An Integrated Approach for the Assessment of Environmental Sustainability in Agro-Industrial Waste Management Practices: The Case of the Tequila Industry

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Sustainable waste management is a key component needed to achieve multiple of the Sustainable Development Goals established by the United Nations for the year 2030. Such waste management can reduce the degradation of superficial water sources and can contribute to the sustainable and efficient use of resources. Due to their usually high nutrient and organic loads, agro-industrial wastes pose a threat to soil and water resources and are a major contributor to greenhouse gas generation. In this study, a novel approach was proposed to assess the environmental sustainability of vinasse management practices, integrating an extensive physicochemical characterization of tequila vinasses, a GIS-based weighted overlay analysis and a scenario analysis. Mathematical models were applied for the determination of discharged pollutants (nitrogen, phosphorus, BOD₅), as well as greenhouse gas emissions. This methodology was applied to an environmental sustainability assessment of the management practices of tequila vinasses, which are one of the main waste streams generated by the agro-industry in the Mexican state of Jalisco and are one of the main contributors to organic and nutrient loads affecting the water quality of Jalisco's superficial water sources. Through this integrated approach, critical regions for the management of tequila vinasses were determined and an extensive physicochemical characterization of tequila vinasses was performed and applied to assess the environmental sustainability of four management scenarios for tequila vinasses. These results can be used by decision-makers for the implementation of public policy and infrastructure for the improvement of local and regional waste management systems. Additionally, these data may be used to increase the

Abbreviations: Bₚ, Methane production capacity; BOD₅, Biological oxygen demand; BOD₅, Biological oxygen demand load in the discharged effluent; BOD₅, Total Biological oxygen demand; CFC₃₁₅, CO₂eq conversion factor for nitrous oxide; EF, N₂O Emission factor; FOG, Fat oil and grease; MCF, Methane conversion factor; N, Nitrogen concentration; ND, Nitrogen load in the discharged effluent; NT, Total nitrogen; P, Phosphorus concentration; PD, Phosphorus load in the discharged effluent; pH, Hydrogen potential; Pₚ, Total phosphorus; V, Vinasses production volume; W, Weight of a selected parameter.
environmental sustainability of the tequila industry. The proposed methodology has the potential to be applied to different waste-intensive regions as well as different organic waste streams for the assessment of the environmental sustainability of specific management practices considering the local and regional context.

**Keywords:** integrated waste management, agro-industrial waste, tequila vinasses, GIS analysis, scenario analysis, physicochemical characterization, integrated methodology

**INTRODUCTION**

The management of agro-industrial waste poses a great challenge for production-intensive (and waste-intensive) regions, as the inappropriate disposal of large volumes of solid organic waste and wastewater can cause many environmental and health problems (Madurwar et al., 2013; Bedoč et al., 2019). Consequently, waste management is a key component to achieving multiple of the United Nations (UN) Sustainable Development Goals (SDG) established for 2030. The sustainable management of waste contributes to integrated water resource management for the protection and restoration of water-related ecosystems and to achieving the sustainable and efficient use of natural resources (UN, 2017).

Tequila is a fermented alcoholic beverage exclusively made from *Agave tequilana* Weber var. azul (DOF, 2012b). Tequila has been given a protected geographical status that restrains where the agave plants, and tequila itself, can be produced. As a result, tequila and agave plants can only be produced in certain municipalities in the Mexican states of Jalisco, Michoacán, Tamaulipas, Nayarit, and Guanajuato, as shown in Figure 1 (DOF, 2012a; CRT, 2019). Tequila is one of the most commonly consumed alcoholic beverages both in Mexico and globally (Bowen and Zapata, 2009; CRT, 2021). Mexico produces a yearly estimate of 1,501,081 tons of *A. tequilana* Weber var. azul over an approximate surface area of 87,000 ha. The state of Jalisco alone contributes 75% of the national agave production (SIAP, 2020). The total tequila production in 2019 reached an all-time high with 374 million liters. Seventy percent of the produced tequila is destined for exportation and the remainder is distributed nationally (CRT, 2021).

Tequila production can be divided into four stages: 1) agave processing and sugar extraction, 2) fermentation, 3) distillation, and 4) maturation and bottling (Cedeño, 1995). Tequila vinasses are the liquid sludge generated during tequila production and are usually made at a 7–15:1 ratio of vinasse to tequila volume

![Figure 1](image.png)

**FIGURE 1** | Distribution of tequila-producing states in Mexico.
Tequila production, such as in the state of Jalisco (Macías, 1997). This is especially a concern in regions with high rates of footprint assessment (Ibanescu et al., 2018), among others. 2010), waste streams (Bani et al., 2009). New integrated methodologies are required to generate adaptive environmental sustainability assessments that can be easily applied by decision-makers to establish public policy and infrastructure to improve local and regional waste management systems, especially for waste-intensive regions.

As a contribution to the literature, this study presents a novel approach to spatially characterize the environmental impacts (nutrient and organic matter discharge and GHG production) of the tequila vinasses generated in the state of Jalisco. This work herein also quantitatively assesses different management scenarios, combining the physicochemical characterization of vinasses collected in field, GIS-based multicriteria analysis and scenario analysis. Due to the lack of academic literature regarding the spatial variations of the physicochemical characteristics of tequila vinasses, an extensive physicochemical characterization of Tequila vinasses was carried out including samples from Tequila Production Units (TPU) across the state of Jalisco. In order to identify the most critical regions to establish vinasse management strategies, a weighted overlay analysis (WOA) was implemented to evaluate the potential pollution risk for the entire territory of the state, integrating five productive and environmental parameters: 1) vinasse production at the nearest tequila production unit (TPU), 2) total vinasse production for the municipality, 3) distance to the nearest TPU, 4) distance to the nearest water body and 5) distance to the nearest urban community. Furthermore, the environmental impacts generated as a result of the current management practices of tequila vinasses were evaluated in addition to the environmental benefits that could be gained if other management practices were implemented. This was accomplished using information generated through the physicochemical characterization and focusing on the critical regions previously determined through the WOA. Nutrient (nitrogen and phosphorus) and organic matter discharge estimations, as well as GHG production estimations were performed for the critical regions as well as for the entire state, based on the existing models reported for the management conditions of each scenario.

METHODS

The general methodology used in the present study is shown in Figure 2.

Data Collection and Processing

The geographic information and the annual production of tequila production units (TPU), expressed in m$^3$ year$^{-1}$, was obtained from the National Statistic Directory of Economic Units in Mexico (DENUE by its acronym in Spanish) (INEGI, 2021a) and validated with official records provided by the Environment and Land Development Ministry of the state of Jalisco (SEMADET by its acronym in Spanish) (SEMADET, 2019b). When possible, this information was further corroborated directly with the producers and updated. TPU were then classified into production categories according to the internal classification system of the Tequila Regulatory Council (CRT by its acronym in Spanish). This classification was based on the tequila production volumes presented in Table 1, and production...
records were used to estimate the production of vinasses for each individual TPU. The current management practices of vinasses within the TPUs in the state were also identified from official records (SEMADET, 2019b) in order to ascertain the most common practices by the production category according to the CRT classification system for the TPUs (Table 1).

Information related to the hydrographic structure, runoff network, digital elevation model, official municipal limits, and location of urban areas within the study region was obtained from the National Institute of Statistics and Geography (INEGI) (INEGI, 2021b). A geographical information system (GIS) was created on ArcGIS 10.5 to integrate the data corresponding to the TPUs and the previously mentioned environmental and geographical parameters. All raster images had a 15 m × 15 m resolution.

### Selection of Parameters for the WOA

The critical regions for the management of tequila vinasses were determined based on vinasse production records and environmental parameters. A weighted overlay analysis allows for the integration of multiple classified raster layers into a single weighted resulting raster based on a weighted index matrix to classify the evaluated parameters (Yazdani et al., 2015; Al-Anbari et al., 2018). A weighted index matrix was generated to classify and rank the rasters comprising each individual point within the territory of Jalisco according to their potential risk of environmental degradation as a result of inadequate management of vinasses. The following parameters were transformed into raster format for the weighted overlay analysis for the establishment of the critical regions: 1) vinasse production at the nearest TPU, 2) total vinasse production for the municipality, 3) distance to the nearest TPU, 4) distance to the nearest water body, and 5) distance to the nearest urban community. A similar approach was reported by (Díaz-Vázquez et al., 2020). These parameters were selected as they are commonly used for the evaluation of the pollution risk as well
as the spatial suitability for the implementation of management strategies and infrastructure for organic waste and wastewaters (Comber et al., 2015; Mukherjee et al., 2015; Venier and Yabar, 2017; Díaz-Vázquez et al., 2020). These parameters are further explained in the following paragraphs.

