ENCIT₂024



20th Brazilian Congress of Thermal Sciences and Engineering

20th Brazilian Congress of Thermal Sciences and Engineering November 10th-14th, 2024, Foz do Iguaçu – PR - Brazil

ENC-2024-XXXX MATHEMATICAL MODEL OF RISK MANAGEMENT IN A DEVICE FOR GENERATING A SUSTAINABLE HYDROGEN PRODUCTION UNIT

Luiz Fernando Joly Assumpção

Federal University of Paraná - (UFPR)
Graduate Program in Materials Science and Engineering at UFPR - (PIPE)
Fuel Cells Laboratory (LaCelC) and Sustainable Energy Research and Development Center - (NPDEAS) luiz.joly@ufpr.br

Eduarda Zeni Neves

Federal University of Paraná - (UFPR)
Graduate Program in Chemical Engineering at UFPR - (PPGEQ)
Fuel Cells Laboratory (LaCelC) and Sustainable Energy Research and Development Center - (NPDEAS) eduarda.neves@ufpr.br

Lauber de Souza Martins

Federal University of Paraná - (UFPR)
Graduate Program in Materials Science and Engineering at UFPR - (PIPE)
Fuel Cells Laboratory (LaCelC) and Sustainable Energy Research and Development Center - (NPDEAS) lauber.martins@ufpr.br

José Viriato Coelho Vargas Dhyogo Miléo Taher

Federal University of Paraná - (UFPR)
Graduate Program in Mechanical Engineering at UFPR - (PGMEC)
Polymers Laboratory (LaPol) and Fuel Cells Laboratory (LaCelC)
Sustainable Energy Research and Development Center - (NPDEAS)
rodrigo.cesar@ufpr.br
viriato@ufpr.br

Abstract: This research aims to identify the ideal parameter for sustainable hydrogen production with zero or negligible level of risk of an interesting alternative that can be obtain this gas through the chemical reaction between aluminum and water catalyzed by an alkaline solution. Although hydrogen is an important form of energy, its production involves peculiar aspects. For the proposed study, the great advantage of generating hydrogen in a simple way, with very low electricity consumption and low cost it is associated with some relevant aspects. The chemical reaction is strongly exothermic, the gas produced is flammable, asphyxiating, has high calorific value and the chemical agents and residues involved present causticity and considerable toxicity. This represents risks to the people, to the environmental conditions and also to fire. Thus, in order to this project to receive definitive approval from government authorities for environmental inspection, occupational health and safety and the Fire Department, a complementary Risk Management Project (RMP) becomes decisive. In order to offer an effective study, a methodology was identified that has innovative characteristics, such as a new conceptualization of risk, unmistakable technical conducts for the unequivocal identification of all associated risks and the best practices of conducts to neutralize or eliminate and control the related risks and others very interesting ones. The research will be developed through zero-order mathematical simulations to determine optimal design and operating parameters with zero risk or at least at an acceptable level. The study will start from the initial condition, when the yield of the gas production will be evaluated. At the same time, a RMP will be developed to manage the risks. Once defined, the risk control actions will be implemented in the system and another round of tests will be carried out and the new results can be compared with the initial condition. Identifying differences, adjustments both in the operating conditions of the system and in the RMP guidelines should be made and new and subsequent tests should be carried out until the ideal condition for hydrogen production with minimum acceptable risk is obtained. Then, in an innovative way, a project for the technical development of a device of relevance to the community that will generate sustainable hydrogen will be offered properly optimized and under strict and effective risk management conditions to offer absolute safety to users, to the environment and to facilities with a focus on fires.

Keywords: Risk Management, Mathematical Model, Hydrogen production.

1. INTRODUCTION

This research aims to offer to the community, a mobile, autonomous and sustainable prototype that will serve as a Hydrogen Station. The generation of the gas, based on the reaction between aluminum and water catalyzed by an alkaline solution will be developed inside a small reactor, using aluminum wasted pieces (soda cans, food packaging and others) and a simple alkaline solution. A great differential of this idea is that the system will operate with low electricity consumption only to supply a small gas pressurization pump. The assembly is simple involving only a reactor, a pressurization pump, a usual cylinder for gas accumulation and the gas supply system to customers. Due to its simplicity in construction, it can be easily moved and located in places where the gas consumption is interesting.

