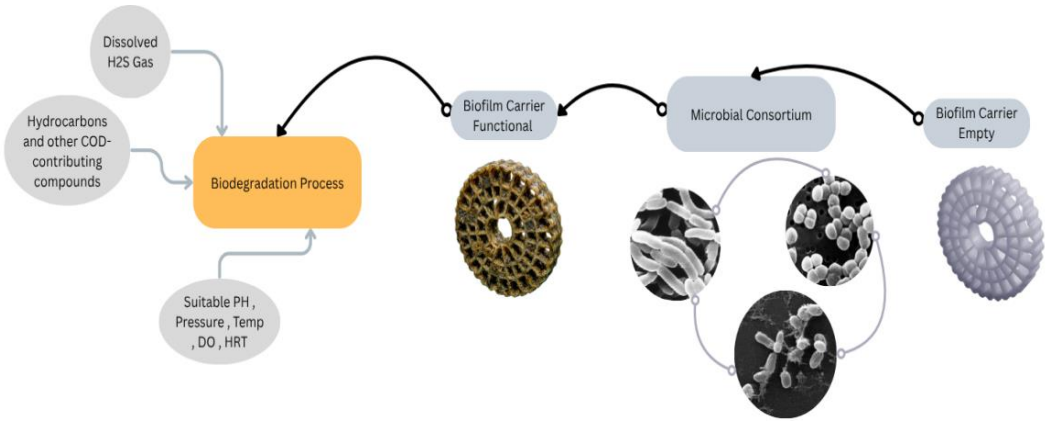


Figure 3. Workflow of biofilm development and biodegradation of H2S and COD.

2.4.2 Hydraulic Retention Time and Kinetic Validation

Hydraulic Retention Time (HRT) is another design parameter, yet there exists no one literature value which could be considered as a universal optimum for treating highly saline produced water. Performance of the MBBR process depends on various factors including organic load, TDS, temperature, carrier arrangement, aeration, and biofilm formation. There are studies conducted on saline produced water with HRT both moderate and low [4]. Accordingly, a 12-hour HRT is used here as a defined design basis for simulation, not as a generally applicable recommended value.

A Monod-type specific-growth model was adopted and extended in this study with dissolved-oxygen, temperature, and salinity-response terms. The extension is a reduced-order modeling choice informed by Monod kinetics and environmental biotechnology; it is not presented as a direct standard equation from a single reference [10].

$$\mu = \mu_{max} \times [S / (K_s + S)] \times [DO / (K_{DO} + DO)] \times \theta^{(T-20)} \times [1 / (1 + (TDS / K_{TDS}))] \quad (1)$$

where μ is the specific growth rate (day^{-1}), μ max the maximum specific growth rate, S the substrate (COD) concentration (mg/L), Ks the half-saturation constant (mg/L), KDO the oxygen half-saturation constant (mg/L), θ the temperature correction factor, and KTDS the salinity tolerance constant (mg/L).

For the COD-degrading consortium (μ max = 2.5 day^{-1}, Ks = 100 mg/L, KDO = 0.5 mg/L, KTDS = 150,000 ppm, θ = 1.05) at a design COD load of 1,200 mg/L, T = 35°C, DO = 3.5 mg/L, and TDS = 35,000 ppm, the model yields:

Substrate term: 1200 / (100 + 1200) = 0.923, Oxygen term: 3.5 / (0.5 + 3.5) = 0.875, Temperature term: 1.05^(35–20) = 2.08, Salinity term: 1 / (1 + 35000/150000) = 0.811

This results in an actual specific growth rate of $\mu = 2.5 \times 0.923 \times 0.875 \times 2.08 \times 0.811 = 3.40\ day^{-1}$, corresponding to a required liquid retention time of:

$$HRT_{required} = 1/\mu = 1/3.40\ day = 0.294\ day \approx 7.06\ hours \qquad (2)$$

This is well below the design HRT of 12 hours, confirming a stable safety margin (Table 3).