(1) Vinasse production rate at the nearest TPU.

The rate of vinasse production at each individual TPU (V) was determined based on the mean, minimum, and maximum production ratio of vinasses (liter of vinasses per liter of tequila) (R) previously reported in the literature (Table 2) and the tequila production volume reported for each individual TPU (T), as shown in Eq. 1. The mean production rates of vinasses were used for the WOA based on the mean production ratio of vinasses (R_mean) reported in Table 2.

\[ V_i = T_i \times R_i \]  

(1)

TPUs can act as both point and non-point sources of pollution to water sources, as the generated vinasses can be discharged directly from the TPUs into water bodies and municipal wastewater systems or they can be transported for field application as fertilizers and then be transported to water bodies by rainfall-runoff processes (Fuess and Garcia, 2014). Therefore, the vinasse production rate at the nearest TPU has a great influence on the pollution risk at every point in the territory.

(2) Total TPUs within the municipality

The total count of TPUs for each municipality in Jalisco was determined based on the TPU inventories. The TPU density within each municipality was included in the analysis as it is related to the density of vinasses that require to be disposed of within the municipal area. Additionally, according to current legislation, all waste of special management is the responsibility of the state, including vinasses (DOF, 1988; SADER, 1989). Therefore the state has the authority to set specific guidelines and regulations for the management of special wastes, as well as the right to establish strategies and region-specific programs in order to improve management of high priority waste, like vinasses (DOF, 1988; SADER, 1989). Higher densities of TPU can facilitate the implementation of pollution prevention strategies within specific regions or small clusters of TPUs rather than at a state level. Additionally, high densities of point sources can lead to the accumulation of pollutants in the areas nearby. Therefore, it is important to locate possible high-density regions in order to establish preventive measures and regulations to reduce pollution risk (Nobre et al., 2007).

(3) Distance to the nearest TPU

The distance from every point in the territory in Jalisco to the nearest TPU was determined using the Euclidean distance tool in ArcGIS 10.5. High production rates of vinasses, and organic waste in general, imply elevated transport costs due to the high water content of vinasses. As a consequence, vinasses tend to be disposed of and accumulated in areas nearby the TPUs in an attempt to reduce disposal costs (Carral et al., 2011; Shahmoradi and Isalou, 2013; Fuess and Garcia, 2017; Díaz-Vázquez et al., 2020). This leads to soil degradation, waterbody eutrophication and, in extreme cases, health hazards for nearby populations (Fuess and Garcia, 2014; Chowdhary et al., 2018).

(4) Distance to the nearest waterbody

The distance from every point in the territory in Jalisco to the nearest water body or water flow were determined using the Euclidean distance tool in ArcGIS 10.5 based on the hydrological data available for the state of Jalisco (INEGI, 2021b). The disposal of vinasses can have a direct effect on the water quality of nearby superficial water bodies (Carral et al., 2011; Shahmoradi and Isalou, 2013). Therefore, it is important to determine how close the evaluated point in the territory is to the nearest superficial waterbody.

(5) Distance to the nearest urban community

The distances from every point in the territory in Jalisco to the nearest urban area were determined using the Euclidean distance tool in ArcGIS 10.5 based on the geographical data available for the state of Jalisco (INEGI, 2021b). The disposal of vinasses to local sewage systems can overload the treatment capacity of local wastewater treatment plants due to the high concentration of pollutants in vinasses. While this is a common management strategy used by TPUs located within urban areas (Beltrán et al., 2001), current legislation requires that each TPU is responsible for the management and disposal of their wastewaters and should not transfer this responsibility to municipal wastewater treatment plants (DOF, 1988; SADER, 1989). Additionally, the accumulation of untreated vinasses in soils and water bodies can generate foul odors due to organic matter degradation (Carral et al., 2011; Shahmoradi and Isalou, 2013).

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**TABLE 2 | Vinasse production ratio used for the estimation of the TPUs vinasses production volumes.**

| Vinasse production ratio (liter of vinasses per liter of tequila) (R) | Mean (R_mean) | Minimum (R_min) | Maximum (R_max) |
|---------------------------------|----------------|-----------------|-----------------|
| 10 Löpez-López et al. (2010)    | 9.75           | 7               | 12              |
| 12 Löpez-López et al. (2010)    |                |                 |                 |
| 7 Iguez-Covarrubias and Peraza-Luna (2007) |         |                 |                 |
| 10 Iguez-Covarrubias and Peraza-Luna (2007) |         |                 |                 |
Development of Classified Raster Images

Raster images were constructed for the five selected parameters. The raster pixels within each raster image of each selected parameter were classified into non-dimensional values ranging from 1 to 5 according to the ranges presented in Table 3. These values were assigned based on how each of the selected parameters increases the risk of environmental pollution from the inadequate management of vinasses at every point in the territory of Jalisco. 1 was assigned to the areas with the lowest pollution risk, and 5 represents the highest pollution risk (Al-Anbari et al., 2018; Díaz-Vázquez et al., 2020).

To evaluate the overall risk of pollution as a result of the inadequate management of vinasses, at every point in the territory, weights were assigned to each parameter based on the literature and studies that evaluate similar parameters (Yager, 1988; Al-Hanbali et al., 2011; Shahmoradi and Isalou, 2013; Vaissy and Sharifi, 2019; Díaz-Vázquez et al., 2020). A WOA was performed using the five generated classified raster images according to Eq. 2, where $RF$ represents the risk factor for every individually analyzed pixel (1–5 scale), $W_i$ represents the assigned weight for the selected parameter and $S_i$ represents the reclassified raster value of the selected parameter (1–5) for the analyzed pixel. Weights were distributed evenly between all parameters based on previous studies (Yager, 1988; Al-Anbari et al., 2018; Vaissy and Sharifi, 2019; Díaz-Vázquez et al., 2020).

The WOA was performed on ArcGIS 10.5 using the Weighted Overlay Analysis tool.

$$RF = \sum_{i=1}^{S} W_i \times S_i$$  \hspace{1cm} (2)

The resulting classified raster, with a 15 m x 15 m resolution, represents the overall pollution risk in each point of the territory (each pixel on the map) considering all five selected parameters expressed on a 1–5 scale. Contiguous municipalities showing zones with a pollution risk of 5 were classified as critical regions.

Collection of Vinasses and Physicochemical Characterization

The physicochemical characterization of vinasses was required due to the lack of information regarding the spatial variability of tequila vinasse physicochemical characteristics in the existing literature. Vinasses were collected from 20 TPUs distributed across the previously identified critical regions. A stratified sampling was performed to include all TPU size categories within the study. 5 L grab samples were taken the same day that these were produced, transported in refrigeration (4°C) for less than 5 h and kept at 4°C until further processing within the next 24 h, as established by the applicable regulation (DOF, 1997). No composite samples were prepared as all samples were analyzed individually in duplicate. Hydrogen potential (pH) was measured at the collection site by the potentiometric method while total suspended solids (TSS), settleable solids (SS), biological oxygen demand (BOD5), total Kjeldahl nitrogen (TKN), total phosphorus (TP), and fat oil and grease (FOG) were determined upon arrival by the Analytical and Metrologic Services Unit (USAM by its acronym in Spanish) of the Centro de Investigación y Asistencia Tecnológica del Estado de Jalisco (CIATEJ). TSS and SS were determined by gravimetric methods, BOD5 was determined by the respirometric method, TKN was determined using the Soxhlet extraction method. All determinations were made following the Federation, W. E., and American Public Health Association methods (Eaton et al., 2005).

A physicochemical characterization was required for the evaluation of the management scenarios. One-way ANOVAs and Tukey tests were performed on Minitab 19.2020.1 to determine significant spatial differences between the sampled vinasses collected from different regions of the state of Jalisco according to the productive records provided by SEMADET (SEMADET, 2019b) as well as the most effective vinasse management practices reported in the literature (López-López et al., 2010; España-Gamboa et al., 2011; Robles-González et al., 2012; Moraes et al., 2017). Complete scenario descriptions are shown in Table 4.

Management Scenarios Analysis

Four scenarios (A, B, C, and D) were proposed based on the most frequent vinasse management practices reported for Jalisco and according to the productive records provided by SEMADET (SEMADET, 2019b) as well as the most effective vinasse management practices reported in the literature (López-López et al., 2010; España-Gamboa et al., 2011; Robles-González et al., 2012; Moraes et al., 2017). Complete scenario descriptions are shown in Table 4.

