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A Joint Computer-Aided Simulation and Water-Energy-Product (WEP) Approach for Technical Evaluation of PVC Production

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Abstract: Recently, polyvinyl chloride (PVC) has emerged as one of the most widely used polymers on the planet due to its versatile mechanical properties and chemical resistance. Suspension polymerization is the most employed method for its production, owing to its ability to control polymer characteristics and cost-effectiveness. However, issues such as water and energy consumption and management in the process have sparked interest in researching the performance and sustainability of the process. In this study, an approach for the technical evaluation of the PVC production process by suspension is proposed, using 11 indicators related to Water, Energy and Product (WEP), based on technical parameters and process simulation for the diagnosis of the process, framed under sustainability criteria. The simulation included the purification and drying stages of the polymer, along with a monomer recirculation stage. The properties of PVC obtained through the process simulation were over 90% accurate when compared to the literature. The technical analysis found that the process has high performance in the handling of vinyl chloride monomer (VCM) and PVC, with a production yield of 99% and an index of reused unconverted material of 99%. On the other hand, there are opportunities for improvement in the process, related to water usage management, since the indicator of wastewater production was 80% and the fractional water consumption was 1.8 m^3/t. Regarding energy use, the process exhibits high consumption and an energy-specific intensity of 4682 MJ/t of PVC, but it has a low overall cost due to the use of natural gas in some stages of the process.

Keywords: CAPE; particle size control; process simulation; suspension PVC; sustainability; WEP evaluation

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1. Introduction

PVC is the third most prevalently utilized polymer globally [1], attributable to its cost-effectiveness and advantageous properties such as durability, flexibility and versatility [2]. Primary applications include the construction industry (pipes, doors and window frames), coatings, textiles, food packaging, healthcare-related materials, electrical insulation, automobiles and common objects such as toys and credit cards [3]. Approximately 80% of worldwide PVC production is performed via suspension polymerization, occurring within VCM droplets containing a dispersed initiator in an aqueous suspension with stabilizers, under continuous agitation at a constant temperature. The reaction is highly exothermic (100 $kJmol^{-1}$) and yields an insoluble polymer within the VCM, resulting in a multiphasic system [4]. This production methodology is characterized by high productivity, flexibility in polymer composition, enhanced control of operations and favourable economic returns [5].

Computer Aided Process Engineering (CAPE) is a multidisciplinary tool focused on the management and development of mechanisms that can recreate reality under specific conditions using software. It allows the saving of resources and time, as well as the analysis of process behavior in response to changes and perturbations (operative or not).

CAPE promotes the development of a variety of molecular, genetic and thermodynamic phenomenon-based systems, products and processes at different scales (molecular to industrial). CAPE is applicable across multiple scales (molecular, pilot and industrial) via modelling, synthesis, design, control, optimization and problem solving domains encompassing products, processes, and associated sustainability changes [6].

Since the establishment of the Sustainable Development Goals (SDGs) by the United Nations (UN), new regulations and laws have increased the pressure on the industrial sector to adapt its systems to operate in a greener and more intelligent way [7]. Diagnosis, assessment and optimization have turned into important tasks in process lifetime and help to improve the sustainable performance of chemical processes. In this matter, the suspension PVC process has serious environmental problems associated with intensive energy usage, high water consumption and emission of toxic substances and greenhouse gases, among others [8].

Process modeling has been applied in some studies to analyze PVC suspension process production, primarily focusing on the modeling of the polymerization reaction, as the operating conditions of this stage critically influence the polymer's characteristics and properties. Various aspects of the reaction have been studied, ranging from kinetics and thermodynamics to process control and others. Methods to model the complexity of the phenomenon, such as those suggested by Bárkányi et al. [9], have proposed a population-balanced model using the Monte Carlo method in MATLAB software to study the effects of agitation conditions on droplet formation.

Kiparissides et al. [10] developed an integrated multiscale, multiphase model to describe the dynamic operation of PVC suspension polymerization and the properties of the polymer generated in a batch reactor through a detailed mathematical formulation of macro/microscopic phenomena and a population balance model. Kiparissides et al. [11] also developed software to model the dynamic behavior of suspension polymerization in a batch reactor using a mathematical approach considering reaction kinetics, thermodynamics and reactor parameters such as geometry and controllability.

In other studies, the focus shifted the extent of the models to include the tank suspension system and reactor controllability. Lewin analyzed the effects of cooling and initiator loading (two initiators) on operation and polymer quality in suspension polymerization in a batch reactor using mathematical models adjusted with plant operation data. [12]. Mejdell et al. [13] applied a rigorous model to study the cooling system of an industrial-scale PVC polymerization reactor using the method of characteristics. This model focused on predicting conversion and reaction kinetics through heat balance.

Miller et al. modelled the temperature control system of a PVC suspension reactor using a nonlinear triple cascade system in order to examine its ability to maintain the reaction temperature [14]. Zhang et al. [15] developed a mathematical method to study the polymerization process of industrial suspension polymerization reactors for vinyl chloride, taking into account the properties and conditions of both the polymer and the reactor. Wieme et al. [16] developed a model for the comprehensive study of operational conditions (kinetics, thermodynamics, heat transfer and PID control) of a suspension polymerization reactor at laboratory and industrial scale.

Regarding simulation of stages beyond the reactor (downstream), or complete processes, commercial simulators have been effective tools to reproduce petrochemical processes. Hoa et al. [17] used Designer software to simulate the s-PVC process (118 t/day and 90% conversion) with VCM removal and the drying stage but without reusing unreacted VCM. Beltrán [18] carried out the design and simulation of a PVC production plant with an annual capacity of 56,000 tons and an 85% conversion using Aspen Plus. The process includes VCM removal and drying stages; however, the unreacted VCM is not treated. Mangili et al. [19] simulated the VCM production process in Unisim software along with an evaluation of the water consumption index. For the process utility systems (liquid and vapor), Astorayme et al. [20] used CAPE to simulate a plant producing VCM and PVC by suspension. The process was simulated in Unisim, with a capacity of 200,000 tons of PVC per year.

Karasek et al. [21] used Aspen Plus to simulate two VCM production processes to produce 5 tons of VCM per hour, one through direct chlorination of ethylene and another with oxychlorination of ethylene using hydrogen chloride (HCl).

