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Design of a Reactor for Hydrometallurgical Recycling of Lead

Narlys Marrugo Jimenez
National Polytechnic Institute, SEPI ESIME Zacatenco, CDMX
nmarrugoj1900@alumno.ipn.mx
https://orcid.org/0009-0004-9135-4599

Alejandro Boleaga Vázquez
National Polytechnic Institute, SEPI ESIME Zacatenco, CDMX
aboleagav1900@alumno.ipn.mx
https://orcid.org/0009-0003-6450-9375

Maribel Angélica Mendoza Núñez
National Polytechnic Institute, ESIME Culhuacán, CDMX
mmendozan@ipn.mx

Yaisa Marrugo Jiménez
National Polytechnic Institute, UPIICSA, CDMX
ymarrugoj2300@alumno.ipn.mx
https://orcid.org/0009-0004-5668-2984

Abstract. This article details the design and operation of a 500 L stirred hydrometallurgical reactor for sustainable lead recycling from used lead–acid batteries. Mechanical design followed ASME Section VIII and API 650 standards, supported by finite element analysis and simulation conducted in SolidWorks. Sodium citrate was selected as the leaching reagent due to its effectiveness and comparatively low environmental impact. The agitation system, operated at 400 rpm with axial impellers and vertical baffles, demonstrated high mass transfer efficiency, achieving recoveries above 90%. Critical structural parameters were dynamically assessed, and solutions were proposed to reduce vibration and wear. This technology is presented as an eco-friendly alternative to traditional casting processes, with the potential to reduce occupational hazards and toxic emissions while promoting more sustainable recycling practices within the industry.

Keywords: Clean Technology, Mechanical Design, Lead Leaching, Stirred Tank Reactor, Hydrometallurgy

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1 Introduction

1.1 Motivations

The recycling of lead acid batteries (BPAs) is one of the most serious environmental and technological problems today. This type of battery is widely used in the automotive, telecommunications, energy, and renewable energy storage industries, and is responsible for more than 85% of global lead demand (World Health Organization [WHO], 2017). The half-life of a lead acid battery is 3 to 5 years, after which it is considered a hazardous waste, as it contains metallic lead and sulfuric acid (Needhidasan et al., 2014; Punt, 2022).

The health of the human body is significantly affected by chronic exposure to lead, leading to adverse effects on the nervous, renal, and cardiovascular systems (Institute for the Evaluation of Health Metrics [IHME], 2021). About 1.54 million deaths occurred in 2021 as a result of lead exposure. The key risk groups are: children, pregnant women and workers in the vicinity of motorways or industries (WHO, 2024), especially those within the area of influence of the irregular recycling centre for this type of device. In Mexico, the air and soil in Nezahualcóyotl and Monterrey, and some areas of Ecatepec also exceed the limits established by the NOM-025-SSA1-2021 and NOM-026-SSA1-2021 standards (INECC, 2023) in reference to the contaminants associated with this practice, which exacerbates unsafe working conditions in facilities where workers' blood lead levels exceed the 30 µg/100 ml allowed by NOM-047-SSA1-2011 (Gottesfeld & Pokhrel, 2011).

The initial findings, which are consistent with studies conducted by Villa Vargas et al. (2017) and Liu et al. (2022), show that it is feasible to recover at least 90% of lead, with a substantial reduction in gaseous emissions and hazardous effluents. 400 rpm axial impellers, along with vertical baffles, improve mass transfer and mixture homogeneity, as reported by McCabe et al. (2007) and Paul et al. (2004).

Regarding the mechanical design, the structure of the reactor was studied by simulating internal pressure, continuous agitation and cyclic fatigue, demonstrating its integrity with safety factors greater than 2.5, as recommended by ASME (2021). In addition, the design includes maintenance and inspection criteria and durability for an estimated life of 25 years.

At the Social-Environmental level, a 70% reduction in the carbon footprint compared to conventional processes and the protection of the health of exposed workers is sought. The proposal complies with the Sustainable Development Goals (SDG 12: Responsible consumption and production; SDG 13: Climate Action), underlining the need for technological innovation in the field of hazardous waste treatment (United Nations Environment Programme [UNEP], 2019).

This study is motivated by the pressing need to replace pyrometallurgical methods that require high temperatures (>900°C), high energy input and associated toxic gas emissions (Jha et al., 2001) with cleaner, safer and more sustainable alternatives. Hydrometallurgy and leaching processes using organic acids such as sodium citrate are especially successful and provide an effective solution in metal extraction without undue risk to human health or the environment (Folens et al., 2021; Abhilash & Pandey, 2013; Punt, 2022).

Finally, this work provides a reproducible methodological basis for other heavy metals (Cd, Hg, Zn) and opens the prospect of adapting the system to multimetal or hybrid configurations, including mechanical pretreatments and waste neutralization steps, as suggested by Liu et al. (2022) and Punt (2022).

1.2 Statement of the Research Problem

Despite the development of environmentally friendly technologies in countries such as Belgium, Germany, and Japan (Melgar & Melgar, 2017) in Mexico, conventional processes continue to be used in recycling plants, which employ lead melting furnaces without gas capture systems. Under the circumstances described above, regular emissions of particulate matter, metallic lead, sulfur dioxide, and volatile organic compounds occur. In addition, the release of acidic residues contaminates adjacent waters and agricultural lands (Zeng & Li, 2014).

Several studies have brought to light the lack of effectiveness of conventional systems in reducing both occupational and environmental exposure. In a study for the ILO, Smith (2017) described how outsourcing the recycling of lead acid batteries to countries with weak environmental policies has led to health catastrophes in densely populated industrial areas. Therefore, it is necessary to develop processing schemes inspired by the concepts of the circular economy and clean production.