The potential nutrient and organic matter release into the environment, as well as the potential GHG emissions (CO2eq)

### Table 3: Weight index table.

| Parameter | Unit | Value (S) | Weight (%) |
|-----------|------|-----------|------------|
| Vinasses production at the nearest TPU to the site | m³/year⁻¹ | 0–1,000 | 20 |
| Total TPUs in the municipality | Units | 0–1 | 20 |
| Distance from the point in the territory to the nearest TPU | M | 0–2,500 | 20 |
| Distance from the point in the territory to the nearest superficial waterbody or water flow | | 0–250 | 20 |
| Distance from the point in the territory to the nearest urban area | M | 0–500 | 20 |
| Scenario | Scenario description | Treatment process | Nutrients (N and P) and biological oxygen demand (BOD5) | Greenhouse gas emissions | B0* | MCF* | EF* | CFCH4* | CFN2O* | RN* | RP* | RDBO* |
|----------|---------------------|-------------------|------------------------------------------------------|--------------------------|------|-------|------|--------|--------|------|------|--------|
| A        | Vinasses are disposed of by direct field irrigation as well as direct disposal into water bodies. This disposal scenario is the most commonly used in Jalisco. | Field irrigation | Complete nutrient (N and P), as well as BOD5 loads, are deposited in soil and water bodies Fuess and Garcia, (2014). | Organic matter is degraded into CO2 and CH4 in soil and receptive waterbodies. A fraction of the nitrogen load is transformed into volatile N2O. The remaining organic matter load in the effluent is discharged into soil and water bodies De Klein, (2006); Doorn et al. (2006); Fuess and Garcia, (2014). | 0.6 Doorn et al. (2006) | 0.1 Doorn et al. (2006) | 0.01 Doorn et al. (2006) | 25 Forster et al. (2007) | 279 Forster et al. (2007) | 0 | 0 | 0 |
| B        | Vinasses are treated in activated sludge wastewater treatment plants | Aerobic oxidation lagoons | Nutrient and BOD5 loads are reduced in the treatment process. A fraction of the removed nitrogen load is transformed into volatile N2O and the rest recovered and reprocessed as biofertilizer. The remaining nutrient and BOD5 load in the effluent is discharged into soil and water bodies Eckenfelder, (1998); Calik and Stenstrom, (2005). | Organic matter is degraded into CO2 and CH4. A fraction of the nitrogen load is transformed into volatile N2O. The remaining organic matter load in the effluent is discharged into soil and water bodies De Klein, (2006); Doorn et al. (2006); Fuess and Garcia, (2014). | 0.6 Doorn et al. (2006) | 0.3 Doorn et al. (2006) | 0.006 Kampschreur et al. (2009) | 25 Forster et al. (2007) | 279 Forster et al. (2007) | 40% von Sperling, (1996) | 45% von Sperling, (1996) | 93% von Sperling, (1996) |
| C        | Vinasses are treated in anaerobic digestion systems and the generated CH4 is harnessed for energy generation | Anaerobic digestion | Nutrient and BOD5 loads are reduced moderately. Removed nutrient loads are recovered and reprocessed as biofertilizer. The remaining nutrient and BOD5 load in the effluent is discharged into soil and water bodies Eckenfelder, (1998); Franklin, (2001); Calik and Stenstrom, (2005). | Organic matter is degraded mainly into CO2 and CH4. CH4 is then valorized for energy production so no CH4 is released. N2O generation is negligible. The remaining organic matter load in the effluent is discharged into soil and water bodies Calik and Stenstrom, (2005); Doorn et al. (2006); Eackenfelder et al., (2006); Kampschreur et al., (2009). | 0.6 Doorn et al. (2006) | 0.8 Doorn et al. (2006) | 0 Doorn et al. (2006) | 2.75 Díaz-Vázquez et al. (2003) | 279 Forster et al. (2007) | 25% von Sperling, (1996) | 20% von Sperling, (1996) | 80% von Sperling, (1996) |
| D        | Vinasses are treated in anaerobic-aerobic sequential treatment, the generated CH4 is harnessed for energy generation | Anaerobic digestion | Nutrient and BOD5 loads are highly reduced in the sequential treatment process. A fraction of the removed nitrogen load is transformed into volatile N2O during the aerobic stage and the rest of the removed nutrient load is recovered and reprocessed as a biofertilizer. The remaining nutrient and BOD5 load in the effluent is discharged into soil and water bodies Frostell, (1983); Chan et al, (2009); Sably et al. (2009). | Organic matter is degraded mainly into CO2 and CH4 during the anaerobic stage. CH4 generated during the anaerobic stage is then valorized for energy production. The remaining organic matter load in the effluent is discharged into soil and water bodies Calik and Stenstrom, (2005); (Doorn et al., 2006); Cakir and Stenstrom, (2005). | 0.6 Doorn et al. (2006) | 0.8 Doorn et al. (2006) | 0 (Doorn et al., 2006) | 2.75 Díaz-Vázquez et al. (2003) | 279 Forster et al. (2007) | 25% von Sperling, (1996) | 20% von Sperling, (1996) | 80% von Sperling, (1996) |

*B0, Maximum methane production; MCF, Methane correction factor; EF, Emission factor; CFCH4, Methane conversion factor; CFN2O, Nitrous oxide conversion factor; RN, Nitrogen removal rate; RP, Phosphorus removal rate; RDBO, Biological oxygen demand removal rate.
from the disposal of the vinasses within the critical regions, were determined based on the characterization of vinasses performed in the present work for the four proposed scenarios (A, B, C, and D).

**Nutrient Release to the Environment**

The total vinasse production, TN production, and TP production were estimated based on the total production volumes reported for each individual TPU and the physicochemical characterization of the sampled vinasses using the minimum, mean and maximum values (for both vinasse production rates and physicochemical parameters) as shown in Table 1 and Table 6, for each of the critical regions. These estimations are total nutrient productions without the differentiation of the bioavailability.

The total nitrogen (\(N_T\)) (Mg year\(^{-1}\)) potential release was determined according to Eq. 3 for each scenario. This was based on the total vinasses generated (\(V\)) (m\(^3\) year\(^{-1}\)) in each critical region and the mean, minimum, and maximum nitrogen concentration in the sampled vinasses (\(N\)) (Mg m\(^{-3}\)) displayed in Table 6. The nitrogen load (\(N_D\)) (Mg year\(^{-1}\)) in the discharged effluent was determined according to Eq. 4, where \(R_N\) (nondimensional) represents the nitrogen removal rate under each scenario.

\[
N_T = V \ast N
\]

(3)

\[
N_D = N_T \ast (1 - R_N)
\]

(4)

The total phosphorus (\(P_T\)) (Mg year\(^{-1}\)) potential release was determined following the same method used for the calculation of the total nitrogen potential release, as shown in Eq. 5, where \(V\) is the total vinasse generation (m\(^3\) year\(^{-1}\)) in each critical region and \(P\) is the phosphorus (mean, minimum, and maximum) composition of the sampled vinasses (Mg m\(^{-3}\)) as displayed in Table 6. The phosphorus load in the discharged effluent (\(P_D\)) (Mg year\(^{-1}\)) was determined according to Eq. 6, where \(R_P\) (Nondimensional) represents the phosphorus removal rate under each scenario.

\[
P_T = V \ast P
\]

(5)

\[
P_D = P_T \ast (1 - R_P)
\]

(6)

**Organic Matter Release and Greenhouse Gas Emissions**

The mean, minimum and maximum organic matter content present in the untreated vinasses and the discharged effluent for each respective scenario was calculated according to Eqs. 7, 8, respectively. \(BOD_T\) (Mg year\(^{-1}\)) represents the total BOD\(_5\) content in the untreated vinasses according to BOD\(_2\) (Mg m\(^{-3}\)) values shown in Table 4. These were obtained as a result of the physicochemical characterization of the sampled vinasses. \(BOD_D\) (Mg year\(^{-1}\)) represents the remaining BOD\(_5\) present in the discharged effluent after the proposed treatment, according to the specific organic matter removal factors of each process as reported in the literature (Table 4).

The mean, minimum and maximum GHG emissions (\(GHG\)) (Mg CO\(_2eq\) year\(^{-1}\)) generated though the proposed scenarios were calculated for each scenario (A, B and C, and D, respectively) according to Eqs. 9–11, using the mean, minimum and maximum values from the vinasse production rates and the physicochemical characterization. These equations were adapted from the IPCC Guidelines for National Greenhouse gas inventories based on process specific factors, summarized in Table 4 (Doorn et al., 2006). The factors proposed by the IPCC are region specific in most cases and, thus, the Latin-America values were used when available. When not available a mean parameter was used, as suggested by the IPCC (De Klein, 2006; Doorn et al., 2006).