Considering the above, it is evident that to date, there are no studies in the literature that perform simulation and technical evaluation based on WEP indicators of an industrial-scale PVC suspension production process, including residual VCM purification and water removal stages. Therefore, this work aims to use CAPE to evaluate a PVC suspension production process at an industrial scale combining process simulation and 11 technical indicators related to water use, energy use and unconverted material use, including production yield, fractional water consumption and energy specific intensity among others.

2. Methods

Figure 1 illustrates the approach proposed in this work for the technical evaluation of the PVC suspension production process, based on four components: the simulation of the process using specialized software in the first stage, which is fed by a preliminary material balance, preliminary economic information for water and energy and the properties of the chemical species involved in the process (Figure 1). In this stage, the equations of the stage and solution models are selected according to the nature of the process in order to calculate the thermodynamic properties of pure substances and mixtures to obtain the extended mass balance and energy balance. After that, the simulation is validated by comparing the properties of intermediates and products with experimental information. As a result of the simulation and validation of the results, information about the process related to water, energy and products is obtained and eight process parameters are calculated: product-related parameters are the flowrate of products, flowrate of waste and flowrate of unconverted material; the water-related parameter is the flowrate of wastewater; and the energy-related parameters are energy flow, energy consumption, natural gas consumption and electricity consumption. With these parameters, in the third stage, eleven technical indicators that will allow diagnosis of the process are calculated, two of them related to the product (production yield and index of reused unconverted material), three of them related to water (fractional water consumption, total cost of freshwater and wastewater production ratio) and six of them related to energy (total cost of energy, energy specific intensity, net energy ratio, energy usability index, natural gas consumption index and electric energy consumption index). For the fourth stage, upper and lower technical limits were defined for each indicator based on characteristics of the production process and, based on those limits, an evaluation of the performance of the indicators was made on a percentage basis.

2.1. Process Description

In general terms, the PVC suspension production process includes a reaction section, a residual VCM recovery section, a VCM purification section and a PVC drying section. In the Supplementary Material, Figure S1 shows the block diagram of the topology to be simulated and evaluated by technical indicators.

The polymerization zone typically consists of several reactors (with sizes ranging from 50 to 200 m^3) that normally operate in batch mode (4–8 h) and in parallel, at a temperature of 70 °C and a pressure of 10 kg-f cm^{-2}. A stream of liquid VCM (stream 5) enters the reactors at room temperature and a pressure of 4.5 kg-f cm^{-2}, containing fresh VCM (stream 1) and recirculated VCM (stream 14), along with demineralized water (stream 2) at 3.5 kg-f cm^{-2} and 85 °C, dissolved polyvinyl alcohol (PVA) (stream 3) at 20% and 3-hydroxy-1,1-dimethylbutane-2-ethyl-2-methylheptane peroxide as initiator (stream 4) dissolved at 20%, both at 10 kg-f cm^{-2} and 32 °C. The polymer is produced within the VCM droplets with the help of the initiator within a water suspension and the stabilizer (PVA) under agitation at a constant temperature. This reaction is exothermic, so the excess energy must be removed and the reaction conversion is usually around 80% to 90%. The generated

PVC enters a new phase, as it is not soluble in the VCM, and forms particles of different sizes. At the end of the reaction, a heterogeneous mixture, known as slurry and containing the suspended PVC, unreacted VCM, water, initiator and PVC, is obtained. This mixture is at a pressure of 3.5 kg-f cm^{-2} and a temperature of around 70 °C. The slurry stream (stream 6) leaving the reactor has a high residual VCM content that must be removed due to its high toxicity; according to international regulations, the VCM content in the polymer must not exceed 1 ppm. To purge the monomer, a gasification stage is used, where the pressure is reduced to 1.8 kg-f cm^{-2}. This change in pressure allows the unconverted VCM to separate from the liquid phase of the suspension (around 95%). Subsequently, the resulting liquid stream (stream 8) retains a fraction of the VCM (5%) which must be removed; the stream enters a stripping column consisting of a tray tower (21 trays), in which a stream of high-pressure steam (stream 15) generated in a boiler enters from the bottom at a high temperature (225 °C) and pressure (14 kg-f cm^{-2}) and carries the VCM from the mixture falling through the tower, resulting in an overhead stream (stream 9) rich in VCM and a bottom stream free of VCM (stream 16) with less than 1 ppm of the monomer.