For the sulfide-oxidizing bacterial (SOB) consortium, a maximum specific growth-rate parameter of μ max = 1.3 day^{-1} was adopted as an initial model/calibration value informed by reported growth behavior of sulfur-oxidizing bacteria and H_2S-biofiltration studies (Oyarzun et al., 2003; Ramírez et al., 2009). For the defined design conditions (K_{H2S}= 0.5 mg/L, K_{DO}= 0.5 mg/L, K_{TDS}= 150,000 ppm, and θ = 1.07), the model predicts μ = 2.42 day^{-1} at an H_2S concentration of 10 ppm, corresponding to a characteristic kinetic timescale of approximately 9.93 h. This timescale is shorter than the selected 12-h liquid HRT. Because MBBR systems retain microorganisms as attached biofilm on mobile carriers, this comparison is used as a kinetic screening metric rather than as a universal washout criterion. Final values of μ max and other kinetic parameters require calibration against strain-specific or consortium-specific experimental data.

Bacteria Type	Pollutant	Conc. (mg/L)	μ (day^{-1})	Required HRT (hr)
COD bacteria	COD	400	2.95	8.13
COD bacteria	COD	1,200	3.40	7.06
COD bacteria	COD	2,500	3.55	6.76
SOB	H_2S	2	2.04	11.73
SOB	H_2S	10	2.42	9.93
SOB	H_2S	25	2.5	9.61

Table 3. Kinetic Assessment of the Selected HRT Based on Modeled Specific Growth Rates

2.4.3 Reactor Geometry and Sizing

The reactor was sized as a vertical cylindrical tank for a design flow rate of 100,000 bbl/day (15,900 m^3/day). At the design HRT of 12 hours (0.5 day), the required operational volume is:

$$V = Q \times HRT = 15{,}900\ m^3/day \times 0.5\ day = 7{,}950\ m^3 \qquad (3)$$

For a tank diameter of 30 m (cross-sectional area A = 706.86 m^2), this corresponds to an operating water level of:

$$H = V / A = 7{,}950 / 706.86 = 11.25\ m \qquad (4)$$

Allowing for internal volume displacement by the air-diffuser piping network (approximately 254.34 m^3, equivalent to a height displacement of 0.36 m) and a safety freeboard (1.24 m) to prevent overflow, the total geometric volume required is 9,084.5 m^3, corresponding to a total internal reactor height of 12.85 m. The resulting hydrostatic pressure at the reactor base is approximately 110.4 kPa (gauge) or 211.7 kPa (absolute), a key input for blower and diffuser selection.