\(B_T\) (nondimensional) is the most commonly used methane production capacity in the calculation of GHG inventories, which indicates the fraction of organic matter that can be transformed to CH\(_4\) and tends to be independent of the degradation process and its conditions, assumed as 0.6 (Doorn et al., 2006). \(MCF\) (nondimensional) represents the methane conversion factor used to estimate the conversion of BOD\(_5\) into methane under specific degradation conditions (Doorn et al., 2006). \(V\) (m\(^3\) year\(^{-1}\)) represents the generation of vinasses in the individual TPU. \(N_T\) (Mg year\(^{-1}\)) represents the nitrogen concentration in the untreated effluent, and \(N_D\) (Mg year\(^{-1}\)) represents the nitrogen present in the discharged effluent after the proposed treatment. The fraction of nitrogen transformed and released into the atmosphere as N\(_2O\) is expressed as \(EF\) (nondimensional). Both \(CFCH_4\) (nondimensional) and \(CFN_2O\) (nondimensional) represent the conversion factors used to transform the CH\(_4\) and N\(_2O\) into CO\(_2eq\), respectively. Eqs. 9–11 were adapted from the equations proposed by De Klein, (2006) and Doorn et al. (2006), as they are the most common methods for estimating GHG resulting from waste management and agricultural practices (De Klein, 2006; Doorn et al., 2006). The GHG estimation for scenarios C and D includes only the direct GHG generated by organic matter and nutrient degradation; it does not include possible GHG reductions due to energetic net reduction or even energetic surplus due to the energetic revalorization of CH\(_4\).

\[
BOD_T = BOD_5 \ast V
\]

(7)

\[
BOD_D = BOD_5 \ast (1 - R_{BOD})
\]

(8)

\[
GHG_A = (B_T \ast MCF \ast BOD_T \ast V \ast CF_{CH_4})
\]

\[
+ \left( V \ast N_T \ast EF \ast \frac{44}{28} \ast CF_{N_2O} \right)
\]

(9)

\[
GHG_{BC} = (B_T \ast MCF \ast BOD_T \ast V \ast CF_{CH_4})
\]

\[
+ \left( V \ast N_T \ast EF \ast \frac{44}{28} \ast CF_{N_2O} \right)
\]

+ \left( B_0 \ast MCF \ast BOD_D \ast V \ast 25 \right)

\[
+ \left( V \ast N_D \ast 0.01 \ast \frac{44}{28} \ast 279 \right)
\]

(10)

\[
GHG_D = (B_T \ast MCF \ast BOD_T \ast V \ast CF_{CH_4})
\]

\[
+ \left( V \ast N_T \ast EF \ast \frac{44}{28} \ast CF_{N_2O} \right)
\]

\[
+ (B_0 \ast MCF \ast BOD_T \ast 0.2 \ast V \ast CF_{CH_4})
\]

\[
+ \left( V \ast N_T \ast 0.75 \ast EF \ast \frac{44}{28} \ast CF_{N_2O} \right)
\]

\[
+ (B_0 \ast MCF \ast BOD_D \ast V \ast 25)
\]

\[
+ \left( V \ast N_D \ast 0.01 \ast \frac{44}{28} \ast 279 \right)
\]

(11)
RESULTS

Characterization of the Tequila Production Sector and of Current Producer Management Practices

The total production of tequila in Jalisco is accomplished by 158 TPUs, from which 109, 17, 14, and 18 units are categorized as micro, small, medium, and large, respectively. This is according to the internal classification system used by the CRT, which is based on the tequila production volume shown in Table 1. The mean estimated vinasse production rate in Jalisco was found to be 2,645,655.69 m$^3$ year$^{-1}$. The TPUs classified as large contribute 84.3% of the state vinasse production, while the remaining 15.7% is generated by micro, small and medium TPUs contributing with 1.7, 4.1, and 9.8% respectively. Almost 80% of the state’s vinasse production is accomplished by only seven municipalities: Tequila, Zapotlanejo, Atotonilco el Alto, Amatitan, Arandas, Tlaquepaque, and Tototlan. The complete vinasse production and size distribution for the municipalities responsible for 80% of the vinasses within the state is displayed in Table 5. Tequila and Amatitan are located within the middle-western region of the state, Atotonilco, Arandas and Tototlan belong to the eastern region, and Zapotlanejo and Tlaquepaque are located in the central region of the state.

Most small, micro, and medium TPUs used pH neutralization and direct field application as their management practices for vinasses, while large TPUs used a variety of treatment alternatives, mainly categorized as biological treatment (aerobic or anaerobic) and, with a lower frequency, sequential anaerobic-aerobic treatment.

Critical Region Determination

Five classification maps were generated, each corresponding to one of the selected parameters (Figure 3) used to evaluate the risk of environmental degradation due to inadequate management of tequila vinasses. High values (5), which indicated a higher risk of pollution, were located within the middle-western and eastern regions of the state of Jalisco. This can be attributed to the higher density of TPUs, and their high tequila production rates, within these regions as well as the abundance of urban settlements across these areas.

As a result of the WOA, a classification map was obtained to identify the critical regions (Figure 4) weighting all five selected parameters. Two main critical regions were found to be located in the western region of the state (Valles region) and in the eastern region of the state (Altos region). These critical regions, Valles and Altos, have the highest possible risk of environmental pollution as a result of nutrient and organic matter release and the highest potential to produce GHG emissions resulting from poor management of the tequila vinasses. The contiguous municipalities displaying critical zones (Figure 4) were selected and clustered, as shown in Figure 5. The Valles critical region comprises the municipalities of Tequila, Amatitan, and El Arenal, while the Altos critical region consists of the municipalities of Tepatitlan de Morelos, Atotonilco el Alto, Arandas, and Jesus Maria, as displayed in Figure 5. The municipalities of Tequila, Amatitan, Atotonilco el Alto, and Arandas belong to the municipalities responsible for 80% of vinasse production in the state, as shown in Table 5.

Characterization of Vinasses

The results of the physicochemical characterization, summarized by descriptive statistics, of vinasses collected at 20 TPUs distributed across the critical regions are displayed in Table 6. Additionally, based on the current Mexican legislation (DOF, 1997), the newly proposed Mexican legislation (DOF, 2018), the European Union water directive (Council directive, 2014) and the EPA guidelines for centralized waste treatment point discharges (EPA, 2021), the permissible limits are shown to compare the results to the applicable federal discharge guidelines as well as to international standards. While the physicochemical characteristics of vinasses from other alcoholic production processes (molasses, sugarcane, sugar beet, etc.) are well documented (España-Gamboa et al., 2011; Christofoletti et al., 2013; Chowdhary et al., 2018; Mikucka and Zieelińska, 2020), there is a lack of information regarding tequila vinasses because most of the existing reports on the physicochemical characteristics have been obtained from single production units and thus fail to represent the variability in vinasse characteristics resulting from a wide variety of productive processes used across the state (Íñiguez-Covarrubias and Peraza-Luna, 2007; López-López et al., 2010).

The pH values of the sampled vinasses exhibited the lowest coefficient of variation (CV = 5%) while FOG displayed the highest coefficient of variation of all analyzed parameters (CV = 158%). This indicates that variations within the tequila production process have a great influence on the FOG content of the discharged vinasses. TP and SS also presented elevated coefficients of variation, at 156 and 133%, respectively.

According to Table 6, vinasses surpass the permissible discharge limits established in the current Mexican legislation for all of the regulated parameters. Furthermore, neither of the vinasse samples were within acceptable limits for any of the seven analyzed parameters according to current legislation. Therefore, a treatment process would be required in order to fulfill the current local legislation standards (DOF, 1997). The local permissible limits for wastewater discharge are currently under a revision process since a new legislation was recently proposed (DOF, 2018). New lower permissible limits may be established within the short term due to the new legislation proposal, which would increase the need for effective wastewater management strategies in order to fulfill the new standards that not only reduce current permissible limits but add new parameters to be regulated, as is the case of color and toxicity (DOF, 2018). Both international discharge guidelines presented in this study (Table 6) exhibit lower limits than the current local legislation, making it unacceptable to discharge untreated vinasses under those guidelines (Council directive, 2014; EPA, 2021).

The mean concentrations of phosphorus and nitrogen (42.01 mg L$^{-1}$ and 131.63 mg L$^{-1}$) were closer to the current...
permissible limits, 40 and 110% higher than the current legislation, in comparison to the mean concentrations for other parameters. However, when compared to international standards, tequila vinasses display concentrations of phosphorus and nitrogen that were 2,100 and 400% higher than the permissible limits set for the European Community (Council directive, 2014). BOD₅ is the water quality parameter that most highly exceeded the current local and international guidelines, reflecting the extreme organic load in the vinasses and emphasizing the need for effective vinasse management practices in order to prevent environmental degradation.