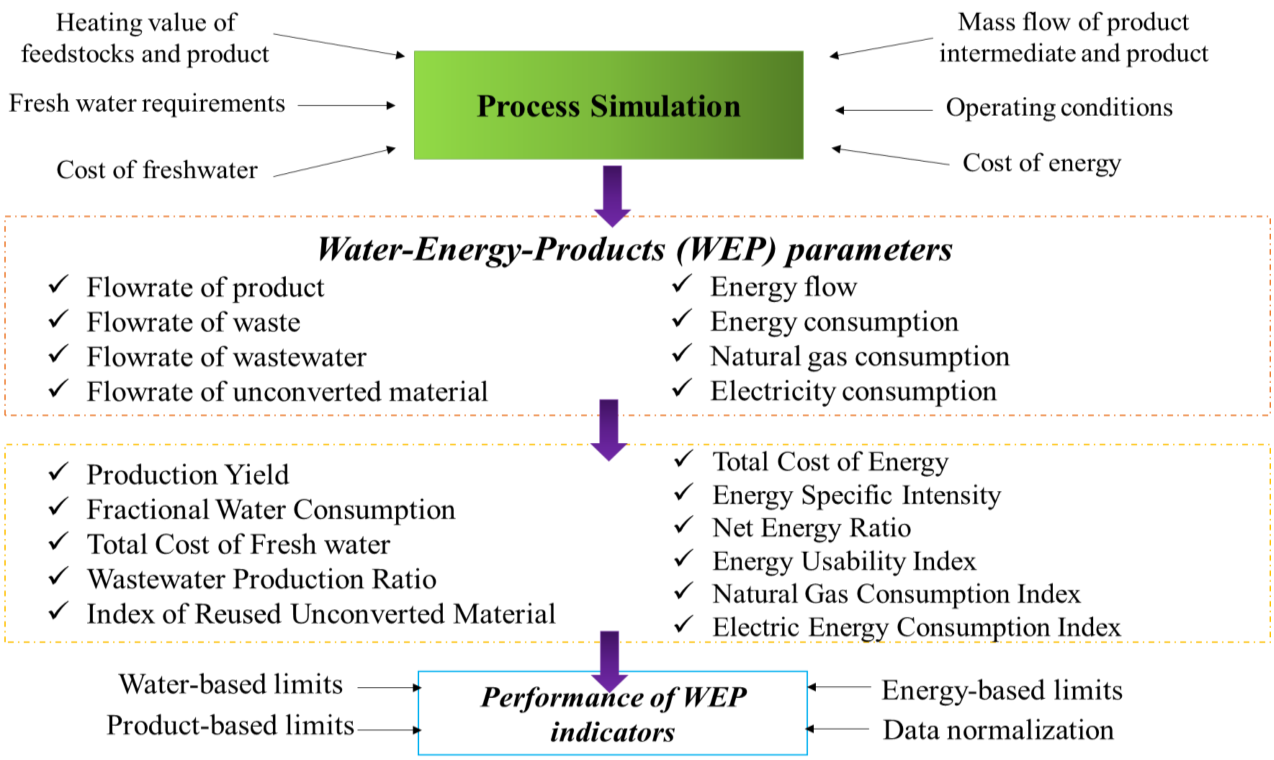

Figure 1. Systematic method for the technical evaluation of the PVC suspension production process.

The VCM-rich overhead stream (stream 11) enters the residual monomer recovery system, which consists of a series of compressors and heat exchangers that condition the residual VCM for recirculation (removal of water and conversion of the VCM to a liquid state). This stream first enters a heat exchanger to be cooled to 50 °C, then passes through a vacuum pump (compressor) that brings the vapor to the saturation point before entering a condenser and separating the water (stream 13) from the MVC gas stream. Next, the gas streams exiting the condenser (stream 15) and the gasification stage stream (stream 7) enter a compressor and are brought to a pressure of 3.5 kg-f cm^{-2} to be conditioned near the VCM saturation pressure, making it easily condensed through a heat exchanger and recirculated to the process (stream 18). The bottom stream (stream 19) from the stripper, containing the monomer, is mostly water (approximately 70%) that needs to be removed. The suspension enters a centrifuge spinning at 1800 rpm, where about 75% of the water in the slurry is removed. The residual water stream (stream 20) carries PVC fractions, almost all PVA and the initiator. The product stream (stream 21) exiting the centrifuge is in the form of a wet paste that must be dried. In the drying stage, the remaining moisture inside the PVC is removed by an air stream (stream 24) that is collected and heated to approximately 250 °C; this is done in a dryer where the streams are mixed, reaching a temperature of 70 °C at the end of the operation. The resulting moisture content of the polymer stream that leaves the dryer is 0.01% by weight [22].

The stream exiting the dryer is a gas stream (stream 25) consisting of air, vapor and entrained PVC particles. To separate the dry polymer from the residual gas mixture, a cyclone is used, which operates at atmospheric pressure conditions (1.03 kg-f cm^{-2}). In this stage, the solid particles of the dry polymer are removed from the gas phase by the inertia of the particles. The stream exiting the top (stream 26) is air and water vapor along with polymer fractions (0.2% of the total produced) and the bottom stream (stream 27) is the dry and granulated PVC with 0.01% of water.

2.2. Computer Aided Process Simulation

For the simulation of the PVC production process by suspension, Aspen Plus v12 software was used. This is a sequential modular software widely used due to its ease and robustness in handling topics related to industrial-scale processes, allowing work with a large number of operations, chemical substances, mass and energy streams, among others [23].

For the reactor, the *rstoic* model was selected, which allows the simulation of the reactor from a macroscopic viewpoint. The model works based on calculations derived from mass and energy balances, using data such as conversion and stoichiometric reaction relationships. The stoichiometric polymerization reaction is defined as n mass units of VCM converting into one mass unit of PVC, as shown in Equation (1).

$$\mathrm{n(VCM)} \rightarrow \mathrm{(PVC)n} \tag{1}$$

The reaction has an 80% conversion and occurs at a temperature of 70 °C and a pressure of 10 kg-f cm^{-2}. For the polymer characterization, the polymerization degree of PVC is needed, with a value of 1000 and a polydispersity index of 2. The reactor is designed to represent the operation of 8 jacketed tanks with a volume of 70.5 m^3, working in cycles between 4 and 5 h long (48 cycles/day). The reactor follows the following proportionality relationships: 1 t of water/1 t of VCM and for the initiator and stabilizer, 1 kg/t of VCM for both [24].

For gasification, the standard model for instantaneous vaporization separators was used, in which the most volatile compound is separated from the stream by changing the pressure (in this case, the VCM). The stripping column was simulated using the simulator's *radfrac* model since it is the only scheme that allows the simulation of gas absorption with a mass carrier such as steam, which is heated in a boiler using the standard heat exchanger model for simplicity. For this tower, the conditions used in the work of Carmona et al. [25] were applied: 21 plates, a pressure of 1.02 kg-f cm^{-2}, counter-current operation (steam enters at the bottom and the suspension enters at the top) and without the presence of a reboiler or condensers. For the centrifugation stage, the general centrifuge model was selected, which uses a *solid separator* method to separate part of the water from the suspension. This is done by knowing the desired water content for the product stream and the operating conditions of the stage. The dryer was simulated using the software's standard dryer model and the centrifuge uses a shortcut method, considering the water content of the solid at the entrance and the desired content at the exit (0.01%).

For the MVC purification stage, the standard compressor and condenser models were used. Both use simplified mass and energy balance methods to calculate the conditions of the streams. For the compressors (vacuum pump, compressor and blower), the isentropic method was selected, which adjusts to an isentropic regime and only requires the outlet pressure. Moreover, the vacuum pump was operated as a standard compressor, considering only the discharge pressure and omitting the vacuum generation. All temperature change units (coolers, condensers, boilers, burners, etc.) were simulated using the heat exchanger model, which only needs the outlet temperature and pressure to calculate the changes in the energy content of the streams; it also allows the separation of insoluble compounds with water in liquid phase mixtures such as free water. Table 1 lists the conditions used for simulating the process, with mass flows in t/day, temperature in °C and pressure in kg-f cm^{-2}.

Table 1. Summary of the conditions of the PVC production process by suspension at a large scale.