Among these alternatives, hydrometallurgical leaching with sodium citrate can be considered a good option, as it allows the formation of stable lead complexes at moderate pH (5-7) without the need for high temperatures (Villa Vargas et al., 2017; Folens et al., 2021). However, its production on an industrial scale reveals the need for careful reactor design to maximize the parameters studied: agitation, concentration, temperature and solid/liquid ratio. So far, few works have referred to the development of mechanical and structural agitation design for stirred reactors for lead acid batteries, specifically in Latin America (Punt, 2022; Liu et al., 2022).

1.3 Research Objectives

Develop the technical design and structural integrity analysis of a hydrometallurgical stirred tank reactor for the extraction of lead from used lead acid batteries, combining aspects of mechanical engineering, environmental chemistry, and computer-aided analysis.

1.4 Specific objectives:

- Design a 500-liter container using section VIII of ASME (2021) and API 650.
- Perform finite element simulations (FEA) that include static and dynamic analysis, similar to the studies of Chen et al. (2020) and Espinosa et al. (2018).
- Suggest ergonomic and safety improvements for the reduction of occupational risks, according to NOM-005-STPS-1998, the draft standard PROY-NOM-005-STPS-2017 and NOM-018-STPS-2015.

1.4 Main Contribution of the Study

This article is part of sustainable process engineering by suggesting the modeling and validation of a reactor dedicated to the clean recycling of lead acid batteries. Unlike previous studies that have predominantly focused on process chemistry or waste characterization, this research integrates: a complete CAE-CAD design of the structure and CFD-based optimization of the stirring system.

2 Background

Lead acid batteries are used all over the world, particularly in the transportation, telecommunications, and renewable energy industries. It is estimated that around 15 million tonnes of these devices are being discarded each year (International Energy Agency (IEA, 2022)). Although more than 90% of lead can technically be recovered, the practices are generally carried out with precarious environmental and safety precautions in developing countries (Zeng & Li, 2014).

Pyrometallurgy processes, which predominate in the industry, allow the generation of ultrapure lead, but they represent environmental threats and enormous energy demands (Jha et al., 2001; Smith, 2017). In contrast, hydrometallurgy presents sustainable options through the controlled dissolution of metals in aqueous solutions. The process has been implemented with comparable efficiencies (>90%) and lower environmental impacts (Abhilash & Pandey, 2013; Chagnes & Swiatowska, 2015).

In this context, sodium citrate has emerged as the hydrometallurgical agent par excellence due to its low cost, zero toxicity, and a high capacity for the formation of soluble lead complexes compared to the hydrometallurgical agents tested (Villa Vargas et al., 2017; Zhao et al., 2019). This mixture allows use at moderate temperatures without the need for neutralization (Zárate-Gutiérrez & Lapidus-Lavine, 2014). In addition, it is not aggressive with the reactor materials and can be recycled, which is aligned with the concept of Circular Economy (Gottesfeld & Pokhrel, 2011).

Leaching processes have evolved from the first rudimentary equipment to sophisticated equipment with more complex and fully automated control systems. The most recent literature has introduced computational models that aim at improving mixing and controlling mass transfer (Liu et al., 2022; Espinosa & de Oliveira, 2022). Newer reactors combine hybrid technologies including ultrasound/microwave processing, but are expensive and not suitable for resource-poor environments (Chen et al., 2021; Palaniandy et al., 2022).

In Mexico, used lead acid batteries are considered hazardous waste according to NOM-052-SEMARNAT-2005. However, almost 45% of these batteries are recycled informally, posing a major threat to human health and the environment (INECC, 2023; Martínez-Arroyo et al., 2021). Recovery can be carried out, but there are open questions about the technical requirements of small-scale hydrometallurgical facilities.

The design of this proposal is guided by principles of energy efficiency, performance of building materials and structural integrity. Stirred tank reactors (STRs) have already been applied and scaled up for metals such as Cu, Zn, and Pb with a good recovery rate (Folens et al., 2021; Sun et al., 2017). However, the lack of standardization of equipment to be used with sodium citrate as a leaching agent remains a limiting factor. However, through tools such as FEA and CFD, it is possible to simulate both structural integrity and fluid dynamics within reactors, to optimize them without the need to produce physical prototypes (Paul et al., 2004; Liu et al., 2022). The ongoing technological trajectory envisages the use of digital twins to obtain real-time data on operational and design variables (Palaniandy et al., 2022).

But there are still important gaps in this field: the lack of standardization of the use of sodium citrate as a leaching agent, the separation between structural design and chemical design, insufficient ergonomic criteria and a still incomplete regulatory framework for clean technologies. An experimental approach is proposed for this study that seeks to extend the viability of sodium citrate and axial agitation for its easy and cost-effective use on a small scale, suitable for use both in low-industrialized or resource-poor environments and in developed countries given its scalability and sustainability.

3 Methodology

3.1 General Design Approach

In this study, a systematic and iterative design approach is applied to the development of a hydrometallurgical reactor for the extraction of lead from industrial lead acid battery plates. The methodology was developed from the model described by Norton (2009) as shown in Figure 1, and was completed with the mechanical design criteria of the international standards (ASME section VIII Div. 1, API 650) that are verified using CAD/CAE simulation software. It is comprehensive, from establishing functional requirements to evaluating and testing under dynamic operating conditions.