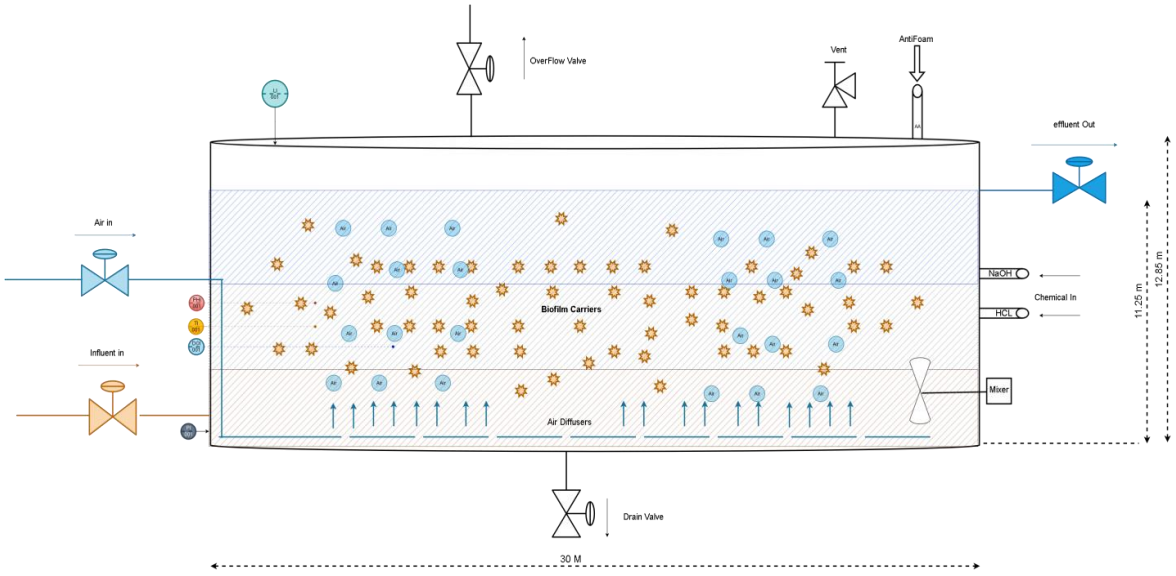


Figure 4: Process Schematic of the Moving Bed Biofilm Reactor (MBBR)

2.5 Aeration and Oxygenation System Design

A dissolved oxygen (DO) design target of 2.5–3.5 mg/L is adopted to support aerobic heterotrophic activity and sulfide oxidation while accounting qualitatively for reduced oxygen transfer under saline conditions. The 0.8 $Nm^3/(m^3 \cdot h)$ aeration rate and 15% OTE are engineering assumptions for preliminary sizing rather than universal biological constants; actual oxygen-transfer performance depends on diffuser type, depth, salinity, alpha factor, bubble hydrodynamics, and process loading (WEF, 2017).

Using a design volumetric aeration rate of 0.8 $Nm^3/(m^3 \cdot h)$ and a reactor volume of 7,950 m^3, the required air flow is:

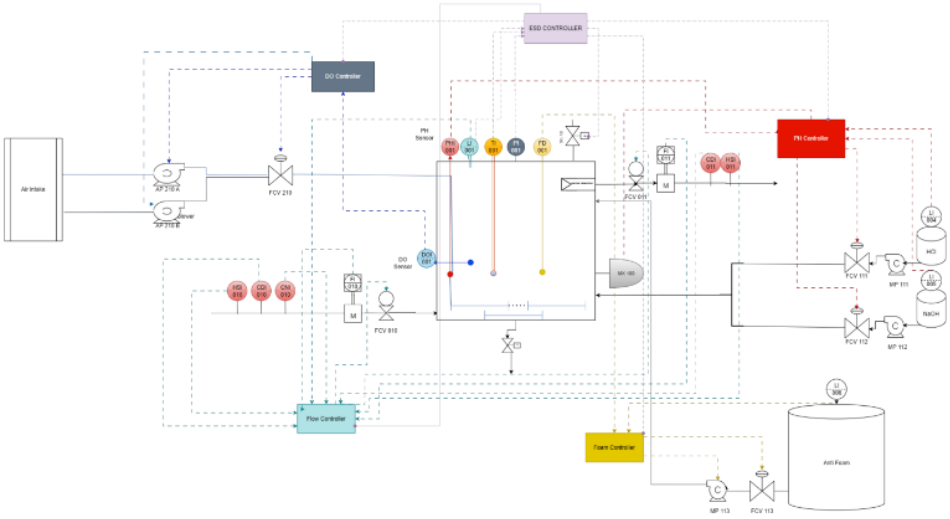
$$V_{air} = 0.8\ Nm^3/(m^3 \cdot h) \times 7{,}950\ m^3 = 6{,}360\ Nm^3/h \approx 1.77\ Nm^3/s \qquad (5)$$