Stage	Variable	Value	Reference
Reaction	Temperature (°C)	70	[10]
	Pressure (kg-f cm^{-2})	10	[10]
	Flowrate of MVC (t/day)	1440	Calculated
	Flowrate of fresh water (t/day)	1440	Calculated
	Reaction	n(VCM) → (PVC)n	[17]
	Conversion (%)	80	[15]
	Polymerization degree	1000	Assumed
MVC removal			
Gasification	Pressure (kg-f cm^{-2})	1.8	Calculated
	Final percentage of MVC (%)	5	Calculated
Stripping	Pressure (kg-f cm^{-2})	1.03	[25]
	Final percentage of MVC (%)	<0.01	[26]
	Flowrate of vapor (t/day)	20	Calculated
	Temperature of vapor (°C)	225	[25]
	Pressure of vapor (kg-f cm^{-2})	14	[25]
	Number of plates	21	[25]
PVC Drying			
Centrifuge	Pressure (kg-f cm^{-2})	1.03	Calculated
	Flowrate of water removed (t/day)	1136	Calculated
	Percentage of water removed (% w/w)	75	[25]
Drying	Temperature (°C)	70	[25]
	Flowrate of hot water (t/day)	6231	Calculated
	Final percentage of water (%)	0.01	[25]
	Flowrate of vapor (t/day)	367	Calculated
Cyclone	Separation efficiency	0.99	Calculated
	Flowrate of gases separated (t/day)	6898	Calculated
Purification of residual MVC			
Cooler	Final temperature (°C)	50	Calculated
Vacuum pump	Pressure of discharge (kg-f cm^{-2})	2.5	Calculated
Condenser 1	Final temperature (°C)	50	Calculated
Compressor	Pressure of discharge (kg-f cm^{-2})	3.5	Calculated
	Mass flow of MVC (t/day)	288	Calculated
Condenser 2	Final temperature (°C)	8	Calculated
	Flowrate of water separated (t/day)	18	Calculated

2.3. Technical Evaluation of the Process

Figure 1 shows the stages of the technical evaluation of processes involved; in this methodology, 11 indicators for describing process performance are quantified using the equations displayed in Table 2, which shows the indicator, the equation for the calculation and their description. These indicators are based on aspects such as material use, energy use and water and energy costs of the process from the simulation. Additionally, these indices allow us to establish assessments that serve as a reference for more detailed process engineering studies (benchmarking) [6].

Table 2. Description of technical process indices.

Variable	Units	Description	Equation
Production Yield	%	Amount of product obtained per unit of feedstock	$\gamma_i = \frac{\text{mass flow of product}}{\text{mass flow of main feedstock}} \times 100\%$
Fractional Water Consumption (FWC)	m^3/t	Volume of water consumed to obtain the products	$FWC = \frac{\text{volume flow of freshwater}}{\text{mass flow of product}}$
Total Cost of Freshwater (TCF)	$/day	Toral cost of fresh water consumed per unit of time	$TCF = \text{flowrate of freshwater consumed} \times \text{cost of freshwater}$
Wastewater Production Ratio (WPR)	%	Quotient between the amount of fresh water required by the process and the wastewater produced	$WPR = \frac{\text{wastewater volumetric flow}}{\text{freshwater volumetric flow}} \times 100$
Index of Reused Unconverted Material (IRUM)	%	Percentage of raw material reused with respect to the flowrate of unconverted raw material	$IRUM = \frac{\text{reused material i mass flow}}{\text{unconverted material i mass flow}} \times 100\%$
Total Cost of Energy (TCE)	$/day	Total cost of energy consumed per unit of time	$TCE = \text{total energy consumed} \times \text{cost of energy}$
Energy Specific Intensity (ESI)	MJ/t	Energy consumed per tonne of product	$R_{ESI} = \frac{\text{total energy consumed}}{\text{product mass flow}}$
Net Energy ratio (NER)	Dimensionless	Quotient between the energy content of the products and energy enters the process	$NER = \frac{\text{product calorific power} \times \text{product mass flow}}{\text{total consumed energy} + (\text{feedstock calorific power} \times \text{feedstock mass flow})}$
Energy Usability Index (EUI)	Dimensionless	Quotient between the energy content of the products and the energy required for its production	$EUI = \frac{\text{product calorific power} \times \text{product mass flow}}{\text{total consumed energy}}$
Natural Gas Consumption Index (NGCI)	m^3/t	Amount of natural gas consumed per tonne of product	$NGCI = \frac{\text{total natural gas consumed}}{\text{product mass flow}}$
Electric Energy Consumption Index (EECI)	kWh/t	Amount of electric energy consumed per tonne of product	$EECI = \frac{\text{total electricity consumed}}{\text{product mass flow}}$

For the fourth stage, the indicators obtained in stage three are compared to obtain a first general overview of how this process performs in relation to defined goals with values showed in Table 3. The analysis is carried out by normalizing the technical indicators using reference parameters (best and worst scenarios).

Additionally, the Energy Usability Index (EUI) was established as a benchmark index for energy capacity if the product is used as fuel, considering that the main use of PVC is not for energy purposes. This is done in view of the new trends in generating energy from plastic waste (PtE, polymer to energy). For the NER and EUI, the higher heating value (HHV) values of substances such as PVC and MVC were considered.

Table 3. Description of technical indicators and their reference values.

Variable	Worst Case	Best Case
Production Yield	0%	100%
Fractional Water Consumption (FWC)	4 m^3/t	0.5 m^3/t
Total Cost of Fresh Water (TCF)	1.3 $/$m^3$	0.1$/$m^3$
Wastewater Production Ratio (WPR)	100% of water utility	0% of water utility
Index of Reused Unconverted Material (IRUM)	0% of unconverted material	100% of unconverted material
Total Cost of Energy (TCE)	0.41 $/kWh (100% of the energy consumed comes to electric energy)	10$/MMBTU (100% of the energy consumed comes from natural gas)
Energy Specific Intensity (ESI)	5000 MJ/t	3500 MJ/t
Natural Gas Consumption Index (NGCI)	0%	100% of the energy entering the process
Electric Energy Consumption Index (EECI)	100%	0% of the energy required

3. Results

3.1. Simulation of the PVC Production Process by Suspension

Table 4 shows the compounds selected for the simulation. The process is designed to produce a standard polymer without additives, with the same specifications as PVC k67. The suspension stabilizer chosen was 71% hydrolyzed-PVA and the initiator selected was 3-hydroxy-1,1-dimethylbutane-2-ethyl-2-methylheptane peroxide, along with compounds such as water, in addition to nitrogen and oxygen to simulate air. On the other hand, considering that the process involves polymers, the simulator needs not only the polymer or the monomer, but also the so-called live segments and termination segments, which are part of the polymerization reaction kinetics and allow for product characterization.

Table 4. Compounds used in the simulation of the PVC production process by suspension.