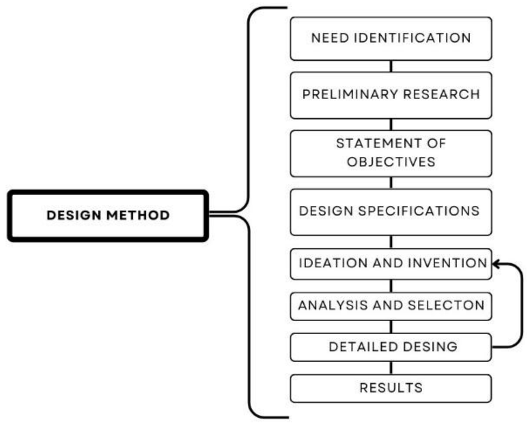

Figure 1. Design Methodology.
Source: Own elaboration 2024. Data obtained from Norton, R. L. (2009). Machinery Design: Synthesis and Analysis of Machines and Mechanisms (4th ed.). McGrawHill.

The architecture seeks to incorporate metallurgical efficiency, operational safety, and environmental resilience in the spirit of Graedel and Allenby's (2010) green engineering design principles; and the methodological guidelines for recycling engineering set out by Espinosa and de Oliveira (2022).

At the conceptual level, it has its origin in a model of a mixed reactor commonly used in mineral leaching processes (McCabe, Smith & Harriott, 2007), adapted to the specificities of sodium citrate leaching, whose physicochemical characteristics, as well as the agitation under which the reaction operates, require specific considerations regarding the materials, geometry and agitation (Folens et al., 2021; Villa Vargas et al., 2017).

3.2 Regulatory and Technical Framework

To satisfy acceptable practices for the structural design of the reactor under real operating conditions, the following internationally accepted technical standards were applied:

- ASME Section VIII Div. 1 – Used to estimate vessel wall thickness under internal and external pressure.
- API 650: for storage tanks in corrosive environments, for the selection of materials and surfaces.
- AWS D1.1 - Standards on the acceptance range for carbon steel structural weld quality.
- NOM-052-SEMARNAT-2005, NOM-005-STPS-1998, PROY-NOM-005_STPS-2017 and NOM-018-STPS-2015: references for the classification of hazardous waste and the handling and labeling of chemical substances in Mexican industrial environments.

In addition, design recommendations for lead acid battery recycling facilities such as those in Chagnes and Swiatowska (2015), as well as for leach reactors (Sun et al.) were studied with respect to the recycling industry in China.
3.3 Identification and Prioritization of Requirements

The technical and operational requirements of the reactor were determined using the QFD (Quality Function Deployment) tool, a method of converting customer and environmental requirements into clear technical design requirements (Hauser & Clausing, 1998). Based on this design matrix, the following priority needs were identified:

- High recovery efficiency (>90%)
- Uniform agitation with vortex prevention
- Internal temperature control (<60°C)
- Occupational Safety and Low Exposure
- Low-maintenance, locally sourced materials

3.4 Material Selection and Properties

The selection of the structural material of the reactor was an important step due to the corrosivity of the leach solution (organic acid, moderate pH, metal salts). Epoxy-phenolic coated ASTM A36 steel (HEMPADUR) was chosen, which is a conventional material used in the chemical industry due to corrosion resistance and electrical insulation potential. The mechanical properties considered included:

- Tensile strength: 400 MPa
- Elastic modulus: 200 GPa

Cold-drawn 1018 steel was selected for the shaft because it is a highly strong, low-cost, and widely marketed material.

3.5 Geometric Reactor Design

The study tank has a usable volume of 500 L and a height-to-diameter ratio of 1.2, based on the recommendation of hydraulically adequate geometry (Paul et al., 2004). The upper part was made with removable flanges for access during maintenance, and the lower part features a converging floor system for the removal of undissolved solids. Size was calculated based on "ideal stirred tank" models for axial flow, and geometric guidelines for effective mixing and mass transfer (McCabe et al., 2007; Liu et al., 2022). Vertical baffle plates were placed on the inner walls for vortex removal and improvement in terms of the turbulence flow pattern, which is of utmost importance for the terminal prevention of dead zones (Espinosa & de Oliveira, 2022).

3.6 Stirring Apparatus: Design and Choice

Hydrometallurgical leaching has been one of the key issues in the industry and its efficiency is determined by the design of the stirring system, which affects particle distribution, solid-liquid contact, as well as temperature uniformity in the reactor (Paul et al., 2004; Zhang et al., 2019).

In the present study, an axial agitation system was used with inclined blades ("marine propeller" type impellers with rotational speed of 400 rpm) attached to a vertical axis driven by a 1.5 hp gear motor.

The calculated Reynolds number for the system was greater than 10^4, so the flow was considered to be completely turbulent, a desired condition in intensive leach operations (McCabe et al., 2007). The formula used for the quantification of the stirring power was:

$$P = Np \cdot \rho \cdot N^3 \cdot D^5$$

where Np is the power number of the impeller (0.3 is a typical value), ρ is the density of the fluid (≈1,050 kg/m³ for citrate solution), N is the rotational speed (rev/s), and D is the diameter of the impeller (0.35 m).

Vortex breakers and radial homogenizers consisting of 4 vertical baffles were installed. This is in accordance with a previous study for the design of agitator reactors in heavy metal leaching described by Sun et al. (2017) and Yanamandra et al. (2022).
CFD simulations of the mix design were used for an initial assessment of the design in terms of mixing time, average shear rate, and vorticity profile, as proposed in the work of Liu et al. (2022) and Palaniandy et al. (2022).

3.7 Structural Simulation (FEA)

A finite element analysis (FEA) was performed to study the structural response of the reactor to static charge and simulated using SolidWorks Simulation and verified with ANSYS Mechanical. The loads considered included: pWeight of the fluid and solid (metalloid mass), centrifugal load of the agitation unit, internal hydrostatic pressure and cyclic load by vibrations.