At an assumed oxygen transfer efficiency (OTE) of 15% and an oxygen content in air of 0.275 kg O_2/Nm^3 (based on standard air density of 1.293 kg/Nm^3 and 21% oxygen by volume), the mass of oxygen actually transferred to the liquid is:

$$O_{2\ transferred} = OTE \times O_{2\ conc} \times V_{air} = 0.15 \times 0.275 \times 6{,}360 = 262.35\ kg\ O_2/h \qquad (6)$$

Oxygen transfer efficiency is enhanced through fine-bubble diffusers (reducing bubble size and increasing interfacial area), the 12.85 m reactor depth (increasing bubble contact time and hydrostatic pressure, improving solubility per Henry's law), and a mixing pattern designed to maintain a high oxygen concentration gradient near the diffusers (WEF, 2017). Diffusers are arranged across the entire reactor floor on fixed supports to ensure uniform air distribution and prevent the formation of anaerobic dead zones.

2.6 Simulation Model Digital Twin



(**Figure 4.0:** Overview of the reactor utilities and control loops)

To evaluate the designed bioreactor under dynamic operating conditions, an interactive digital twin was developed in Unity using C#. The model links hydraulic balances, reduced-order biochemical kinetics, attached-biomass states, sensors, actuators, process-control logic, and simulated fault conditions. This architecture follows the general concept of a wastewater digital twin while remaining a reduced-order model that requires experimental calibration for quantitative plant prediction [2].

2.6.1 Fluid Dynamics and Mass Balancing

The simulator uses Euler numerical integration based on Unity's frame time (Δt), multiplied by a simulation-speed slider. This allows real-time calculation of fluid levels and volume changes. The balance-tank volume change is calculated using a standard mass-balance equation:

$$dV_{BT}/dt = Q_{in}(t) - Q_{out}(t) - Q_{overflow}(t) \quad (7)$$

where Q_{in}(t) is the incoming flow, Q_{out}(t) is the flow sent to the reactor, and $Q_{overflow}$(t) is any excess water diverted to overflow.

Inside the bioreactor, COD and H_2S removal rates are calculated directly from the Hydraulic Retention Time (HRT) and biological performance, rather than by tracking individual biomass growth frame-by-frame.

2.6.2 Reactor Removal-Efficiency Model (Gaussian Inhibition, Monod Kinetics, and Biofilm Diffusion)

Removal efficiency for each pollutant p (COD, H_2S) is calculated sequentially from: (1) environmental inhibition, (2) substrate-limited Monod growth, (3) hydraulic sufficiency, (4) attached-biofilm dynamics, and (5) diffusion effectiveness. These terms are then combined into the final removal-efficiency relation. Environmental factors are applied once, inside the growth-rate term, to avoid double-counting inhibition.

Stage 1: Environmental Inhibition Factor

Bacterial activity is represented by phenomenological response functions that peak near selected operating optima and decrease as pH or DO move away from those optima. This representation is used as a reduced-order approximation of environmental stress; the selected numerical optima and tolerance widths are model parameters rather than universal species constants. The pH/DO response treatment is informed by wastewater microbiology and saline-wastewater literature [10].

$$f_{pH,i} = exp\ exp\ -\left(\frac{pH - pH_opt_i}{\sigma_pH_i}\right)^2 \quad (1)$$

where $f_{pH,i}$is the pH performance factor of species *i* (0–1); *pH* is the current bulk pH; $pH_opt_i$is the optimum pH for species *i*; and σ_pH_i is the pH tolerance width for species *i* a larger value means the species tolerates a wider pH range.

$$f_{DO,i} = exp\ exp\ -\left(\frac{DO-DO_opt_i}{\sigma_DO_i}\right)^2 \quad (2)$$

where $f_{DO,i}$, is the DO performance factor of species *i* (0–1), mg/L; *DO* is the current dissolved-oxygen concentration (mg/L); $DO_opt_i$is the optimum DO for species *i* (mg/L); and σ_DO_i is the DO tolerance width (mg/L).