From the seven analyzed parameters, significant mean differences between the vinasses produced by TPUs of different size categories were only found when considering SS ($p = 0.011$). No significant differences were found between the vinasses produced in the different regions (Altos and Valles) of the state of Jalisco, indicating there is no difference between the vinasses generated in either of the tequila producing regions.

Critical Regions and Scenarios Analysis

Table 7 displays the estimated vinasse production volumes for the municipalities within the established critical regions. The complete scenario-based estimations for organic matter, nutrient and GHG release is shown in Tables 8, 9 for both Altos and Valles critical regions as well as for the entire state of Jalisco.

DISCUSSION

Critical Regions for the Management of Vinasses

All of the tequila producers registered in the official records in Jalisco were classified in four categories, as shown in Table 1. Similar proportions of all categories (micro, small, medium, and large) were found for both critical regions, Valles and Altos (SEMADET, 2019b) While most of the vinasses generated in Jalisco are produced by large TPUs (83%), a great majority of these producers already report vinasse treatment systems that offer complete or partial treatment. Large producers generally have the resources and technical knowledge to implement effective wastewater management systems. However, medium, small, and micro-producers generally lack these resources and technical knowledge and thus release higher volumes of untreated vinasses discharged to soils and waterbodies across the state (SEMADET, 2019b).

Both the critical regions determined in this study displayed similar overall vinasse production volumes, as shown in Table 7. However, these regions present different spatial configurations. Most of the TPUs within the Valles critical region are in a smaller area (within a 5 km radius, approximately), which favors the implementation of centralized treatment units. This is not only because of the constant supply of vinasses, but due to the relatively short distances between most TPUs. The TPUs within the Altos critical region are more dispersed across the region (within a 30 km radius), which can be a disadvantage for the implementation of large-scale centralized treatment units due to higher transport costs (Flotats et al., 2009; Fuess and García, 2014). Areas with lower densities of wastewater production may require different approaches in order to achieve effective and economical wastewater management like small-scale clustering or other diverse onsite treatment options (Massoud et al., 2009).

Besides being the top Tequila producer, Jalisco is the leading state for the production of crops and livestock in Mexico (SIAP and SAGARPA, 2018). This agricultural productivity increases the overall organic waste and nutrients released to the environment as a result of inadequate management practices (Montoya et al., 1997; Martínez Rivera, 2004; Jayme-Torres and Hansen, 2018; Díaz-Vázquez et al., 2020). Both critical regions identified in this study, Altos and Valles, display high agricultural and industrial activity that influences the soil and water quality of the region. Additionally, the tequila industry in these regions generates larger volumes of agro-industrial waste compared to other industrial categories and therefore has a great influence on the environmental degradation (Montoya et al., 1997; SEMADET, 2017; Jayme-Torres and Hansen, 2018). Furthermore, these regions are located within the Santiago river basin, which is known to be highly polluted with nitrogen, phosphorus, and organic matter (Abrol and Sharma, 2012). The spatial identification of critical regions can be a powerful tool to identify areas that require special policies or management in order to prevent environmental degradation or health hazards to nearby populations (Delivand et al., 2015; Díaz-Vázquez et al., 2020). Although it is out of the scope of the present work, the identification of waste-intensive regions would open up the possibility for the implementation of synergic waste management systems. Different waste streams could then be integrated and valorized to higher levels than the ones from individual revalorization of waste streams. One example of this is the anaerobic co-digestion of waste, where the biogas yields from mixed waste stream feeds are significatively higher than the ones from individual waste feeds (Muhammad and Chandra, 2021; Rincón-Pérez et al., 2021).

Potential Environmental Effects of Untreated Vinasses

As shown in Table 6, the mean pH of the analyzed samples is within the range previously reported for tequila vinasses (3.4–4.5) (López-López et al., 2010). If vinasses are discharged without previous pH neutralization, the receptive soils and water bodies can be severely affected due to the high acidity of this agro-industrial waste (Fuess and García, 2017). Acidification of soil and water is known to increase nutrient mobility, altering its uptake in crops as well as increasing its transport by runoff or leaching to receptive waterbodies or groundwater, respectively (World Health Organization, 2006). The most common method used by TPUs to regulate this parameter is to utilize neutralizing agents, such as CaO, Ca(OH)₂, and NaOH. However, special care must be taken, as large amounts of neutralizing agents can increase the content of specific ions in the effluent (Fuess and García, 2017; Chowdhary et al., 2018), which over time can cause soil degradation, heavy metal transport, as well as damage to aquatic species due to increased ion concentrations in receptive...
The mean BOD$_5$ value (Table 6) in the sampled vinasses (119,011.77 ± 104,097.12 mg L$^{-1}$) was greater than previously reported values for tequila vinasses as well as for other vinasses (20,600–60,000 mg L$^{-1}$) (López-López et al., 2010; España-Gamboa et al., 2011). The higher BOD$_5$ concentrations in the sampled vinasses can be linked to the high TSS content also found in the characterized vinasses (9,875.80 ± 11,958.41). This is due to the fact that TSS in tequila vinasses are mainly composed of organic unfermentable solids like cellulose and pectin, which are present in the agave juice that was not degraded during the alcoholic fermentation stages (Íñiguez-Covarrubias and Peraza-Luna, 2007; España-Gamboa et al., 2011). Because of these substrates’ composition, the TSS content in the sampled vinasses (9,875.80 ± 11,958.41) is above the higher limit reported by López-López (2000–8,000 mg L$^{-1}$) (López-López et al., 2010; España-Gamboa et al., 2011). The mean TSS content in the sampled vinasses (9,875.80 ± 11,958.41) is due to the high TSS content also found in the characterized vinasses (9,875.80 ± 11,958.41). This is due to the fact that TSS in tequila vinasses are mainly composed of organic unfermentable solids like cellulose and pectin, which are present in the agave juice that was not degraded during the alcoholic fermentation stages (Íñiguez-Covarrubias and Peraza-Luna, 2007; España-Gamboa et al., 2011). The implementation of other sugar extraction processes, such as diffusion extraction, increase the total unfermentable solid content in the agave juice, which is discarded in the vinasse effluent (España-Gamboa et al., 2011). Because of these substrates’ composition, the TSS content in the sampled vinasses could have been affected due to natural sedimentation during the time prior the sampling.

The TKN content (Table 6) in the analyzed vinasses (131.63 ± 97.59 mg L$^{-1}$) was approximately three times higher than the previously reported values for tequila vinasses (20–50 mg L$^{-1}$). However, it was still lower than the values reported in the literature for vinasses from mezcal production, which uses different varieties of agave; likewise, the TKN content reported herein was lower than in vinasses obtained from the fermentation of other substrates like corn, beet, and sugarcane (660–5,650 mg L$^{-1}$, 2,000–2,680 mg L$^{-1}$, 1,800–4,750 mg L$^{-1}$, and 1,000–7,000 mg L$^{-1}$, respectively) (Robles-González et al., 2012; Fuess and García, 2017). An important fraction of the total nitrogen content in tequila vinasses is in an organic form, which reduces its potential as a crop fertilizer since it requires mineralization by soil microorganisms to be of use for crop fertilization (Fuess and García, 2017). Organic nitrogen is mineralized in soils or water bodies, into ammonium which can be easily used by plants as a nitrogen source. However, high ammonium concentrations may lead to elevated concentrations of nitrates and nitrites in soil and waters, causing eutrophication, or may also cause increased N$_2$O emissions through nitrification or denitrification processes (Kirchman, 2018). The mean phosphorus content of the tequila vinasses analyzed in the present study (42.01 mg L$^{-1}$) corresponds to the values reported for tequila vinasses by España-Gamboa (40 mg L$^{-1}$) (España-Gamboa et al., 2011). Tequila vinasses present lower phosphorus contents compared to vinasses obtained from other common substrates (71–1,990 mg L$^{-1}$) (sugar cane, sorghum, sugar beet, molasses, etc.), which can be attributed to the natural phosphorus content in these other substrates (España-Gamboa et al., 2011). Because phosphorus exhibits lower volatility compared to nitrogen, there is the risk of accumulation of phosphorus in soil and receptive waterbodies if vinasses are inadequately managed (World Health Organization, 2006) either by the direct discharge of or by the transport of accumulated phosphorus in the soil through superficial runoff and groundwater (Fuess and García, 2017).
The disposal of untreated vinasses by field irrigation or direct discharge to water bodies can be a powerful driver for phosphorus accumulation due to its excessive phosphorus content and reduced volatilization rates, leading to eutrophication of water bodies due to surface runoff and groundwater phosphorus transport (Carpenter et al., 1998; Fuess and Garcia, 2017).