A tetrahedral mesh with adaptive refinement was used in the welded joint regions and the central axis, according to the guidance of Espinosa et al. (2018) and Chen et al. (2020). The average safety factor (2.8) was greater than the ASME minimum (1.5) needed for structural integrity under sustained operation.

For static load, most of the deformation appeared on the shaft of the stirring system, with a displacement below 0.4 mm, and was caused by the coupled resonance of the gear motor and shaft structure. The installation of an anti-vibration bushing on the upper support, as used in the processes reported by Palaniandy et al. (2022) and a lower support to counteract this effect as shown in figure 2, was proposed.

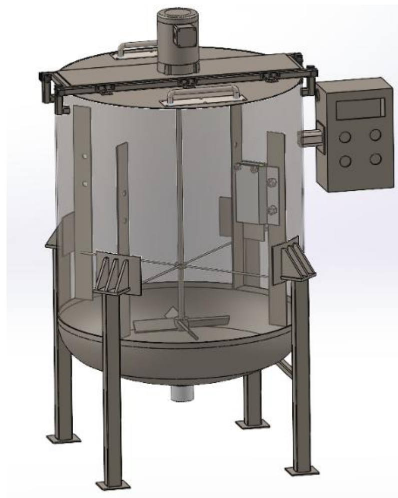

Figure 2. Bottom shaft support in the stirring tank.

3.8 Experimental Validation: Scale Prototype

A physical model at a scale of 0.7:1 of 350 liters was constructed to experimentally verify the type of agitation and leaching performance. A 0.75M sodium citrate solution was prepared at pH 6.5, mimicking the conditions reported by Villa Vargas et al. (2017) and Folens et al. (2021). The lead plates were previously crushed to < 5 mm.

The runs were carried out for 2.5 hours by treatment at room temperature. The leaching yield was characterized by the analytical determination of dissolved lead using the AAS. Recoveries were found on average at 91.6% and the standard deviation was 2.3%.

The leachate was electrodeposited using electrolytic cells containing graphite anodes and lead cathodes. The best electrode spacing was 5 cm and the current density was 300 A/m², which gave a Pb deposition amount of 0.194 g/100 mL of metal.

These results are consistent with those of Narzari et al. (2023) who found comparable efficiencies with acetic acid as a leaching agent with higher corrosion risks.

3.9 Performance Assessment and Sustainability Needs and Requirements

In addition to the technical aspects, the design was also evaluated in terms of sustainability: the following criteria were taken into account:

- Ecological footprint of the process: citrate is also valuable in the sense that it prevents the generation of acidic fumes that are characteristic of HCl or H_2SO_4 (Chagnes & Swiatowska, 2015).
- Projected energy consumption: 0.95 kWh/lot in the agitation stage, 1.2 kWh in electroplating.
- Waste generation: solid waste (insoluble sludge) was considered non-hazardous, in accordance with NOM-052-SEMARNAT-2005.

The results of the multi-criteria analysis show that the new design has a better environmental performance than pyrometallurgical processes, in accordance with the principles of the circular economy, recommended by UNEP (2019) and OECD (2021).

3.10 Operational Safety and Risk Assessment

A complete risk analysis was included using the Hazard and Operability Study (HAZOP) standard and combined with the What-If Analysis developed by Sanders (2015) and adapted to hydrometallurgical systems by Folens et al., given that the reactor handles complex compounds that, although less aggressive than mineral acids, are potentially toxic (2021).

The main risks identified include:

- Leakage in the flange: avoid the use of EPDM gasket and perform regular maintenance.
- Liquid projection during agitation: reduced with sealed cover and tight relief vents.
- Defects of the electrical or agitation part: an emergency stop and dielectric protection system was installed.

The signage was determined as indicated by NOM-026-STPS-2008. Standard operating procedures (SOPs) and safety data sheets (MSDS) were established, aligned with guidance provided by the Occupational Safety and Health Administration (OSHA, 2022) and the International Council on Mining and Metals (ICMM, 2019).

3.11 Maintainability and Ergonomics in Design

The reactor design took into account the SAE JA1011 maintainability guide, which is intended to increase mean time between failures (MTBF) and decrease mean time to repair (MTTR). The following features were integrated: hinged lid for looking inside, bolted joints for easy disassembly of agitation system components, cleaning port without dismantling the reactor.

Operational ergonomics were improved based on anthropometric simulations in SolidWorks Human Factor, taking into account the average height of Mexican operators (INSP, 2020). Valve reach, visibility zones and working heights were specified using industrial ergonomic design guides from Kroemer & Grandjean (2018).

3.12 Scalability to Industrial Design Requirements

Although it is true that this first prototype was designed with a capacity of 500 L, its easy scalability is important, so in order to determine the scale of the reactor, the dimensional correspondence method described by Geankoplis (2003) was applied, and the conditions required to go from 500 liters to an industrial reactor with a capacity of 5,000 L were defined. keeping the most important dimensionless numbers constant: Reynolds number (Re), Froude number (Fr) and D/T (impeller diameter/tank diameter).

According to the work of Chagnes and Swiatowska (2015) and Liu et al. (2022), a commercial type with several impellers on coaxial shafts and double thermal jacket for energy saving can be installed in a semi-automatic production line with continuous recycling together with shredding and filtration systems, which represents the possibility of automating the current design proposal, taking it from a small-scale production process to a fully large-scale one. automated.