Compound	Type	Formula
Vinyl chloride	conventional	C_2H_3Cl
Polyvinyl chloride	polymer	$(C_2H_3Cl)_n$
Polyvinyl alcohol	conventional	$[CH_2CH(OH)]_n$
Water	conventional	H_2O
3-hydroxy-1,1-dimethylbutane-2-ethyl-2-methylheptane peroxide	conventional	$C_{16}H_{32}O_4$
Nitrogen	conventional	N_2
Oxygen	conventional	O_2
Vinyl chloride-r	segment	C_2H_3Cl
Vinyl chloride-e	segment	C_2H_3Cl

For the selection of property models, their ability to calculate the properties of polymers was considered. In this case, Aspen Plus software has exclusive models for reactions involving polymers. On the other hand, the process pressure and temperature conditions were considered, with the knowledge that there are both moderate and high pressures along with high temperatures. Considering these conditions, the POLY-NRTL-SRK model was selected. This model is characterized by its extension of the standard Non-Random-Two-Liquid (NRTL) model to systems with polymers, adding calculations of the contributions of polymer segments, using models such as Van Krevelen's for the calculation of properties based on the contribution of functional groups, among others. For the gas phase, the Soave–Redlich–Kwong equation of state was used, which adequately predicts the behavior of common and organic gaseous substances such as short-chain hydrocarbons, as well as working appropriately under variable conditions (high and/or low pressure and temperature) [27].

In the simulation shown in Figure 2, streams 2, 3, 4 and 5, which correspond to demineralized water, PVA, the initiator and the VCM, respectively, enter the reactor (REACTOR). Stream 2 enters at a temperature of 85 °C and a pressure of 4.5 kg-f cm^{-2}; the established temperature allows preheating the suspension before starting the reaction. Stream 3 and stream 4 are aqueous solutions, with the PVA stream at 5% and the initiator stream at 50%. Both substances enter at a temperature of 32 °C and a pressure of 10.2 kg-f cm^{-2}. Stream 5 is the mixture of stream 1, which is fresh VCM, with stream 17, which is recirculated VCM from the residual VCM purification zone; it is approximately 80% fresh and 20% residual at an approximate pressure of 5 kg-f cm^{-2} and 32 °C. The valve (VAL) maintains the outlet pressure of the reactor effluents at 3.5 kg-f cm^{-2} [28].

For the gasification stage (GASIF), the pressure decreases to a value of 1.8 kg-f cm^{-2} to remove 95% of the unreacted VCM. The gaseous stream 8 mainly contains the VCM, but it also carries some water (18 t/day) and very small fractions of initiator and PVA (less than 1% for both). The purged stream 9 is in the liquid phase and contains approximately 600 ppm of VCM, which must be reduced to less than 1 ppm. Stream 9 enters the stripper to remove the remaining 99% of VCM from the suspension, using a 225 °C steam stream entering at the bottom of the tray column (21 trays). The steam stream, generated from raw water in a boiler (BOILER), enters the bottom of the tower with a flow of 20 tons of steam per hour at 225 °C and a pressure of 14 kg-f cm^{-2}. This stream is counter-current to the suspension stream entering at the top. This column has a pressure of 1.02 kg-f cm^{-2}.

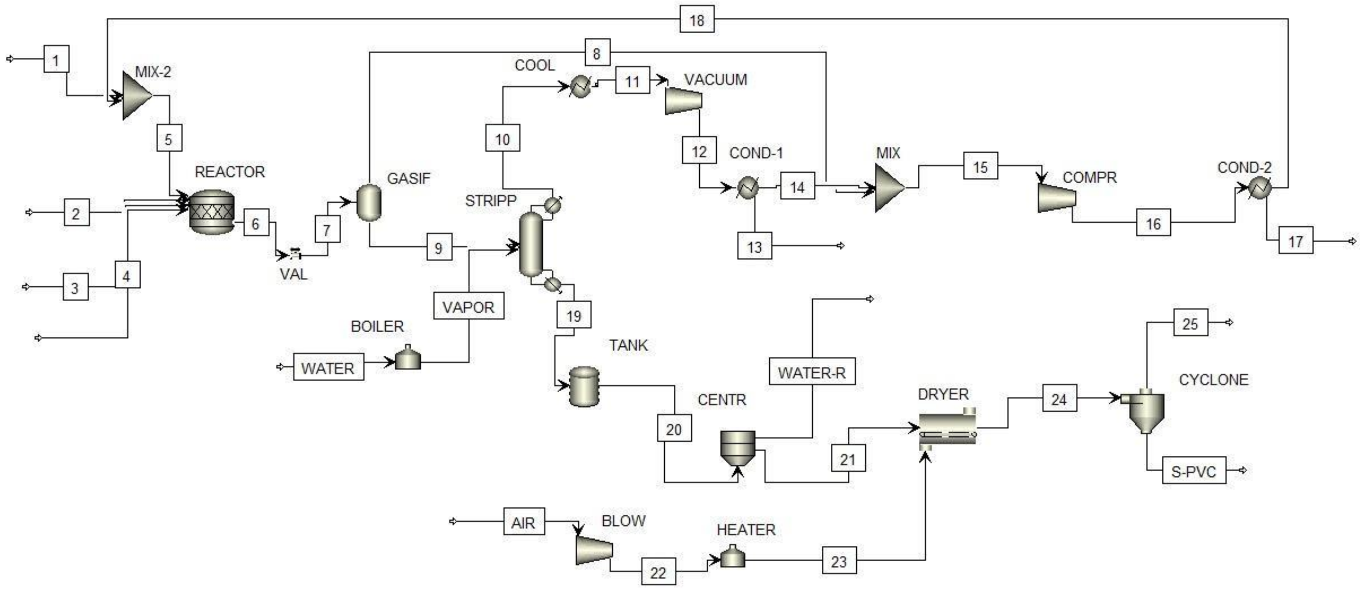

Figure 2. Simulation diagram of the PVC suspension production process.