For total dissolved solids, no inhibition occurs while TDS ≤ TDS_limit,i ($f_{TDS,i}$ = 1). Above the threshold, a one-sided Gaussian applies:

$$f_{TDS,i} = exp\ exp\ -\left(\frac{TDS-TDS_{limit,i}}{TDS_{sens,i}}\right)^2 \quad (3)$$

Where $f_{TDS,i}$ is the salinity performance factor of species *i* (0–1); *TDS* is the current total-dissolved-solids concentration (ppm); $TDS_{limit,i}$ is the salinity threshold below which species *i* is unaffected (ppm); and $TDS_{sens,i}$ is a sensitivity constant (ppm) controlling how quickly performance falls once TDS exceeds the limit a larger value means slower, more tolerant decline.

The three factors are combined with a species strength coefficient to give a per-species performance factor:

$$F_i = f_{pH,i} \cdot f_{DO,i} \cdot f_{TDS,i} \cdot k_i \quad (4)$$

where F_i is the overall performance factor of species *i* and k_i is its strength coefficient, a fixed weighting that reflects the species' relative competitiveness within the consortium. For each pollutant, the pollutant-level environmental factor $f_{env,p}$ is then taken as a weighted blend of the best-performing species (70%) and the consortium average (30%), bounded to a maximum $f_{env,max}$ (default 1.0), since one dominant strain carries most of the removal while the remaining species provide functional redundancy.

Stage 2: Substrate-Limited Growth Rate (Monod)

The Monod relationship is used to combine substrate availability with the environmental factor and obtain the fully loaded specific growth rate (Monod, 1949; Rittmann & McCarty, 2001). In the dynamic model, μmax values are expressed on a day^{-1} basis as model inputs and converted to hr^{-1} only where required for the HRT calculation.

$$\mu_p = \mu_{max,p} \cdot \frac{S_p}{K_{s,p}+S_p} \cdot f_{env,p} \quad (5)$$

where μ_p is the fully-loaded specific growth rate for pollutant *p* (hr^{-1}); $\mu_{max,p}$ is the maximum specific growth rate (hr^{-1}, converted from a day^{-1} input); S_p is the influent substrate concentration (mg/L or ppm); $K_{s,p}$ is the half-saturation constant , the substrate concentration at which growth is half its maximum (mg/L or ppm); and $f_{env,p}$is the environmental factor from Stage 1.

Stage 3: Hydraulic Sufficiency Factor

The retention time required for the biomass to process the pollutant at rate μ, and how the actual HRT compares to it, is:

$$HRT_{req,p} = \frac{1}{\mu_p} \quad (6)$$

where $HRT_{req,p}$ is the retention time (hr) required to sustain growth rate μ_p for pollutant *p*.

$$HRT_{fac,p} = \left[\frac{HRT_{actual}}{HRT_{req,p}}\right]_0^1 \quad (7)$$

where $HRT_{fac,p}$ is the resulting hydraulic sufficiency ratio (0–1) and $HRT_{actual}$is the current retention time of the reactor (hr), obtained from the fluid mass balance.

Stage 4: Biofilm Mass Balance

Attached biomass density is tracked as a dynamic state variable. The formulation follows the general biofilm modeling framework of [11], while a logistic carrier-capacity term is introduced here as a reduced-order model choice to prevent unbounded biomass growth in long digital-twin runs. Biomass increases with the current growth rate and decreases through endogenous decay and detachment.

$$\frac{dX_{f,p}}{dt} = \left[\mu_{p,day}\left(1 - \frac{X_{f,p}}{K_p}\right) - b_p - k_{det}\right] \cdot X_{f,p} \quad (8)$$

where $X_{f,p}$is the areal attached-biomass density for pollutant *p* (g VSS/m²); $\mu_{p,day}$ is μ_p converted to day⁻¹ (μ_p× 24); K_p is the biofilm carrier capacity (g VSS/m²); $b_p$is the endogenous decay rate (day⁻¹); and k_{det} is the detachment (shear/sloughing) rate (day⁻¹).