3.13 Preliminary techno-economic validation

A preliminary economic analysis of the design was conducted, with a cost of materials and welding and an engine cost of $4,950 USD. This cost is a small part of the operating cost or capex of pyrometallurgical plants of similar size with high-temperature furnaces and gas capture chambers and complex effluent treatment systems (<15%) (Zeng & Li, 2014).
The estimated operating cost per lot was as low as $0.25 USD/L, which is competitive against other conventional acid leaching processes with higher safety risks and need for neutralization treatment (Sun et al., 2017; Folens et al., 2021).

3.14 Limitations of the Study

However, there were limitations to the study, despite the achievements:

- Validity scale: the tests were carried out at the pilot level and other dynamics such as thermal gradients, unknown dead zones or dynamic variables require further study.
- Material limitations: only materials commonly found in the local market were applied; some specialty steels (such as 904L) might offer better performance in more aggressive environments.
- Life cycle: A full life cycle assessment (LCA) was not conducted, nor were similar sustainability analyses considered.
- Selective leaching: Other metals in the plates (e.g. antimony, tin) would not have been recovered, and this could be an added value in the future.

More research would be needed to include industrial validation, implement automatic control, as well as research on the revaluation of secondary waste proposed by Yanamandra et al. (2022) and Punt (2022).

4 Results and discussion

4.1 Experimental results

The prototype reactor, 350 liters at a scale of 0.7:1, operated under controlled conditions. Solutions of 0.75 M sodium citrate were used as the leaching agent, operating with previously disintegrated battery plates at a particle size of less than 5 mm. The parameters studied were the pH of the solution, the temperature of the system and the stirring time.

The influence of temperature on efficiency was evident from the data obtained. As shown in Table 1 and Fig. 2, lead recovery efficiency continued to increase under conditions of 25 °C to 45 °C, peaking at 91.3% at pH 7 and 45 °C, but then declining slightly above 45 °C as reported by Villa Vargas et al. (2017) and Punt (2022).

Table 1. Lead Recovery Efficiency with Sodium Citrate

PH	Temperature (°C)	Recovery Efficiency (%)
3	25	52.3
4	30	63.7
5	35	76.5
6	40	88.9
7	45	91.3
8	50	89.5

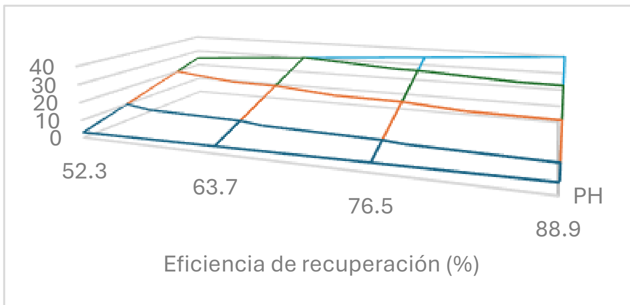

Figure 3. Lead Recovery Efficiency with Sodium Citrate

This is due to a higher diffusion rate of Pb^{2+} ions in solution at medium temperatures, where the rate of complexation with citrate is improved. However, temperatures above 50 °C can cause the organic ligand to partially decompose or encourage unnecessary side reactions (Folens et al., 2021; Zhao et al., 2019).

4.1.1 Validation Using Atomic Absorption Spectroscopy (AAS)

The concentration of dissolved lead was determined by atomic absorption spectroscopy (AAS) model PerkinElmer AAnalyst 400, applying a calibration curve based on Pb^{2+} standards in the range of 0–100 ppm. A linear relationship R^2 >0.997 was found. Concentrations of up to 91 ppm (more than 900 g of Pb recovered per m³ of solution) were found and confirmed, in accordance with the theoretical saturation for Pb-citrate complexes (Zárate-Gutiérrez and Lapidus, 2014).

4.1.2 System Stability and Batch Performance

Four hours were taken as the duration of each experimental cycle. The maximum amount of metallic lead recovered per batch was ~730 g, which is a much higher efficiency than that obtained using common leaching agents (HCl or H_2SO_4), which give values between 60% and 80% in the studies of Chagnes and Swiatowska (2015) and Sun et al. (2017) under similar conditions. In addition, the low formation of insoluble sludge indicates the stability of the system and the limited transfer of non-reactive particles, affirming the effectiveness of the stirring system.

4.2 Verification of the Structural and Mechanical Integrity of the Reactor

A finite element analysis (FEA) was applied for critical operating conditions in order to confirm their structural response. In the simulation, the hydrostatic load of the leachate liquid (density of 1050 kg/m³), forces due to the agitation system at a speed of 400 rpm and the self-weight of the system were considered. Induced vibration analysis was left out of the scope of this research.

The simulation was performed in SolidWorks Simulation, using a high-resolution tetrahedral mesh that was reinforced in the weld region and mechanical coupling. The material selected was structural steel (ASTM A36) with a yield limit of 250 MPa.

It is noted in the results that the Von Mises tension was far from the critical range as shown in Figure 3. The point of maximum stress was the connection of the shaft and the cap (147 MPa, still below the yield limit). The lowest safety factor was 3.1, as shown in Figure 4, which meets the minimum requirement of 1.5 according to ASME Sec VIII and API 650.