Stream 10, exiting at the top of the stripper, enters the conditioning zone of the residual VCM stream where it first enters a cooler (COOL) to lower the temperature to 50 °C, while maintaining the quality of the gases entering the compression system. Stream 12 passes through a vacuum pump (VACUUM), which sucks gases from containers (gasification tanks) and expels them at a certain pressure to reduce pressure changes in other equipment, with a discharge pressure of 2.5 kg-f cm^{-2}. The compression of the gases generates an increase in temperature, so stream 13 enters a condenser (COND-1) to maintain the temperature at 50 °C and separate water fractions from the gaseous stream before entering the compressor along with the stream exiting the gasification stage (stream 8). The water-free stream 14 and stream 8 pass through a compressor (COMPR) that raises the pressure of the VCM to close to its saturation pressure and then to a heat exchanger (COND-2) to condense at 8 °C. Additionally, if there is still water in the residual VCM stream, it is purged (stream 18) as it is not soluble in the VCM, and stream 17 is recirculated to the beginning of the process at a pressure of 3.5 kg-f cm^{-2} and 8 °C.

Stream 19, when exiting the bottom of the stripper, enters a tank that allows the suspension to rest and reduce its temperature to 65 °C, which is done to protect the polymer and adapt it for the centrifugation stage. In the centrifuge (CENTR), 75% of the water is removed from stream 20. This unit generates the largest amount of wastewater (WATER-R) in the process and contains a large portion of the PVA and initiator. Stream 21 has a moisture content of 25% when entering the dryer (DRYER); the remaining moisture is removed using a hot air stream at 250 °C coming from a burner (HEATER) and a blower (BLOW) with a flow of 6360 t/day. This stream leaves the polymer with a water content of 0.01% by weight. Stream 24 exits the dryer as a mixture of hot gases and dry polymer that needs to be recovered, so it is introduced into a cyclone. The cyclone separates the gaseous phase from the dry polymer particles and from this unit, stream 25 is formed, which consists of air, steam and some traces of polymer, along with a stream of dry, granular polymer (S-PVC) containing traces of VCM and water necessary to maintain the product's structure.

From the information in Table 5, it can be said that the WATER-R stream contains 60% of the water entering the process, along with most of the initiator and PVA; the steam stream has the highest pressure in the process at 14 kg-f cm^{-2} and is used to recover the VCM; stream 21 has the highest temperature in the process at 250 °C and is composed of air that exits the process at 70 °C in stream 23. This stream has remnants of PVC that could be recovered. Additionally, the product stream (S-PVC) has a minimal VCM content, which, according to international regulations [26], must be less than 5 g of VCM per ton of S-PVC, as VCM is a highly toxic compound. This allows PVC to be used for medical applications. The production capacity of the simulated plant is comparable to some industrial chemical plants that produce PVC (400,000 tons annually), such as the Vestolit plant in Germany that produces 415,000 tons of PVC per year [29], the Qihua plant of ChemChina that produces 380,000 tons annually [30] and the Westlake Chemical plant in Calvert City, Kentucky with a capacity of 650,000 tons per year [31].

Table 5. Operating conditions of the main process streams.

Stream	1	2	3	4	5	18	20	25	VAPOR	23	WATER-R	S-PVC
T-°C	32	85	32	32	32	8	60	70	225	250	65	70
P-kg-f cm^{-2}	3.5	3.5	10.2	10.2	5	3.5	1.03	1.03	14	1.03	1.03	1.03
Flowrate-t/day	1152	1440	8.64	1.73	1440.11	288.11	2667.87	6610	480	6230.53	1136.62	1150.54
Composition in mass fraction												
MVC	1	0	0	0	0.99	0.99	0	0	0	0	0	0
PVC	0	0	0	0	0	0	0.431	1×10^{-3}	0	0	2×10^{-3}	0.98
PVA	0	0	0.2	0	0	0	0	0	0	0	1×10^{-3}	3.7×10^{-4}
Water	0	1	0.8	0.8	3.9×10^{-4}	3.9×10^{-4}	0.568	0.055	1	0	0.998	0.010
Initiator	0	0	0	0.2	0	0	1×10^{-4}	0	0	0	2×10^{-4}	7.4×10^{-5}
Nitrogen	0	0	0	0	0	0	0	0.669	0	0.71	0	0
Oxygen	0	0	0	0	0	0	0	0.273	0	0.29	0	0

The validation of the simulation was performed to demonstrate the accuracy of the simulation development compared to the literature-reported information. For comparison, properties that the software could calculate under the models were selected. Many other representative properties of commercial polymers can only be obtained through laboratory-scale tests. Properties chosen for validation were density, heat capacity, thermal conductivity, glass transition and melting temperatures. All properties are taken at the temperature at which the polymerization was performed, which was 70 °C for this work.

The results in Table 6 show that the simulation predicts the properties of the PVC with high accuracy. Important values in the process to ensure proper operation, such as glass transition and melting temperatures, had accuracies higher than 94%. Density, despite being a complex property because it depends on many factors determined in the reaction stage, such as polymer crystallinity, particle size and temperature, etc., reached an accuracy higher than 90% compared to the PVC density value at 25 °C. This indicates that the considerations made to the reaction system and reactor were adequate (selection of compounds and segment specification). On the other hand, thermal properties show results very close to those in the literature (97% and 91%), which depend heavily on polymer structure and temperature, confirming that the thermodynamic models were appropriately chosen since they consider the contribution of monomers that make up the polymer and its chemical structure.

Table 6. Comparison of properties of PVC and their accuracy.

Variable	Unit	Literature	Simulation	Accuracy
Density	Kg m^{-3}	1.368–1.453 [32]	1502.09	90.2%
Heat capacity	$Jkg^{-1}K^{-1}$	1.313 [32]	1285.18	97.9%
Thermal conductivity	$Wm^{-1}K^{-1}$	0.158 [33]	0.144	91.3%
Glass transition temperature	°C	73–80 [33]	76.88	94.7%
Melting temperature	°C	228.85 [33]	236.57	96.2%

3.2. Technical Evaluation of the PVC Production Process by Suspension Using WEP Indicators

In Table 7, the Water–Energy–Products parameters used for the technical analysis of the process are shown. For this, the input streams of raw materials, such as VCM, and other substances used in separation stages, such as steam, air, or water used to make the suspension and separation operations, were considered. These streams influence how the process manages basic resources. Additionally, the amount of product generated is used to determine how efficient the process is using energy or raw materials to produce it. For this table, the VCM was considered the only raw material because it is the only compound that undergoes chemical transformation, unlike water, which is only a mass and thermal carrier.

Table 7. Process parameters related to WEP utilization in the PVC production process by suspension.