Due to its different sectors of activity (industrial chemicals, pharmaceuticals, cosmetics, food, energy, mining, fertilizers, among others), the chemical industry plays an important role in global socioeconomic development. However, most of its facilities have a high accident risk, related to fire, chemicals, explosion and other environmental and safety at work potential accidents, such as the case of Seveso, Minamata, Bhopal and the explosion in the Port of Beirut (Cheng et al., 2021; Assumpção, 2018).

In addition, mainly due to climate problems related to the use of fossil fuels, among the sectors of the chemical industry that have been obtaining attention worldwide is energy. One of the biggest causes of the climate deviations is carbon dioxide that, among others, has been continuously generated by use of fossil fuels. To decarbonize the planet the replacement of energy sources by environmentally balanced ones is urgent.

In this context, the 26th United Nations Climate Change Conference (COP26) reaffirmed the Paris Agreement goal of keeping global average temperature below 2 °C. In order to achieve this goal, efforts are being made to reduce carbon dioxide emissions that contribute to reducing air pollution because greenhouse gas (GHG) emissions and air pollution come from common sources, i.e., fossil fuels (Jiang, 2023).

Thus, contributing to a sustainable energy future and decarbonizing the planet the chemical industry plays a key role in the transition to renewable energies. As a promising alternative solution is to replace the energy source is hydrogen (Dincer and Aydin, 2023).

Therefore, in order to the facilities of the chemical industry have business success and to prevent industrial accidents, even in cases of activities that have risks of low intensity, it is necessary the development of an effective risk analysis and assessment through a well improved and complete Risk Management Project (RMP). The RMP is currently a tool of high importance (De Silva et al., 2022).

In this research, in spite of the fact that favorable, currently, aluminum has a well-established recycling chain, which contributes to the process being considered as sustainable, the assembled set is simple and has low operating cost. However, analyzing the aspects related to the chemical reaction involved there are several aspects to be considered: i) the gas is asphyxiant, flammable and has a high calorific value; ii) the alkaline solution and the residue involved in process have causticity and high toxicity, and iii) the reaction is exothermic, bringing risks to users when it is necessary to interact in the system. Furthermore, because hydrogen is classified as risk level 2 (ONU 1049) (CETESB, 2023), it is considered as a dangerous chemical. These risks can result in accidents of high severity.

It should be noted that a study like this that contains risks of accidents with that great magnitude, devoid of a consistent risk management project, will hardly reach approval from the environmental agencies, from those responsible for the health and safety of workers and will also hardly receive an operating license from the Fire Department of the locations where these devices will be installed.

For these reasons, a risk management system that interacts in the conditions involving the system becomes decisive. Thus, before the operation of this system a detailed analysis from the point of view of the risk must be developed.

Previous works have proposed practical methods for risk management and analysis to the chemical industry, such as hazard and operability (HAZOP), Failure Mode Effect Analysis (FMEA), Layer of Protection Analysis (LOPA), Fault Tree Analysis Method (FTAM) and others (Mokhtarname et al., 2021; Minkowycz et al., 2006; Nguyen et al., 2022; Yan et al., 2022). In this research, it is adopted the HAZOP method with some adjustments.

In terms of the risk/hazard concept, this paper presents a new technical concept that will be decisive for any RMP. While for the risk identification procedure, an unmistakable technical methodology was developed to effectively identify all related. As for the definition of the risk index, this study used the better practices on how to qualify them through new likelihood factors concept.

Therefore, based on the need for a consistent management of risks in the development of an important system that has potentiality to result bodily injuries to the people, damage to the environment and fire to the facilities, this work proposes a modeling and simulation to the process of sustainable hydrogen generation set with zero or negligible level of risk.

Methodology and materials

Initially, it is important to highlight that this study aimed for the development conditions, operating and risk conditions of a sustainable hydrogen generation unit. Thus, in order to be able to characterize the work and demonstrate the innovation of the study, a bibliographic review is conducted on the topics related to the subject, with the objective of characterizing the state-of-the-art in the theme and identifying the existing gaps for scientific advancement in the area.