Stage 5: Diffusion Effectiveness Factor

As the biofilm develops, diffusion resistance can reduce the substrate available to microorganisms within the film. The model therefore uses a reduced-order Damköhler-type effectiveness factor, consistent with the established use of effectiveness factors to represent reaction rates under diffusion limitation in biofilms [12]. The exact algebraic form used here is a reduced-order approximation developed for this digital twin, rather than a direct reproduction of a published full biofilm PDE model.

$$\eta_p = \left[\frac{1}{1 + \left(\frac{\delta}{D_{e,p}}\right)\left(\frac{\mu_{max,p}}{Y_p}\right)\left(\frac{X_{f,p}}{S_p}\right)}\right]_{\eta_{min,p}}^1 \quad (9)$$

where η_p is the diffusion effectiveness factor for pollutant p (0–1); δ is the boundary-layer thickness (m); $D_{e,p}$ is the effective diffusivity (m²/day); Y_p is the biomass yield coefficient; $X_{f,p}$ is the attached-biomass density; S_p is the pollutant concentration; and $\eta_{min,p}$ is a numerical lower bound used to prevent digital-twin efficiency collapse. The $\eta_{min,p}$ value is a numerical/modeling parameter and should not be interpreted as a measured biological minimum.

Combined Result: Removal Efficiency

$$E_p = \left[E_{max} \cdot \left(HRT_{fac,p}\right)^{n_p} \cdot \eta_p\right]_0^{E_{cap}} \quad (10)$$

where E_p is the removal efficiency for pollutant p; E_{max} = 0.95 is the maximum achievable model efficiency; n_p is the selected biofilm-geometry exponent (0.70 for COD and 0.35 for H_2S); and E_{cap} = 0.98 is retained as a numerical ceiling. Because E_{max} = 0.95, the E_{cap} value is non-binding under the present parameterization. The values of E_{max} and n_p are model parameters and require calibration against experimental or pilot-scale data.

$$S_{out,p} = S_{in,p} \cdot \left(1 - E_p\right) \quad (11)$$

where $S_{out,p}$ and $S_{in,p}$ are the effluent and influent concentrations of pollutant *p* (mg/L or ppm), respectively.

Eq. (10) is the model endpoint. It combines hydraulic sufficiency, biofilm geometry, and diffusion effectiveness into a reduced-order removal-efficiency index. Emax, the exponents np, and any numerical ceiling are model/calibration parameters; quantitative values should be fitted or validated against experimental or pilot

data. Because COD and H_2S are chemically different contaminants, their arithmetic mean is reported, when needed, as an "Overall Removal Index (ORI)" rather than as a mass-balance plant removal efficiency.

2.6.3 Process Control Systems

To maintain safe, efficient, and stable operational conditions, the simulation automates the control of key process variables, including pH, dissolved oxygen (DO), liquid level, and flow rates. The automated control loops emulate standard industrial PLC strategies to preserve optimal biochemical conditions and prevent mechanical actuator wear:

pH and Dissolved Oxygen (DO) Control: Chemical dosing and aeration adjust dynamically based on target thresholds, maintaining favorable metabolic conditions for carrier-bound biomass while mitigating rapid valve oscillation.

Level and Flow Rate Control: Regulated using proportional control to maintain hydraulic equilibrium and consistent biomass contact time. The controller output u(t) is defined as:

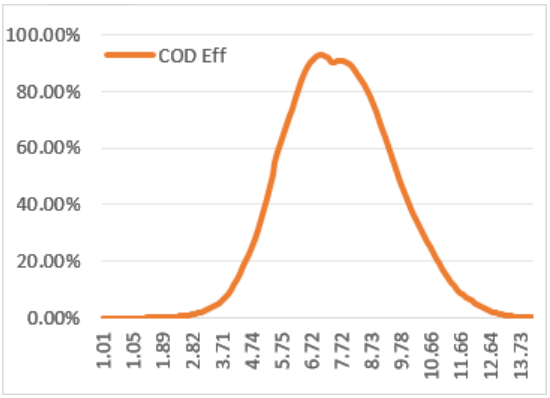
$$\boldsymbol{u(t) = Bias + K_p \cdot e(t)} \quad \mathbf{(12)}$$