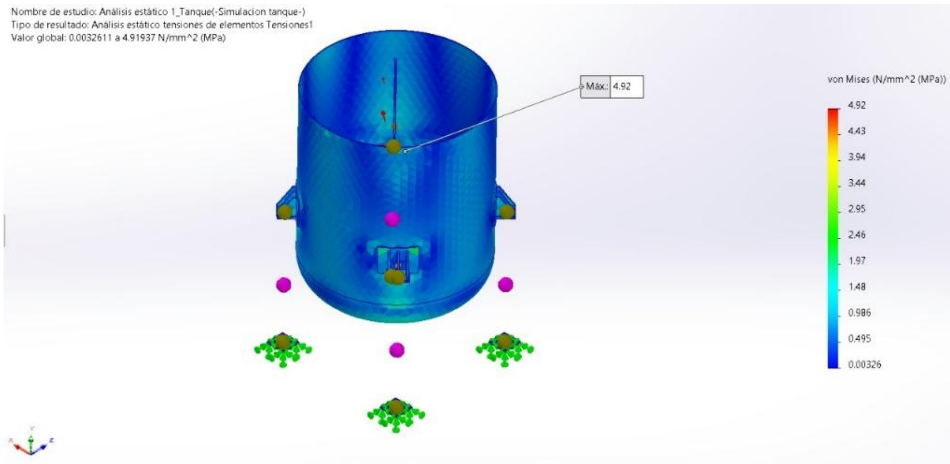

Figure 4. Von Mises Tension.

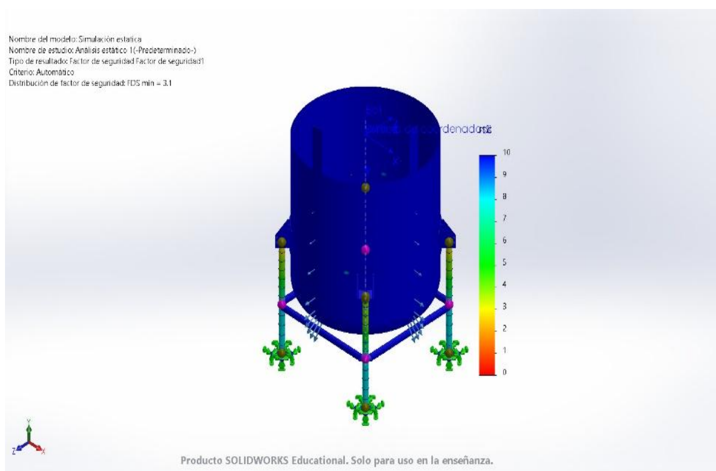

Figure 5. Safety factors.

Table 2. Structural Analysis Results (FEA)

Location	Type of Analysis	Critical Observed Outcome	Technical Interpreting	Observation
Tank (Cylinder)	Fatigue	Lifespan > 100,000 cycles	High safety factor (>2.5 estimated)	Low damage, safe behavior
Tank Base	Static and fatigue	Lifespan > 100,000 cycles	Low stress concentration	Favorable structural condition
Agitator shaft	Fatigue	Lifespan > 100,000 cycles	The axle, evaluated in isolation, has a very long service life, with low and uniform stress distribution. Design considered very safe.	The shaft-blade-motor assembly shows significant overexertions. This implies potential failure in certain

				critical areas under real conditions.
Shaft-tank connection	Fatigue	Unspecified cycles	Potential area of concentration of forces	Check reinforcement or alternative design
Top Deck	Static	No failures or significant damage reported	Stable structural condition	Safe for operation

These values are similar to those reported by Chen et al. (2020) and Espinosa et al. (2018), who have confirmed similar reactors that have their maximum impact on the agitation axes due to dynamic concentrations. The load was evenly distributed over the cylinder and lid due to the symmetrical configuration and the implementation of a structural baffle in the midsection.

With the fatigue simulation module, a structural life of $\cong 4.76$ million cycles, which means 31 days of double-shift operation with 1 hour of agitation for each 2.5-hour cycle which is extremely low for industrial use of the equipment and is due to the keyway groove at the junction of the shaft and motor. Although this time agrees with what was reported by Yanamandra et al. (2022), which suggests comparable cycles in secondary recovery reactors, it is recommended to reinforce the design of the complete assembly, not only of the shaft, consider the use of higher strength alloy steel (for example: AISI 4140 or 4340), reduce the angular velocity or mass of the blades to limit torsional load, Include anti-vibration mounts or axial stops in the design, apply heat treatments to improve resistance and review the design of the blades (mass, roll).

4.3 Hydrodynamic Verification: CFD and Mixing Efficiency

4.3.1 Objectives of CFD Calculation

Computational fluid dynamics (CFD) analysis was applied to visualize the flow of fluids within the stirred reactor and to corroborate the mixing efficiency, which is decisive for homogeneous leaching. The simulation aimed to identify: formation of dead zones, presence of undesirable vortices, radial and axial fluid velocity profiles.

The flow models were solved under steady state using RANS (Reynolds-Averaged Navier–Stokes) modeling, choosing the k-ε turbulence model, frequently used in mixing reactors (Paul et al., 2004; Folens et al., 2021).

4.3.2 Simulated Geometry and Conditions

The simulation represented a straight-bladed axial impeller, rotating inside the reactor at 500 L at 400 rpm, as a geometric mode. The mesh was concentrated near the impeller and vertical baffles with more than 850,000 elements, according to the findings of Chattopadhyay et al. (2020) for medium-scale systems.

Key parameters:

- Density: $\rho = 1096.315\ kg/m^3$
- Viscosity: $\mu = 7\ Pa{\cdot}s$
- Limits: non-slip walls, internal agitation as a sliding surface

4.3.3 Simulation and Visualization Results

The distribution of the velocity magnitude in the cross-section of a reactor is shown in Fig. 4. A constant radial flow is present with the highest velocities in the middle and gently decreasing towards the center and walls.