The FOG mean values (Table 6) obtained in the present study (301.14 mg L\(^{-1}\)) were 300% higher than the upper limit of the reported range by López-López for tequila vinasses (10–100 mg L\(^{-1}\)) (López-López et al., 2010). The high coefficient of variation (Table 6) (CV = 158%) found for FOG in this study is of special interest since the lower measured values of FOG in the analyzed vinasses fall within the acceptable limits for both current and proposed legislation. The cooking process used for the agave heads may be related to the high variation in the FOG values measured in the analyzed vinasses since the agave heads cuticles release waxy compounds under heat treatment. Prior to sugar extraction by milling, agave heads are cooked mostly either by oven cooking or autoclaving (Cedeño, 1995). The use of diffusion extraction, on the other hand, may prevent the release of waxy compounds into the sugar-rich agave juice and can significantly reduce the content of FOG in the vinasses.
(Cedeño, 1995; Tequila Sauza, 2021). However, only a small fraction of producers have implemented extraction alternatives like diffusion (Cedeño, 1995; Tequila Sauza, 2021). When vinasses are inadequately managed and released to the environment untreated, the FOG present in them not only contributes to the overall BOD₅ but can reduce gaseous transfer rates in both water bodies and soils and can cause clogging in transport and treatment piping (Husain et al., 2014).

The differences presented between previous studies and the present work can be attributed to the larger pool of sampled vinasses since the present study characterized 20 different TPUs across the state of Jalisco compared to individual characterizations performed by López-López, Íñiguez-Covarrubias, and España-Gamboa (Íñiguez-Covarrubias and Peraza-Luna, 2007; López-López et al., 2010; España-Gamboa et al., 2011), which may not represent the complete diversity of TPUs and their vinasses. López-López et al. (2010) reported the only physicochemical characterization of Tequila vinasses available in the literature but neither indicated the amount/location of TPUs sampled nor the descriptive statistics from the results.

**Critical Regions and Scenarios Analysis**

Scenario A (field application) is based on the most common management in Jalisco, while scenarios B (aerobic treatment), C (anaerobic treatment), and D (sequential anaerobic-aerobic treatment) are not widely implemented in Jalisco but are generally applied for the management of vinasses in other regions (López-López et al., 2010; España-Gamboa et al., 2011).

**Scenario A: Field Irrigation**

Because scenario A (field application) assumes no treatment previous to the vinasse’s disposal, the complete nitrogen, phosphorus, and organic matter loads are released to the soil through irrigation (348.24 Mg year⁻¹, 111.14 Mg year⁻¹, and 314,864.18 Mg year⁻¹, respectively) (Table 8). Although the estimated GHG emissions for scenario A (473,823.03 Mg year⁻¹) (Table 8) are the lowest of the proposed scenarios, the GHG production rates in scenario A are highly dependent on the environmental conditions (temperature, oxygen, nutrient concentration, microorganism populations, etc.) on which the organic matter and nutrients present in the soils and waterbodies are degraded. The estimated GHG emissions for scenario A are likely an underestimation since the emission factors used assume complete aerobic degradation. Moreover, due to the elevated organic content, vinasses are prone to generate partially anaerobic conditions upon applications, which would significantly increase overall GHG estimations (De Klein, 2006; Doorn et al., 2006; Fuess and Garcia, 2014). Additionally, GHG estimations from scenarios C and D do not include possible GHG reductions due to external energy demand reduction, which would reduce overall GHG estimations, lowering the GHG estimation difference.
The mean GHG production estimated for scenario A represents 82.2% of the total GHG production estimate through wastewater management reported for the state of Jalisco (SEMADET, 2019a) and 1.5% of the state's total GHG emissions (SEMADET, 2019a). However, due to lack of information, it is not clear if the GHG resulting from wastewater management previously estimated for Jalisco includes only urban wastewaters or if it also includes agro-industrial wastewater, therefore explaining the low reported wastewater management GHG values in the state.

Field application, proposed in scenario A, is the most common disposal method of vinasses globally (Moraes et al., 2017). As shown in Table 8, field irrigation of vinasses has several financial advantages, such as low investment and overall disposal costs, in addition to savings in chemical fertilizer or other fertilizer sources.
for crops. However, this management practice also comes with strong disadvantages that reduce its environmental sustainability due to possible environmental impacts generated. Plants mainly assimilate nitrogen in the form of nitrate. Therefore, most of the nitrogen (85–90%) present in vinasses cannot be directly assimilated by plants, reducing the fertilization potential of untreated vinasses (Fuess and Garcia, 2017). Increased nitrogen content in untreated vinasses leads to high volatilization rates by denitrification increasing N₂O generation (World Health Organization, 2006). Phosphorus displays higher stability compared to nitrogen and can be accumulated on the soil’s surface if regularly applied, making it prone to be transported by runoff during rain events (World Health Organization, 2006). Vinasses typically do not contain significant heavy metal concentrations, but the increased soil acidity caused by the regular application of vinasses can increase the mobility of metals present in the soil, causing the accumulation of metals in receptive waterbodies and groundwater (Fuess and Garcia, 2017).

To reduce transport costs, a common practice for tequila producers is to dispose of the vinasses in their own crop fields (SEMADET, 2019b). Since agave is one of the most cultivated crops within both of the critical regions, a great majority of the irrigated vinasses are disposed of in agave fields. However, agave plants display higher soil erosion rates compared to other crops due to their rainfall-concentrating leaf structure, which leads to higher nutrient and solid transport in runoff coming from agave fields (Abrol and Sharma, 2012). Therefore, counterproductive effects can be seen due to excessive vinasse application on crops, as proposed in scenario A. This is due to changes in soil structure and salinity, nutrient bioavailability and microbial communities (World Health Organization, 2006; Fuess and Garcia, 2017).

Jalisco has a total cultivated Surface of 1,649,784.9 Ha in 2019 (SIAP, 2020), with an estimated fertilizer consumption of 54.79 kg Ha⁻¹ and 25.74 kg Ha⁻¹ of nitrogen and phosphorus, respectively (FAO, 2021). While the fertilizer requirements of Jalisco largely surpass nitrogen and phosphorus production from tequila vinasses, which represent only 0.03 and 2.5% of the total nitrogen and phosphorus demand respectively, the production of vinasses in the Valles and Altos critical regions and the distribution of the generated vinasses for its use in other regions of the state by fertigation may be economically unfavorable due to increased transport costs (Fuess and Garcia, 2014).

### TABLE 7 | Estimated vinasse production rates for the municipalities within the established critical regions.

| Critical region | Municipality | Vinasses (m³ year⁻¹) |
|----------------|-------------|---------------------|
| Valles         | Tequila     | Min 471,707.21      |
|                |             | Mean 660,390.09     |
|                |             | Max 808,640.93      |
|                | Arandas     | Min 143,315.77      |
|                |             | Mean 200,642.07     |
|                |             | Max 245,684.17      |
|                | Arenal      | Min 12,458.97       |
|                |             | Mean 17,442.56      |
|                |             | Max 21,358.24       |
| Total Valles   | Min 627,481.95 |
|                | Mean 876,474.72 |
|                | Max 1,075,683.34 |
| Altos          | Atotonilco  | Min 219,028.59      |
|                |             | Mean 307,060.02     |
|                |             | Max 375,991.86      |
|                | Arandas     | Min 132,919.94      |
|                |             | Mean 186,087.92     |
|                |             | Max 227,862.76      |
|                | Tepatitlan  | Min 47,987.30       |
|                |             | Mean 67,182.21      |
|                |             | Max 82,263.94       |
|                | Jesus Maria | Min 43,549.77       |
|                |             | Mean 60,969.67      |
|                |             | Max 74,656.74       |
| Total Altos    | Min 443,785.59 |
|                | Mean 621,299.82 |
|                | Max 760,775.29 |
| Total          | Min 1,889,754.07 |
|                | Mean 2,645,655.70 |
|                | Max 3,239,578.40 |

Values presented in bold represent the sum of the values reported for each individual municipality.