Parameter	Unit	Description	Value
Mass flow of raw material (VCM)	t/day	total flow of VCM entering the process	1158
Mass flow of product	t/day	total flow of PVC leaving the process	1150
Mass flow of recycled raw material	t/day	total flow of VCM being recycled to the process	288
Total volumetric flow of water	m^3/day	volume of fresh water used in the process	1933
Total volumetric flow of wastewater	m^3/day	volume of fresh water used in the process	1552
Total mass feed flow	t/day	total flow of substances entering the process including water, reactants, etc.	9313
Total energy consumed	GJ/day	total energy used during the process (includes cooling and heating)	5327.8

Table 8 shows the summary of technical WEP indicators obtained for the PVC suspension production process. The process yield and the index of reused material were considered for describing the use of raw materials. The obtained production yield (98.8%) is high, which is primarily due to the high conversion of the VCM to the polymer in the reaction zone. Additionally, the units in the PVC purification stages have high separation efficiencies, due to the difference in the chemical properties of the polymer compared to other substances in the process, which allows for minimal polymer loss in process sub-streams. Saeki et al. [5], confirms that the PVC production process is characterized by being mature technology, which means that a wide range of knowledge has been developed that allows for reliable production with high yields. Additionally, the yield obtained by this process is higher than the yield obtained by the simulation performed by Hoa et al. [17], which was 90%. This difference is due to the process benefiting from the recirculation of residual VCM (288 tons), reducing the amount of fresh VCM entering the process. On the other hand, the index of reused material of the process is high (99%), this indicator was applied mainly to VCM, which is the raw material of the process. This value is mainly due to the conditioning and recirculation system of the unreacted VCM from the polymerization stage (288 tons) and the system has a high separation efficiency, allowing the VCM to be separated from water without any observable loss.

Table 8. Results of the technical evaluation of the process.

Indicator	Unit	Value
Production Yield	%	98.8
Wastewater Production Ratio (WPR)	%	80
Fractional Water Consumption (FWC)	m^3/t	1.8
Total Cost of Fresh Water (TCF)	$/year	693,080
Index of Reused Unconverted MateriaL (IRUM)	%	99
Natural Gas Consumption Index (NGCI)	m^3/t	59.4
Electric Energy Consumption Index (EECI)	kWh/t	1.01
Energy Specific Intensity (ESI)	MJ/t	4681.8
Total Cost of Energy (TCE)	$/year	13,552,846
Net Energy Ratio (NER)	-	0.7
Energy Usability Index (EUI)	-	7.4

The index of reused material was not extended to water because it is not transformed but is used as a reaction medium and it is an important resource. Therefore, fractional water consumption and water usage indicators were established to describe how the process uses fresh water. In Table 8, the FWC index is 1.8 m^3 per ton of PVC, which is low compared to what was reported by Olapiriyakul [34], where the studied plant producing 560,000 tons of s-PVC has a water consumption of 4 m^3/t of PVC, or the plant indicated by Pietro et al. [35], with a fractional consumption of 3 m^3 per ton and production of 250,000 tons of PVC. This significant difference is due to this process only considering the demineralized water required for the process, unlike the previously mentioned studies that also consider raw water used to produce demineralized water.

The suspension PVC production process has the peculiarity that most of the water entering the process is demineralized. This water goes through a purification process in which minerals and salts are removed because they interfere with the quality and stability of the resin in the reaction stage [36]. If the amount of raw water used to produce 1933 m^3 daily were considered, the FWC index would increase to 2.83 m^3 per ton, which would put the process closer to the values reported in the literature. Additionally, there are other sources of water consumption, mainly in energy exchange tasks. Cooling towers have the highest water consumption as a result of losses due to evaporation when cooling the hot water used in the process. These losses can cause the index to exceed 3 m^3 per ton of PVC. On the other hand, the residual water indicator was 80%, meaning that of the 1933 m^3 of demineralized water, 80% ends up as residual water. This indicator allows for the affirmation that the application of process optimization techniques concerning materials such as water is possible because there are significant residual water streams leaving the process that could be adapted for use, as in studies such as Hoa [37] or Pietro et al. [35], among others.

The Energy Specific Intensity *(ESI)* index was 4.6 GJ per ton, which indicates that the process has a high energy demand for PVC production, but it is slightly lower than other processes such as the one reported by Wang et al. [38] in their study of a chlor-alkali and PVC plant with an annual polymer capacity of 300,000 tons, where they report a value of 5.8 GJ per ton, or the value reported by Franklin Associates, around 5.11 GJ/t of PVC [39]. This difference can be explained because the consulted studies quantified this indicator in real operating processes including additional equipment beyond process topology. Some operations, such as pumping, cooling towers and control systems, among others, have considerable additional contributions to the total energy used for the proper operation of the process.

Indicators are quantified according to the use of natural gas and electricity per ton of product, indicating how much of each energy source is used within the process. The process uses 59.4 m^3 of natural gas per ton of PVC and 1.01 kWh of electricity per ton of PVC, meaning the process uses low amounts of electrical grid energy, which is mainly used in equipment for material movement in the process, such as compressors, dryers and blowers, among others. On the other hand, the process mostly uses natural gas, so the natural gas consumption indicator is much higher than that of electricity for equipment in which heating occurs, such as boilers, burners and heat exchangers. The energy cost was 13,552,846 USD per year, taking into account both electrical energy and the natural gas used to generate thermal energy to meet the needs of the process. The FWC was USD 694,080 per year, considering the demineralized water used as a compound within the process stages, meaning the water that comes into direct contact with PVC. Comparing these results with works reported, such as Gomes [40], where a pre-feasibility study for a suspension PVC plant was conducted for 800 tons per year of product, a water consumption cost of USD 1200 per year and an energy cost of USD 422,000 per year were obtained. It can be observed that the process has a higher water and energy consumption cost, which is expected since the capacity of the plant studied by Gomes is 500 times smaller than the topology simulated in this work [40].

The Net Energy Ratio (NER) and Energy Usability Index (EUI) yielded values of 0.7 and 7.4, respectively. An NER higher than 1 indicates that the process has a net gain of usable energy, meaning the process has little gain of usable energy associated with the product relative to the process. NER is commonly used for biofuel generation processes, such as the research by Meramo et al. [41], who obtained an NER of 0.13 to produce acetone, butanol and ethanol from cassava waste in a biorefinery topology [40]. On the other hand, Niño-Villalobos et al. obtained an NER of 1.16 for a process of hydrogen and biodiesel production in a biorefinery from African palm and *Jatropha curcas*. When compared to both previous works, the suspension PVC production process has a slightly high NER due to the high but similar energy content of the polymer and monomer (HHV = 18 MJ/kg, PVC and HHV = 16 MJ/kg, VCM). Additionally, the NER of this process is not as high as that of substances used mainly as fuels, such as hydrogen, biodiesel or even natural gas. An Energy Usability Index above 1 indicated that PVC can be potentially used as fuel based on its high energy content, preferably taking advantage of waste with a high polymer content. However, there are restrictions on the direct combustion of PVC due to the emission of toxic and corrosive gases, and pre-treatment processes must be implemented [42]. In any case, other thermal degradation processes, such as pyrolysis and gasification, among others, allow the recovery of some of the energy contained in the polymer as direct energy or through secondary products [43].