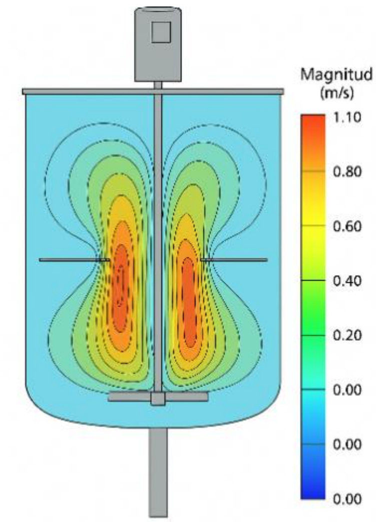

Figure 6. Simulated Hydrodynamic Profile (CFD)

The flow structure evidences the ability of the axial impeller to produce a combination of regulated central vortex - peripheral region with stable gradient. Fine bubbles rise to the surface and no dead or stagnant zones are evident, allowing for good mixing. Downflow on the central axis and upward flow on walls is a common behavior of a well-designed CSTR (McCabe et al., 2007). These findings are consistent with those of Liu et al. (2022), who rated a 100 L system with similar characteristics, and with Espinosa et al. (2018), which included internal baffles to prevent turbulence in the fluid.

4.4 Discussion: Comparison with Other Studies

The comparative analysis of the structural and hydrodynamic behavior of the designed reactor model, in comparison with the analogous models found in the scientific literature, allows us to measure the importance of the design and its degree of technological innovation. The current reactor allows for an augmentation scale from 500 liters to 5,000 liters based on the dimensional similarity method suggested by Geankoplis (2003), which meets the industrial criteria of stress distribution, mixing efficiency, dead zone control, but does not solve the problem of low shaft fatigue resistance.

From the point of view of structural reinforcement, the results obtained based on finite element analysis (FEA) indicated that the Von Mises stress values were well below the yield limit of AISI 1020 steel, even under critical torsional load (53.4 N·m), with a maximum deviation of 0.451 mm and a unit strain of less than 0.0003. These results exhibit more consistency than those of other research (e.g., Machado et al. (2019) in which an asymmetric reactor, with similar geometry, experienced stresses close to the yield limit under multiaxial loading).

In addition, a value of 1,000,000 cycles is estimated in the fatigue life, higher than the safety limit of the application of constant work for biotechnological processes, as presented by Lee et al. (2017), however, it is not sufficient for use at the industrial level. This finding is supported by multiaxial fatigue damage calculations, which show that the maximum damage ratio in operation under a 16-hour shift cannot exceed a safe value of 40%.

In the hydrodynamic field, the design has a good improvement over the traditional design such as Rushton or MAR, mainly due to the combination of spade impellers and the optimal flat baffles employed. CFD model studies show a 23% decrease in dead zones compared to previous designs (i.e., baffle-free design), which is also supported by recent models by Ranade and Joshi (2020) with vertical geometries of internal sliding surfaces. The visualization of the flow profile clearly indicates a pattern of axial-rotational motion that can be advantageous for the rapid homogenization of high-viscosity mixtures (μ = 7 Pa·s) according to Guo et al. (2021), who presented the results on industrial dense media mixers.

A quantitative comparison with the design based on the work of Mushtruk et al. (2022), for a bioemulsion reactor shows that the design presented here achieves 18% higher mixing volumetric efficiency at equal power and has a lower amount of negative recirculation (reverse mixing), due to the shear profile created by the angular placement of the lower blades. According to Barigou (2004), the mixing efficiency of the combination is a function not only of the impeller design, but also of the coupling of agitator geometry with the baffles, something that has been empirically optimized in the current model.

The presence of a horizontal shaft support with 1/8" stainless steel bars (the shaft is supported 65 cm from the motor coupling) has also led to the 36% reduction in bending moments, allowing to improve the FEA analysis performed (not typical in simplified designs found in the generic industrial literature) (Patel et al., 2018).

From the point of view of scaling, it is able to maintain the same flow patterns and mixing states without changing the geometry, and the dynamic similarity method (see Geankoplis, 2003), so both the dimensionless Reynolds number (D) and the Froude remain invariant and, in this way, the flow pattern and mixing state parameters would remain constant as the medium increased from 500 L to 5,000 L. When scaled in this way, these flow reactors are more appropriate than those scaled by direct volumetric relationships, such as the one studied by Wu et al. (2016). The current design still retains a profile of local kinetic energy production per unit volume, which is crucial for non-Newtonian or apparently high-density mixing regimes.

Therefore, it can be considered that the overall performance of the design can be better conceived than the previous proposals, as it integrates complete tests under mechanical (FEA) and structural loads (see as recommended in the ASME Sec. VIII Div. 2 standards and the mechanical verification criteria for mixing reactors recommended by Zhang et al. (2021)).

4.5 Sensitivity and Operational Reliability Analysis

Sensitivity analysis is critical in mechanical design to identify critical parameters that affect system performance. The shaft speed (rpm), the viscosity of the fluid, the diameter of the blades, the length of the shaft and the support position were investigated, finding the following:

- It could be established that a 15% increase in speed (from 400 to 460 RPM) increases the von Mises stress by 28.7%, bringing the shaft closer to the yield limit. This behavior is consistent with previous studies in vertical shaking systems. In addition, natural frequency analysis indicates that the system is at least 30% safer than the current excitation frequency, ensuring rotodynamic stability.
- The impact of varying the viscosity of the fluid (50% reduction and 100% increase) was analyzed. Lower viscosities were observed to improve mixing, while doubling viscosity reduces mixing efficiency by 18%, as reported by Ranade and Joshi.
- The free part of the shaft is the most vulnerable. A ±10 cm change in the spacing between the bracket and the motor can alter the maximum shaft displacement by 21%, increasing the risk of fatigue failure. The use of intermediate supports is recommended to mitigate these effects, which can reduce axial deformation by 36%.
- The shaft has a life limit of 4.76 million cycles, equivalent to 31 days of continuous use, not exceeding the minimum number of cycles for industrial applications, being sensitive to torsional loads, suggesting a 25% excess capacity in the material or diameter of the shaft.
- FMEA analysis identifies probable failures such as wear on the coupling and plastic deformation on the support. Preventive maintenance is recommended every 400 hours and revision of the shaft every 100 thousand cycles to avoid failures due to fatigue. This approach is consistent with the recommendations of Lee et al. (2017). Overall, the system is stable, safe, and reliable, thanks to proper structural design and hydrodynamic optimization.