1.1 Hydrogen generation reactor

For the energy production (hydrogen) one of the components of the set to be installed in the system is the reactor. The basic principle of the process to produce the gas consists in the chemical reaction of metallic aluminum that is added to an alkaline solution. Usually, the alkaline product is the sodium hydroxide used in varying concentration. The chemical reaction that happens inside of reactor is as follows (Soler et al., 2007; Huang et al., 2013; Martinez et al., 2005; Jung et al., 2008).

$$Al_{(s)} + 3 H_2O_{(l)} + NaOH_{(s)} \rightarrow NaAl(OH)_{4(s)} + 3/2 H_{2(g)}$$
 (1)

$$NaAl(OH)_{4(s)} \rightarrow NaOH_{(s)} + Al(OH)_{3(s)}$$
 (2)

$$Al_{(s)} + 3 H_2O_{(l)} \rightarrow Al(OH)_{3(s)} + 3/2 H_{2(g)}$$
 (3)

The general reaction is expressed in Eq. (3). The involved chemicals products are aluminum, sodium hydroxide and hydrogen (Soler et al., 2007; Huang et al., 2013; Martinez et al., 2005; Jung et al., 2008). The aqueous solution of sodium or potassium hydroxide catalyzes the reaction, and they can be recovered. Soler et al., 2007 indicate that in this reaction aluminum can be passivated, and using seawater prepared with NaAlO₂ and this effect can be avoided. Therefore, seawater is more efficient than fresh water for the production of H₂.

The proposed system is sustainable, since there is a low need of energy to its operation, only to supply a small gas pressurization pump.

In addition, aluminum and NaOH are used, which are abundant substances in nature and of low cost.

Despite the chemical viability and abundant supply of reagents, to enable the production of H_2 on a large scale, aspects of yield, safety and risk need to be addressed in depth. It should be also noted that the reaction shown in Eq. (3) is highly exothermic, which allows the understanding that the heat released is disfavored to the H_2 production (Haller et al, 2021). In addition, reactors producing H_2 from Al must be properly sized to withstand high pressures and temperatures and allow for safe operation (Hurtubise et al., 2018).

Figure 1 demonstrates an example of Hydrogen Rector:



Figure 1. An example of Hydrogen Reactor.

1.2 Mathematical modeling

Major accidents can not only result material losses to the facilities or also produce severe damage to the environment, but can also lead to the risk to human life. HAZard and OPerability (HAZOP) method is one of the most widely used and an accept techniques to manage the risks that can result in inconvenient and negative changes and be a tool to identify safeguards to avoid such situations (Mokhtarname et al., 2021; Minkowycz et al., 2006; Nguyen et al., 2022; Yan et al., 2022).

However, this method is a subjective qualitative approach to engineering judgment through a HAZOP team. The integration of a mathematical modeling with a HAZOP study, called HAZOP quantitative dynamic study is necessary for providing new systems evaluation a quantitative analysis of risks in order to avoid bodily injuries to people, environmental impacts on the environment and fire to the facilities. Few studies in the technical literature present the role of quantitative dynamic HAZOP and its capabilities (Mokhtarname et al.; 2021). This then identifies the shortcomings of this integration that need to be addressed in order to achieve the full potential of this approach (i.e., especially for complex systems). Mokhtarname et al., 2021; Minkowycz et al., 2006; Nguyen et al., 2022; Yan et al., 2022).

The actual study is a combination of mathematical model for the identification of the ideal operating conditions of a system of hydrogen production supervised by a HAZOP evaluation aiming to identify if this condition represents the best

alternative for risk management. Initially, the ideal condition of operation of the system is obtained and then the comparison of this condition with others is carried out to verify which is the one that has the best safety conditions for the facilities, for worker and for the environment.

1.3 Risk management

The HAZOP methodology is a Process Risk Analysis technique used around the world to study not only the hazards of a system, but also its operability problems, exploring the effects of any deviations from design conditions. A comprehensively documented HAZOP which covers all risks addressed in a project and gathering the information from books, guidelines, standards, scientific journals and conference proceedings, with the aim of classifying the research conducted over the years can define the state of the art. (Dunjo et al. 2010).