### TABLE 8 | Pollutant discharge potential values calculated for the established critical regions under scenarios A and B.

| Critical region | Scenario A | Scenario B |
|----------------|------------|------------|
|                | Nitrogen (Mg year⁻¹) | Phosphorus (Mg year⁻¹) | BOD₅ (Mg year⁻¹) | GHG (Mg CO₂eq year⁻¹) | Nitrogen (Mg year⁻¹) | Phosphorus (Mg year⁻¹) | BOD₅ (Mg year⁻¹) | GHG (Mg CO₂eq year⁻¹) |
| Valles         | 19.55      | 0.63       | 14,113.57  | 85.72          | 11.73      | 0.35       | 987.95       | 65,095.88         |
|                | Mean 115.63 | 36.9       | 104,548.83 | 157,330.21     | 69.38      | 20.3       | 7,315.94     | 482,055.73        |
|                | Max 444.8   | 301.2      | 308,791.25 | 465,136.98     | 266.88     | 165.66     | 21,615.39    | 1,424,323.82      |
| Altos          | 13.83      | 0.44       | 9,981.80   | 980.33         | 8.3        | 0.25       | 698.73       | 4,289,560.44      |
|                | Mean 81.78  | 26.1       | 73,941.99  | 111,271.53     | 49.07      | 14.5       | 15,287.45    | 340,933.13        |
|                | Max 314.58  | 213.0      | 218,392.11 | 328,967.37     | 186.75     | 118.38     | 15,287.45    | 1,007,350.71      |
| Total          | 58.88      | 1.89       | 42,505.10  | 1,177.87       | 35.33      | 1.04       | 6,604.89     | 196,045.81        |
|                | Mean 346.24 | 111.14     | 314,686.18 | 473,823.03     | 206.94     | 61.28      | 22,040.49    | 1,451,781.65      |
|                | Max 1,329.57 | 907.11     | 929,707.20 | 1,400,829.35   | 803.74     | 500.13     | 65,097.91    | 4,289,560.44      |

aValles critical region comprehends the following municipalities: Tequila, Arandas, and Arenal.
bAltos critical region comprehends the following municipalities: Atotonilco, Arandas, Tepatitlan, and Jesus Maria.
cTotal sum values for the 125 municipalities within Jalisco.
TABLE 9 | Pollutant discharge potential values calculated for the established critical regions under scenarios C and D.

| Critical Region | Scenario C | Scenario D |
|-----------------|------------|------------|
|                 | Nitrogen (Mg year$^{-1}$) | Phosphorus (Mg year$^{-1}$) | BOD$_5$ (Mg year$^{-1}$) | GHG (Mg CO$_2$eq year$^{-1}$) | Nitrogen (Mg year$^{-1}$) | Phosphorus (Mg year$^{-1}$) | BOD$_5$ (Mg year$^{-1}$) | GHG (Mg CO$_2$eq year$^{-1}$) |
| Valles$^a$      | Min 14.66 0.5 2,822.71 22,928.28 8.8 0.38 197.59 31,705.67 | | | | 52.03 22.14 1,463.68 234,750.20 |
| Mean 86.72 29.52 20,909.77 169,749.33 | | | | |
| Max 333.6 240.96 61,758.25 501,704.40 | | | | |
| Atos$^b$        | Min 10.37 0.36 1,986.36 16,215.99 | | | | 5.22 0.27 139.75 22,423.79 |
| Mean 61.33 20.88 14,788.40 120,054.94 | | | | |
| Max 235.94 170.42 43,678.42 354,829.62 | | | | |
| Total$^c$       | Min 44.16 1.51 8,501.02 69,051.89 | | | | 141.56 127.81 3,057.49 490,686.00 |
| Mean 261.18 88.91 62,972.84 511,225.04 | | | | |
| Max 1,004.67 725.69 185,954.04 1,510,956.51 | | | | |

$^a$Valles critical region comprehends the following municipalities: Tequila, Aramilitan, and Arenal.
$^b$Atos critical region comprehends the following municipalities: Atotonilco, Arandas, Tepatitlan, and Jesus Maria.
$^c$Total sum values for the 125 municipalities within Jalisco.

Scenario B: Aerobic Treatment

The aerobic treatment of wastewater (scenario B) is one of the most common processes applied globally for the treatment of organically polluted wastewater since it has proven to be an effective way to remove both organic matter and nutrients from organic wastewaters (SEMADET, 2019b). A downside of this process is the intensive energy requirement to achieve the aeration rates required for the system to operate properly (Rantala and Väinänen, 1985; Eckenfelder, 1998). This energetic demand increases overall treatment costs (Rantala and Väinänen, 1985; Cakir and Stenstrom, 2005). From the four proposed scenarios, the aerobic treatment (scenario B) had the highest GHG emission estimates with a mean of 1,451,781.65 Mg year$^{-1}$ while having the second lowest nitrogen and phosphorus disposed volumes (208.94 and 61.28 Mg, respectively) (Table 8). GHG production from aerobic systems tends to be proportional to the organic load of the wastewater feed (Cakir and Stenstrom, 2005). Aerobic treatment of highly polluted wastewaters, like vinasses, tends to demand elevated oxygen concentrations in order to allow for the aerobic degradation of organic matter. If operated under non-ideal conditions (low aeration, low mixing, low retention times, etc.), partial anaerobic conditions can be generated within the treatment system, which increases GHG release (Doorn et al., 2006). Since none of the CH$_4$ generated by the aerobic process is captured and combusted, the complete CH$_4$ load is released to the atmosphere, increasing overall GHG estimations for the scenario and increasing the GHG production difference against other proposed management scenarios (Díaz-Vázquez et al., 2020).

Scenario C: Anaerobic Treatment

Scenario C had a mean GHG estimate of 511,225.04 Mg year$^{-1}$ (Table 9), which represents a 96% reduction compared to the values estimated for scenario B. This was due to CH$_4$ combustion and transformation into CO$_2$ rather than direct release as CH$_4$. Although scenario C displayed lower GHG and a significant reduction of the discharged nitrogen and phosphorus load (208.94 Mg year$^{-1}$ and 61.28 Mg year$^{-1}$, respectively) (Table 9), the implementation of individual anaerobic systems requires high investment from producers, limiting its implementation to medium and big producers (Anderson et al., 2013). The implementation of centralized anaerobic digestion systems can offer the possibility to micro and small producers to treat their vinasses through greener alternatives, which bypass the required high initial investments but do not significantly increase treatment costs (Díaz-Vázquez et al., 2020). However, the operation of a centralized anaerobic digestion system can present difficulties due to the heterogeneous nature of the vinasses generated by multiple production units as well as the presence of other pollutants due to non-ideal wastewater management systems within the production units. Alterations in the feed composition can cause changes in the microbial populations within the anaerobic system leading to reduction in treatment efficiency and even complete shutdown of the system (Naik et al., 2014). This heterogeneity in the vinasses can be regulated by strictly monitoring the incoming vinasses in order to prevent undesired pollution and to maintain stable feed conditions to prevent inhibitory or toxic effects on microbial population within the anaerobic digester (Álvarez et al., 2010).

The use of effective nutrient (nitrogen and phosphorus) recovery systems, as proposed in scenarios B, C, and D, not only prevents the excessive discharge of nutrients into the soil and water but additionally presents the opportunity to reduce treatment cost by valorizing the recovered nutrients and allowing for a controlled application of nutrients in crop fields. By concentrating the recovered nutrients in both aerobic and anaerobic sludge, the volume of the nutrient mixture is reduced, simultaneously reducing transport and application costs, which in time allows these recovered nutrients to be applied in fields further from the production site, increasing its economical competitiveness against other fertilizer sources (Fuess and Garcia, 2014; Díaz-Vázquez et al., 2020).

Scenario D: Sequential Anaerobic-Anaerobic Treatment

Scenario D displayed the maximum nutrient (nitrogen and phosphorus) and BOD$_5$ reduction and the third lowest GHG
### TABLE 10 | Comparison between the advantages and disadvantages of the proposed vinasses management scenarios.