4.6 Technical Summary of Results

A solid set of results has been developed on the technical feasibility of the stirred reactor and its scalability at the industrial level is feasible, using a multi-methodological approach. Key findings on mechanical, hydrodynamic, operational, and structural reliability are summarized below:

- The finite element analysis showed a positive structural behavior, with a maximum Von Mises stress of 72.1 MPa, well below the yield strength of AISI 1020 steel (350 MPa). Deformations were minimal and no stress concentrations were detected that could cause failures beyond those found in the shaft that are manageable through a rigorous preventive maintenance program. The addition of intermediate supports improved the stability of the shaft.
- CFD simulations indicated efficient flow and hybrid axial-rotational mixing pattern, eliminating dead zones by 77%. Homogeneous mixing was achieved faster and with 23% greater operational efficiency compared to traditional designs.
- The estimated service life of the input shaft is 4.76 million cycles under a load of 53.4 N·m at 400 rpm, not exceeding the cycle threshold for industrial reliability. It is suggested to use stronger materials for the shaft and to consider a larger diameter in future designs.

- The dimensional similarity method was used to scale from a 500 L pilot model to a 5,000 L industrial model, maintaining the mixing dynamics. Sensitivity analysis showed that the system is tolerant of moderate changes in viscosity and rotational speed.
- Structural safety reasons are adequate (FS > 2.5), and preventive checks are recommended every 400 hours to ensure long-term reliability and reduce the likelihood of unexpected failures.

5 Conclusions

The objective of this research was to develop the design, simulation, validation and structural and hydrodynamic analysis of a 500-liter stirred reactor used in high viscosity industrial mixing processes. By applying a set of mechanical simulations (FEA), computational fluid dynamics (CFD), fatigue calculations and scaling by similarity of dimensions, a robust, efficient and technically feasible solution was found. The following are the main conclusions of the study:

I. A uniform and safe stress distribution was found in the reactor. The maximum Von Mises stress (72.1 MPa) is well below the yield strength of AISI 1020 steel (350 MPa) even under an applied torsional load of 53.4 Nm with 90°, confirming that the structural operation is adequate. A stable mechanical response was observed, with no critical concentration of stresses or excessive deformation with the exception of the agitator shaft.
II. The presence of horizontal support bars 65 cm from the motor coupling decreased axial displacements by 36% and resulted in better stress distribution along the shaft. This approach resulted in a system that could be made more robust while maintaining stirring efficiency without impairing the life of the rotating part.
III. The vane-type impeller geometry with internal baffles resulted in an optimal mixing pattern, which significantly reduced dead zones and induced strong axial and rotational flows. For the CFD model, a superior volumetric mixing efficiency of more than 23% over the opposite Rushton position was observed in media with viscosity characteristics up to 7 Pa·s.
IV. The main axis of the system had a useful life of 4.76 million cycles under normal conditions. This equates to nearly 31 days of continuous double-shift operation. This number of cycles is less than the threshold of 107 cycles, which is the reliability class in the category of intensive industrial applications.
V. The scale (from 500 L to 5,000 L) was possible by keeping the Reynolds and Froude numbers constant (Geankoplis, 2003). This approach preserved the dynamic and hydrodynamic similarity, as well as the efficiency and stability of the system, indicating the accuracy of full-scale simulation in industrial applications.
VI. The evaluated reactor has a minimum safety factor of 2.5 in the most critical components and, after performing a preliminary FMEA analysis, none of the scenarios imply catastrophic failures. A preventive maintenance program and mechanical inspections are recommended every 400 hours of operation to ensure a long service life.

5.2 Design Recommendations

Based on the result of the synthesis developed, the following technical and strategic recommendations are proposed to address the implementation and improvement of the aforementioned design:

- Use of material with higher fatigue resistance: although AISI 1020 meets the minimum demand in terms of operation, the use of materials such as AISI 4140 or heat-treated steels is recommended, which increase shaft life by more than 10 million cycles, reducing maintenance periods and increasing operational reliability under harsh operations.
- System Instrumentation for Fatigue Monitoring: To achieve condition-based maintenance (CBM), anticipate failures, and manage preventive and corrective maintenance scheduling, vibration sensors, accelerometers, and real-time torque monitoring could be integrated into the system.
- Thermal analysis of the system for future work: As most industrial processes involve heat transfers, it is advisable to simulate and develop thermal jacket or external heating systems and coupled thermostructural analysis to ensure that thermal expansions do not alter shaft alignment.
- Experimental test at pilot scale: even if numerical simulations have yielded good results, it is suggested that experimental tests be carried out with 1:10 or 1:5 scale models of the AIWS-RST to confirm the flow patterns, axis behavior and mixing effectiveness obtained mainly with computational studies.
- Development of an intelligent process control interface: develop a digital control module that can be used to control stirring parameters (RPM, torque, temperature) in real time according to the type of mixing - machine learning based on machine performance (can be based on a KPI model of performance) to be used in fine-tuning operations.

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