New products often define an industry's competitive advantage and market success. However, only a part of new product development (NPD) initiatives results in success and this therefore represents one of the major causes of wasted investments. In addition, NPD processes have become very complex and risky due to globalization as well as public demands for safe and technologically advanced products (Chauhan et al., 2018).

In this context, it is important to highlight that all decision making is an opportunity to assess the situation of risk-benefit relations and, cause and effect. Therefore, risk assessment, whether carried out or by subjective impulse and even by in-depth and detailed technical analysis of the case, is part of people's daily lives (Chauhan et al., 2018).

In order to substantiate this study, it was necessary to define the technical concept for the term risk. Wagner and Bode (2006) refer that risk, in the context of safety at work and environmental protection techniques, is considered as something that can result in negative consequences. Tohidi, (2010) conceptualizes that risk is a *threat (hazard* and *threat)* existing in systems that can result in adverse effects. Several bibliographic sources offer different technical concepts about risk, however, the one that comes closest to characterizing that risk is a source that can result in adverse effects is the one contained in the glossary of the technical standard ISO 45.001, (2018) that conceptualizes "hazard" as "source with a potential to cause injury and ill health". In the same vein, Mayer et al. (2022) presents as an understanding for the term hazard, the existing condition dependent on the vulnerability of its target object to determine adverse effects of varying intensity. It further conceptualizes risk as the potential for a given threat to exploit the vulnerability of an asset or group of assets causing harm to the organization (Mayer et al., 2022).

According to the information presented above and the development of the practical research, this study defines as risk/hazard the following technical understanding: "forms of energy that when reach man, environmental conditions or some installation result in adverse effects". To consolidate this concept, it can point out that the more intense is the form of energy, more severe the related effects will be. Hence, hazardous energy can be understood as: "A condition inherent in a form of energy (chemical, mechanical, electrical, potential, light energy, radioactive or another) which, when out of control, hits the worker's body resulting bodily injuries or reaches the environmental condition will result adverse impact and when achieves the facilities can result fire of various levels of severity".

Considering that risks are forms of energy and because they are transient, it can be understood that they can be found in the systems inputs and outputs. In this understanding, the safe and effective conduct to proceed to the identification of risks of an activity is through the methodology that is called "Inputs and outputs". This method involves Risk assessment (RA) and life cycle assessment (LCA), which use input-output theory, and two analytical tools used to support decision-making in environmental management (Harder et al, 2015).

In the sequence of the study, the next step is to define the risk index of each identified risk. This task consists of combining the factor of severity of the associated effect with the factor of probability of realizing a risk-related effect. For that, there is a need to identify the effects associated with the risks and the causes related to these effects. To identify the effects, it is necessary to have experience in the object of the study and to be able to identify the causes of the effects, the teachings of Ishikawa recommend that the technique called "Fishbone" must be employed (Assumpção, 2022; Harder, 2015). This methodology indicates that, conceptually, the causes of effects are those related to six factors: i) labor (malpractice, recklessness and negligence), ii) the method used to perform the task, iii) the conditions of the machine or installations, iv) the environmental conditions, v) the materials involved and vi) interference from other aspects (Assumpção, 2022; Harder, 2015).

To define the severity and likelihood factors, the scales were adopted shown in Table 1 and 2.

SEVERITY				
FACTOR	EFFECT	CRITERION		
1	MILD	Accidents that do not cause bodily injury (e.g., light scratches, etc.);		
2	MODERATE	Accidents that cause non-disabling injuries (e.g., burns with redness on the skin, etc.):		

Table 1. Scale for severity of effects (Assumpção; 2018).

SEVERITY					
FACTOR	EFFECT	CRITERION			
3	MAJOR	Accidents that cause disabling injuries without loss of substance (e.g., deep and serious burns, etc.);			
4	SEVERE	Accidents that cause disabling injuries with loss of substance (e.g., loss of part of fingers, etc.);			
5	CATASTRÓPHIC	Death			

Table 2. Escala para probabilidade (Assumpção, 2018).