| Management scenario | Advantages | Disadvantages |
|---------------------|------------|---------------|
| **Field irrigation (A)** | • Reduced disposal costs Fuess and García, (2014) | • The elevated water content of vinasses limits their transportation for them to be used as fertilizer which leads to its accumulation near production sites Fuess and García, (2017) |
| | • Does not require a large initial investment in infrastructure or equipment Fuess and García, (2014) | • Potential for soil acidification as well as waterbody eutrophication due to nutrient transport in runoff and groundwater Fuess and García, (2014); Fuess and García, (2017) |
| | • Low operation complexity Fuess and García, (2014) | • Low nitrogen fertilizer potential due to high content of organic nitrogen Mengel, (1996) |
| | • If applied according to crop needs, vinasses can be used as a cheap source of nutrients Christofoletti et al., (2013) | • Since there is not BOD$_3$ reduction the complete nutrient and organic load of the vinasses is discharged into soil leading to its uncontrolled degradation and the production of GHG Fuess and García, (2017) |
| | • Can help reduce the state dependency on chemical and imported fertilizer Kanagachandran and Jayaratne, (2006) | • The accumulation of organic matter in soil and receptive waterbodies can lead to the production of foul odors España-Gamboa et al., (2011) |
| | • – | • Water removal processes required for its transport reduce the viability of vinasses as a source of nutrients for crops against other fertilizer sources Christofoletti et al., (2013) |
| | • – | • Excessive application of vinasses on crop fields can present phytotoxic effects Singh and Agrawal, (2008) |
| **Aerobic treatment (B)** | • High nutrient and organic load reduction Chan et al. (2009) | • Aerobic treatment increases overall GHG generation due to higher CH$_4$ production rates compared to field degradation Cakir and Stenstrom, (2006) |
| | • Sludge can be used as fertilizer Nguyen and Shima, (2019) | • Its operation increases treatment costs significantly mainly due to aeration needs Rosso et al., (2008) |
| | • Does not require temperature control Chan et al. (2009) | • High initial investment required for the construction of the treatment infrastructure |
| | • Short start-up periods Chan et al. (2009) | • Typically requires large extensions for the construction of the needed infrastructure Chan et al., (2009) |
| | • Does not require alkali addition for its proper operation Beltrán et al. (2001) | • – |
| | • Low operation complexity | • Nutrient and organic load removal rates lower than those of aerobic treatment systems Chan et al., (2009) |
| **Anaerobic treatment (C)** | • Negligible N$_2$O generation Cakir and Stenstrom, (2005) | • High initial investment required for the infrastructure required for both anaerobic treatment and CH$_4$ revalorization Anderson et al., (2013) |
| | • Higher nutrient content and bioavailability in generated sludge Field et al. (1984) | • Anaerobic systems require long startup periods Chan et al. (2009) |
| | • CH$_4$ capitation systems prevent its release into the atmosphere Cakir and Stenstrom, (2005) | • Anaerobic microorganisms present high sensitivity to feed changes and alteration in the vinasses feed can alter the removal rates as well as the CH$_4$ production within the system McLeod et al., (2015) |
| | • CH$_4$ can be used as an energy source either for thermal or electric energy conversion Rantala and Väänänen, (1985); Eckenfelder, (1998) | • Feeds presenting extreme pH values can reduce the productivity of the system and require pH control Chan et al., (2009), which is the case for vinasses |
| | • Low operational costs especially for wastewater with high organic loads Rantala and Väänänen, (1985); Eckenfelder, (1998) | • Require temperature control in order for the system to operate properly Chan et al., (2009) |
| | • Energetic costs can be greatly reduced and even completely covered by the energetic production using CH$_4$ Rantala and Väänänen, (1985); De Bere, (2000) | • High operation complexity McLeod et al., (2015) |
| | • Smaller areas required for its implementation Franklin, (2001); Chan et al. (2009) | • Typically requires additional treatment processes in order to achieve proper effluent qualities Chan et al., (2009) |
| | • – | • Higher GHG emission than the individual anaerobic treatment due to the addition of the aerobic stage Keller and Hartley, (2003); Cakir and Stenstrom, (2005) |
| **Anaerobic-aerobic sequential treatment (D)** | • Higher nutrient and organic load removal rates than both individual treatment processes Frostell, (1983) | • Highest investment required for the implementation of the infrastructure needed for the operation of the anaerobic-aerobic sequential treatment Chan et al., (2009) |
| | • Maximum nutrient recovery and revalorization potential by the production of nutrient-rich sludge Cervantes et al. (2006) | • Anaerobic systems require long startup periods Chan et al. (2009) |
| | • Excess aerobic sludge can be reprocessed into the anaerobic system Frostell, (1983) | | (Continued on following page)
production out of the four proposed scenarios (156.71 Mg, 66.69 Mg, and 706,984.71 Mg, respectively). The higher GHG production through scenario D in comparison to scenario C can be explained by the addition of an aerobic stage, which slightly increases both CH₄ and N₂O production even when the BOD₅ and nutrient loads entering the aerobic system are reduced by the previous anaerobic stage (Cakir and Stenstrom, 2005). Anaerobic digestion of effluents with high organic loads tends to result in lower overall GHG generated compared to other treatment alternatives, even reaching negative values due to the use of produced biogas for energy generation and the consequent reduction of required energy during the treatment process, contrary to aerobic treatment processes in which wastewaters with a high organic load tend to increase overall GHG generation and energy consumption (Cakir and Stenstrom, 2005). The GHG reduction by CH₄ energetic revalorization is not accounted for in scenarios C and D, meaning both have the potential to produce even lower GHG emission rates.

Table 10 displays a comparison of the reported advantages and disadvantages for each of the management strategies proposed in the present work.

### Integrated Management Approaches

The implementation of effective treatment systems, either aerobic (scenario B), anaerobic (scenario C), or sequential anaerobic-aerobic (scenario D), usually requires large investments, which limit the producers that can afford such investments and the corresponding operation costs (Díaz-Vázquez et al., 2020). The implementation of centralized treatment units allows micro and small productive units to access effective treatment systems reducing the initial investment needed for its implementation. Additionally, TPUs located within urban areas, which is the case of most productive units located within the municipality of Tequila (Valles critical region), allows access to treatment systems that would require offsite construction due to spatial constraints, reducing the required investment and reducing the strain of local wastewater treatment plants caused by vinasse discharge into municipal wastewater systems (Flotats et al., 2009; Massoud et al., 2009).

The logistics required for the operation of centralized treatment units can significantly increase treatment costs, especially in waste with elevated water content, which is the case of tequila vinasses. This needs to be taken into consideration by decision-makers in order to prevent an unnecessary treatment cost increase due to logistics (Díaz-Vázquez et al., 2020). The establishment of centralized treatment units within critical regions allows the guarantee of a constant supply of wastewater to maintain the economic viability of the treatment systems and protect the natural resources and services of sensitive regions from degradation, which is the case for most basins within Jalisco (de Anda and Shear, 2001; Martinez Rivera, 2004; Abrol and Sharma, 2012; Jayne-Torres and Hansen, 2018). This is not only applicable to tequila vinasses but for most primary production wastes and byproducts generated in the state, as is the case of livestock production waste and dairy processing wastewater (Díaz-Vázquez et al., 2020).

Since vinasses are generated by most alcoholic beverage and bioethanol production processes, regions in Brazil, Japan, the United States as well as many countries within the European Union that are known for intensive alcoholic production, face similar problems to those found in Jalisco (España-Gamboa et al., 2011). Several other practices have been proposed globally for the management of vinasses, in addition to the ones proposed in the previously discussed scenarios. Some examples include use as animal feed, treatment by electrocoagulation, coagulation-flocculation and advanced oxidation (Ozone) as well as biorefinery approaches using either bacteria, fungi, or algae for the simultaneous treatment and recovery of metabolites, biomass or energy (Waliszewski et al., 1997; López-López et al., 2010; España-Gamboa et al., 2011; Christofoletti et al., 2013; Mikucka and Zieilińska, 2020). Several novel processes have been developed on a laboratory scale that may offer new alternatives with promising effects on the quality of generated vinasses, as they use hydrolytic enzymes to increase substrate fermentability and decrease the discarded vinasses organic load (Ávila-Fernández et al., 2009; Waleckx et al., 2011). These alternative management practices could be analyzed following the methodology proposed here to assess their environmental sustainability applied to Tequila vinasses. It would be important to pay special attention to the scale and economic viability for the implementation of such practices, as well as to the local and regional context.

The existence of strong producer associations and certification organizations for TPUs at state and national levels can assist in the establishment of centralized treatment units. They can act as intermediaries between policymakers, local authorities, academia, technology suppliers and producers in order to establish the best management practices and coordinate efforts to improve the Tequila production sector and achieve international environmental standards.
CONCLUSION

The proposed methodology integrates both physicochemical characterization and GIS-based spatial analysis in order to evaluate management scenarios for the determination of possible environmental impacts derived from management practices, either current or proposed. This can be a powerful tool for policymakers and local authorities to evaluate and propose local or regional integral waste management programs, policies, and infrastructure. It likewise has the potential to incentivize sustainable practices among productive sectors. This approach can be applied to other regions or other waste-producing sectors in order to determine best management practices in a local and regional context.

The proposed methodology could be improved by the generation of site-specific and waste-specific emission, removal, and conversion factors in order to estimate nutrient and organic load discharge as well as greenhouse gas emissions with higher accuracy based on regional and geographical characteristics, either for environmental (soil and water) degradation of waste or for the evaluation of specific treatment alternatives. It would also be useful to include the integration of multiple organic waste streams into the analysis model. This would open up the possibility to evaluate coprocessing alternatives that may prove to have a more positive environmental impact compared to individual management strategies, especially for dense and highly productive regions, such as the Mexican state of Jalisco.

DATA AVAILABILITY STATEMENT

The raw data supporting the conclusions of this article will be made available by the authors, without undue reservation.

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