Figure 3 shows the performance of nine of the evaluated indicators for the suspension PVC production process in terms of best–worst scenarios; given the nature and method of calculating NER and EUI, they do not present worst and best values and cannot be normalized on a percentage basis. From this figure, the performance of the process in terms of mass, energy and product can be diagnosed. Additionally, aspects that can be improved through process optimization methods can be identified. The figure shows that the process has high performance in aspects such as production yield and reuse of unreacted VCM; both indicators are above 95%. This indicates that the process does not require any improvements in raw material management. On the other hand, the indicators associated with water management show a deplorable performance. The indicators show that the process has high water consumption, high wastewater generation (very little effluent reuse) and high costs associated with supply consumption, all without considering raw water and losses. These findings support the application of optimization techniques or methodologies such as process integration to improve this aspect of the process; understanding the importance of water resources forces processes to have intelligent and sustainable use.

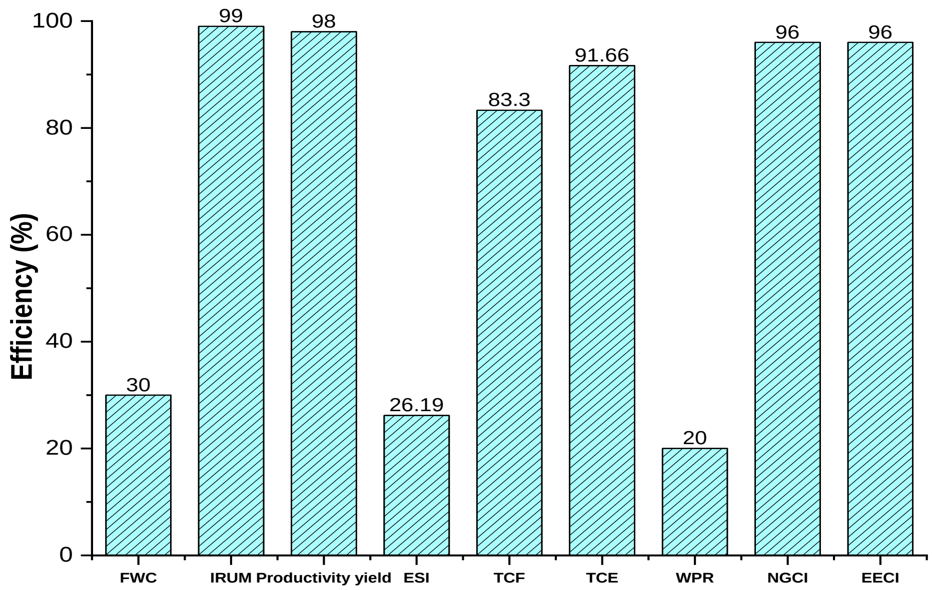

Figure 3. Performance of technical indicators for the suspension PVC production process.

Energy-related indicators show that the process has both advantages and disadvantages. The advantages are centered on aspects such as energy consumption cost, which benefits from the primary use of natural gas to meet energy requirements due to its lower unit cost. However, the energy specific intensity (ESI) indicator presented low performance (26%), indicating that the process has a high energy consumption, even though it is lower than the consumption of other processes in the literature. High consumption can lead to other problems associated with environmental criteria due to pollutant emissions and safety, due to high processing temperatures [44]. On the other hand, there may be unaccounted energy losses that impact the proper use of energy resources. This indicator allows us to point out that there are energy aspects that should be studied; for this, it is appropriate to evaluate not only the quantity but also the quality of energy flows within the stages, for which exergy analysis could be used. In the same vein, it is appropriate to say that there is room for improvement in the process's energy performance by applying process energy integration techniques.

4. Conclusions

In the present study, a methodology for the technical evaluation of the suspension PVC production process was proposed based on process simulation and the calculation of 11 technical indicators related to water, energy and product management (WEP). The simulation data (PVC properties) had an accuracy higher than 90% compared to the reported literature. The FWC and WPR indicators showed that the water management of the process had the worst performance due to high water consumption and low reuse (30 and 20%, respectively); the IRUM and the productivity yield showed product management is the most positive aspect of the process due to high conversion and reuse of unreacted VCM; on the other hand, the TCE, NGCI and EECI indicated energy management has a good performance, thanks to the use of natural gas as primary energy source; however, ESI showed the energy consumption needs improvement (4681 MJ/t of PVC). Nevertheless, these results support the claim that water and energy management can be improved through the use of process integration techniques combined with environmental diagnostics, process safety, technical–economic resilience and energy quality assessments. To conclude, the proposed indicators were useful in diagnosing the performance of the suspension PVC process and are recommended for similar processes such as polyethylene polypropylene production and biomass-based bio-refineries.

Supplementary Materials: The following supporting information can be downloaded at: https://www.mdpi.com/article/10.3390/su15108096/s1, Figure S1: Block diagram for PVC production via suspension polymerization.

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Abbreviations

MVC	Monomer Vinyl Chloride
NRTL	Non-Random Two-Liquid
PtE	Polymer to Energy
PVA	Poly-Vinyl Acetate
PVC	Poly-Vinyl Chloride
s-PVC	Suspension Poly-Vinyl Chloride
WEP	Water–Energy–Product
FWC	Fractional Water Consumption, m^3/t
TCF	Total Cost of Fresh Water, $/day
WPR	Wastewater Production Ratio, %
IRUM	Index of Reused Unconverted Material, %
TCE	Total Cost of Energy, $/day
ESI	Energy Specific Intensity, MJ/t
NER	Net Energy ratio
EUI	Energy Usability Index
NGCI	Natural Gas Consumption Index, m^3/t
EECI	Electric Energy Consumption Index, kWh/t
VCM	Mass Flow of Raw Material, t/day
HHV	Higher Heating Value, MJ/kg

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