	LIKELIHOOD					
FACTOR	OCCURRENCE	CRITERION				
1	UNLIKELY	Very low probability of damage occurring. (One occurrence over a large period of time, one every ten years or so)				
2	POSSIBLE	Low probability of damage occurring. (One occurrence in the last five years)				
3	OCCASIONAL	Moderate probability of damage occurring. (More than one occurrence in the last three years)				
4	REGULAR	High probability of damage occurring. (More than two occurrences in the last two years)				
5	CERTAIN	Very high probability of damage occurring. (at least one occurrence is expected in the next twelve months)				

According to the results obtained with the severity and with the likelihood, it is possible to define the risk index and the corresponding actions according to the information contained in the Table 3:

Table 3. Actions management (Adapted from Assumpção, 2018).

ACTIONS MANAGEMENT					
RESULT S x L	RISK INDEX	ACTIONS			
Up to 3 (severity < 3)	TRIVIAL RISKS	Do not require special actions, neither preventive nor detection.			
From 4 to 6 (severity = 3)	TOLERABLE RISKS	Do not require immediate action. They may be improved at an appropriate time depending on the availability of manpower and financial resources			
From 8 to 10 (severity = 4)	MODERATE RISKS	Requires prediction, definition (short term) and responsibility for the implementation of actions;			
From 12 to 16 (severity = 5)	RELEVANT RISKS	Requires the immediate implementation of actions (preventive and detection) and definition of responsibilities. The work can be released for its execution only with continuous supervision and monitoring. The interruption of work can happen when the conditions present some lack of control;			
> 16	INTOLERABLE RISKS	The work cannot be started and, if it is ongoing, it must be stopped immediand can only be restarted after implementation of containment actions.			

With the information regarding the effects and causes of the accidents, due to the proposed methodology having safe guidelines, a consistent Preventive Action Plan can be developed. It is also important to note that, to avoid adverse effects, hazardous energy can be neutralized or controlled through preventive measures. Preventive actions can neutralize or eliminate the hazardous energy.

Once the effects and causes related to the risks are identified, it is possible to establish the risk indices of each related cause. Subsequently, the Preventive Action Plan must be defined and implemented (Assumpção, 2018; Dunjo et al, 2010; Harder et al. 2015).

When the preventive actions are implemented, it is expected that the likelihood outcomes are likely eliminated or at least minimized. In most technical aspects, such as the installation of energy control devices, the adoption of physical protections (limits, barriers, defenses), the establishment of preventive actions is effective. Above all, according to Assumpção (2022), it should be noted that human behavior is diverse, technical preventive actions do not always effectively interfere in aspects related to negligence and recklessness. It states that, even with well-established and

properly implemented preventive actions, negligent and reckless behaviors are still identified. It states that negligent behavior is more susceptible than reckless behavior. Cases of negligence are more predictable than reckless ones (Assumpção, 2022).

To define the severity factor, regarding the effects that accidents with sodium hydroxide can cause, Schvartsman (1991) states that dermal contact results in severe extremely painful burns. There is an initial edema with formation of vesicles and then occurs necrosis of liquefaction that progressively deepens. In the eyes, rapid and little intense exposure produces conjunctivitis, lacrimation and photophobia. In the most severe cases there are severe pain, edema of the conjunctiva and eyelids and corneal ulceration. It has a lethal dose of 5.0 g.

1.4 Practical development

This research aims to develop a complete risk management study to identify the condition of maximum amount of hydrogen produced under condition of lower risk of accidents when operating the system, focusing on the following aspects:

- Chemicals products: aluminium. alkaline solution, hydrogen and sodium aluminate;
- Equipment and accessories: reactor, pipes and gas pump;
- Activities: preparation of the alkaline solution, removal of waste generated on the reactor, operating conditions of the set.

For this work, only the preliminary part of the research related to the conditions of preparation of the alkaline solution of the hydrogen reactor will be demonstrated.

The study of the following variables will be reported: type of caustic soda to be used (pellet or liquid, concentration 50%) and the concentration of the solution to be defined (1.0; 3.0; 7.0 or 12.5 M). This research will have as final objective to identify the conditions of lower risk to the user, the environment and fire occurrences, associated with the conditions of obtaining the highest yield of hydrogen production.