Where u(t) is the Controller Output

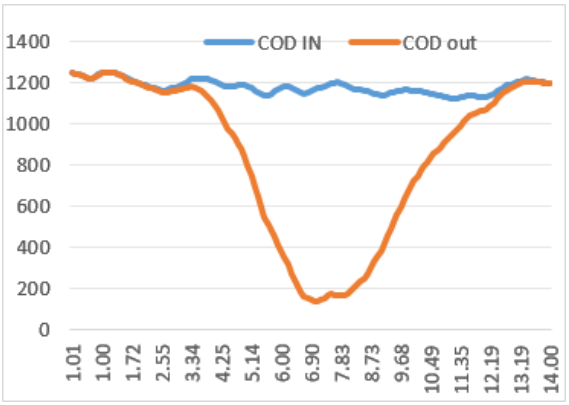
Bias is the nominal output

e(t) is the error signal

And $K_p = 2.5$ is the proportional gain factor.



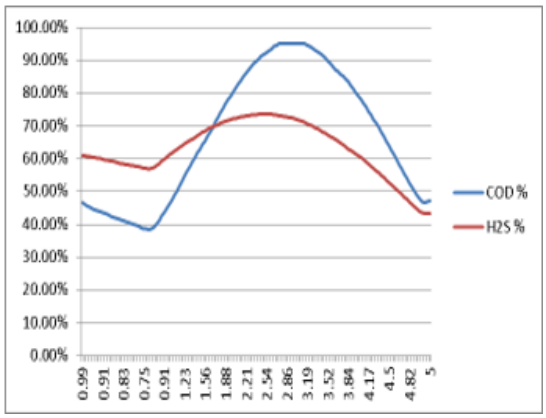
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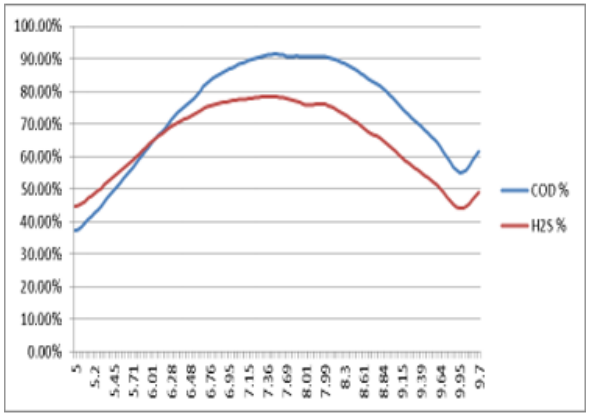


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Graph 1: COD Removal Efficiency vs. pH

Graph 2: Influent and Effluent COD Concentration vs. pH





3 **4**

Graph 3: COD and H2S Removal Efficiency vs. DO **Graph 4**: COD and H2S Removal Efficiency vs. pH

Note: All the Results are an outputs of the simulation model

2.6.4 Emergency Shutdown (ESD) System

An independent safety supervisory layer continuously monitors operational parameters and overrides standard automatic control loops during severe process excursions to prevent structural damage and safeguard the biological culture.

If the reactor reaches a High-High Level (HHL) condition exceeding 12.5 m(or 90% total capacity), the ESD system disables automatic level loops, completely closes the inlet feed valve (0%), and fully opens the emergency relief valve (100%). This rapid diversion prevents hydraulic surcharge, tank overflow, and the irreversible loss of plastic carriers and attached biofilm.