The sequence of the research must be followed as shown in Figure 3.

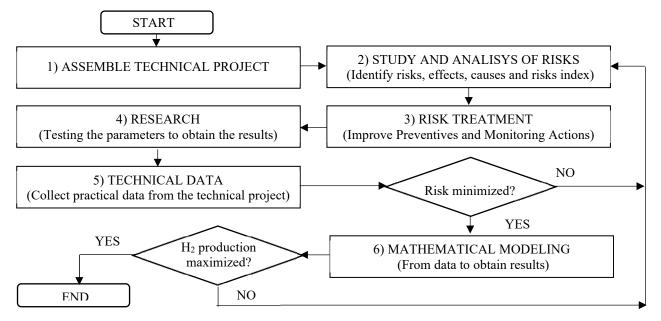


Figure 3. Flowchart adopted for work.

As a reference for the development of this case study, it will be evaluated the risk conditions that a Operator of system undergo when he has to carry out his intervention activities in the system and has to submit to the risks of the process. He has a basic knowledge of the operability and risks existing in the system. At the beginning of his activities, he makes all the preparations of the system by adding the caustic soda lye solution to the reactor. Every 15 minutes he adds one can of soda to the reactor and wait for the next cycle.

The objective of the study is to identify which is the condition of lowest risk for Operator of system, when varying concentrations of alkaline solution are used (caustic soda (1.0 molar, 3.0 molars, 7.0 molars or 50% soda (12.5 molars)) and when solid caustic soda (pellets) or liquid caustic soda (50% by weight), the commercial one, is used. Consider that, through market research, it was identified that liquid caustic soda has a price by weight 30% higher than solid soda.

For the purpose of the research, it was considered that the higher the concentration of the alkaline solution contains a greater amount of energy, the more intense the risks will be. However, the greater the use of the solution and the lower the exposure of users to the risk, which results in a lower probability of accidents.

It should be considered that a can of soda has a weight of 15 grams. The volume of the hydrogen reactor has a capacity of 18 liters and the alkaline solution will occupy 50% of this volume (9 liters). Assuming reaction (3) above, without considering the reaction kinetics and aluminum alloy composition of soda cans, it is understood that 40 grams of caustic soda will be required to consume 27 grams of aluminum from soda cans.

The practical experiment should be conducted as follows:

The research will be developed only in the study of existing risks in the hydrogen production reactor. For this purpose, the methodology of inputs and outputs was used, encompassing the following steps:

<u>1st Step – Identification of risks:</u> for this purpose, the methodology of "*Inputs and outputs*" was adopted and among the results are sodium hydroxide and perform tasks of feeding reactor with alkaline solution (sodium hydroxide).

<u>2nd Step – Characterization of risks:</u> In order to establish the risk indices of each risk, the related effects and the corresponding causes must be defined. After that, the factors related to the effects and causes should be defined. The predictable effects on vehicle users in relation to a sodium hydroxide accident is the burning of the skin or eyes. The corresponding severity of this effect will be a function of the concentration adopted for the alkaline solution.

In order to define the likelihood of accidents with sodium hydroxide, Table 4 was established:

The information shown in the columns in this table is as follows:

Concentration: of the alkaline solution referring to 1.0 M; 3.0 M; 7.0 M (caustic soda in pellet) and 12.5 M (50% liquid caustic soda);

- NaOH pellet: amount of NaOH pellets required to form the alkaline aqueous solution with water;
- NaOH liquid: amount of 50% liquid NaOH to be added;
- Can: number of cans to saturate the solution; obtained from the reaction (3)
- Time to replacement: time of use of the alkaline solution, when one has to replace the solution;
- Intervention factor: Number of times one has to intervene to prepare new solutions. It is taken as a basis (factor equal to 1,0) for the case in which the alkaline solution is used for a longer time (12.5 M alkaline solution).