Under severe environmental stress, such as a High Temperature excursion exceeding 35C or High Pressure exceeding 130 kPa, the system overrides aeration, dosing, and level control. It isolates all chemical dosing lines, shuts the inlet and outlet feed valves, and fully opens the main bottom drain valve (100%) to depressurize the vessel, relieving internal stress and protecting active bacterial populations from thermal cell death.

Additionally, if a Low-Low Level (LLL) condition is detected in the balance tank, the safety layer zeroes the reactor feed output (0%) to protect upstream feed pump impellers from dry-running and cavitation while holding the bioreactor in a safe operating state until normal flow resumes.

3. Discussion

The reactor was evaluated under a conservative design COD load exceeding 2,000 mg/L, selected to ensure the design could absorb sudden organic-load increases characteristic of Libyan field produced water. Based on the kinetic model and simulator outputs, the reactor achieves COD removal efficiencies approaching 90%, attributable to the use of a specialized bacterial consortium capable of breaking down complex hydrocarbon bonds. Hydrogen sulfide concentration is reduced to below 4 ppm through biological oxidation, exceeding the performance required by applicable standards. As expected for a biological process, TDS shows no significant reduction, confirming that biological treatment targets organic and gaseous load rather than the ionic salt content of the water.

Simulator output indicates that COD and H_2S removal efficiency peaks within a near-neutral pH range (7.0–7.9), with a sharp decline in bacterial activity under strongly acidic or alkaline conditions — consistent with the pH sensitivity ranges reported for the selected bacterial strains in Table 2.

Removal efficiency is closely tied to dissolved oxygen concentration; continuous aeration is required to sustain biofilm growth and aerobic bacterial activity, and efficiency declines once DO drops below the strains' minimum thresholds.

The salinity-inhibition simulation confirms that treatment performance is sustained even at high TDS due to the halotolerant strains selected, with efficiency degrading gradually above each strain's tolerance limit rather than collapsing abruptly — reflecting the biological adaptation capacity built into the consortium selection [13].

3.1 Model Limitations and Validation Requirements

The model relies on several assumptions that must be confirmed through laboratory testing. Key parameters—such as carrier capacity, biofilm detachment, effective diffusivity, and the minimum effectiveness factor—are set as inputs, and their actual values depend on the specific carrier, shear conditions, and biofilm growth, so they need to be measured and calibrated experimentally. Likewise, the pH, DO, temperature, and TDS response

functions are simplified approximations rather than true inhibition kinetics, and the sulfide module only accounts for biological oxidation while stripping and other physical losses are not resolved. COD is also treated as a single aggregate load rather than separate biodegradable and recalcitrant fractions.

For these reasons, laboratory and pilot-scale tests under representative salinity and temperature are essential. These tests will provide the data needed to validate the simulation, adjust its constants, and confirm that predicted removal rates match real system behavior before the model is used for design or regulatory decisions.

4.Conclusion

This work presents a framework for using heterotrophs and sulfur-oxidizing bacteria that are tolerant to high salinity as means of high-salinity produced water treatment in an MBBR along with a Unity-based digital twin of such system that accounts for hydraulics, Monod kinetics, biofilm behavior, mass transport, sensing, and control. The 12 hour HRT is considered a design scenario, while the reciprocal growth time (1/μ) is a tool for kinetic screening only and cannot be considered a universal washout criterion, because the biomass is retained regardless of the liquid phase. Strain-specific physiology, microbial community composition, and acclimation effects have to be characterized experimentally before the model can be used for predicting optimal reactor dimensions. In addition, the validation/calibration procedure described in Section 4.1 has to be carried out. Simulation results can be provided only after quality assurance and comparison with the exact conditions of discharge, reinjection, and compatibility with the formation of the selected field. No general regulatory limits are to be considered. Further steps include uncertainty/sensitivity analysis, finishing of the experimental validation/calibration program, and implementation of the digital twin into the PLC environment

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