ITEM	CONCENTRATION	PELLET	LIQUID	CAN	TIME TO REPOSITION	INTERVENTION FACTOR
1	1.0 M (40g/l)	360 g	720 ml + 8,280 ml H ₂ O	17	04h15min	12.5
2	3.0 M (120 g/l)	1.080 g	2,160 ml + 6,840 ml H ₂ O	49	12h15min	4.2
3	7.0 M (280 g/l)	2.520 g	5,040 ml + 3,960 ml H ₂ O	114	17h45min	1.8
4	12.5 M (500 g/l)	4.500 g	9,000 ml + 0 ml H ₂ O	203	31h30min	1.0

Table 4. Likelihood of accidents with sodium hydroxide.

Through what is shown in the right column of the table above, it is identified that for each time when need to replace the alkaline solution using the 50% liquid caustic soda one has to proceed 12.5 times to obtain the 1.0 M solution of the pellet soda.

Usually, to obtain the risk index, the result of multiplying the factors of severity of the effect with the likelihood of effectiveness of this effect is used. One of the innovations of this project is that to obtain the risk index for the factor likelihood is used the factor of the probability of the effect combined with the factor of the probability of the causes. It was observed that when only the probability of effecting the effects is used the interferences of the causes are not considered. Doing as it is being proposed, it is observed that the results obtained are more realistic.

Considering that when using pellet soda at the concentration of 1.0 molar it is necessary to prepare this solution 12.5 times than when using liquid soda. It is admitted that the probability of accidents (effects) for the use of the solution prepared with pellet soda receives the likelihood factor 2 and for the liquid soda factor 1. Then, upon this consideration and combining the likelihood factors of the effects and the causes, the results are as shown in the Table 5:

KIND OF LIKELYHOOD OF EFFECTS LIKELYHOOD OF CAUSES **SOLUTION** (POSSIBLE (2)) Others factors: NaOH contaminated (1) **UNLIKELY (1) IKELIHOOD** (NaOH in pellet; 1.0 M solution) OF CAUSES Environment: noise, rain, and others (2) POSSIBLE (2) Workforce: inexperience. (2) Workforce: reckless, negligence (3) OCCASIONAL (3) POSSIBLE (2) Method: unappropriated utensils (2)

Table 5. Combining the likelihood factors of the effects and the causes.

	Materials: unappropriated PPE, equipment and utensils (2)			
	Machine: feed point is too small (3)	OCCASIONAL (3)		
KIND OF SOLUTION	LIKELYHOOD OF CAUSES	LIKELYHOOD OF EFFECTS (UNLIKELY (1))		
	Others factors: NaOH contaminated (1)	TIMIT HZEL V (1)		
OF OH OH	Environment: noise, rain and others (2)	UNLIKELY (1)		
OOD (NaC 50%)	Workforce: inexperience. (3)	POSSIBLE (2)		
HO ES (Workforce: reckless, negligence (3)			
LIKELIHC CAUSES liquid 3	Method: unappropriated utensils (2)			
CA	Materials: unappropriated PPE, equipment and utensils (2)	UNLIKELY (1)		
	Machine: feed point is too small (2)			

According to the information shown above, the Risk Matrix for the preparation of the alkaline solution with caustic soda in pellets at a concentration of 1.0 molar and with liquid caustic soda 50% is shown on Table 6.

ITEM	DICK	EFFECT	CAUSE		RISK INDICE			
TIEM	RISK	EFFECT			L	SxL	RISK INDICE	
1	G 1'-		Others factors: NaOH contaminated		1	3		
2	Sodium		Environment: noise, rain		2	6	Tolerable risk	
3	hydroxide		Workforce: inexperience.		2	6		
4	(pellet); Perform tasks of feeding		Workforce: reckless, negligence	3	3	9	Moderate risk	
5	reactor with		Method: unappropriated utensils	3	2	6		
6	sodium hydroxide	Burns in	Materials: unappropriated PPE, equipment and utensils		2	6	Tolerable risk	
7	nydroxide	the Skin	Machine: feed point is too small		1	3		
8	G 1:	and eyes	Others factors: NaOH contaminated		1	3		
9	Sodium	and eyes	Environment: noise, rain.		1	3		
10	hydroxide (liquid 50%); Perform tasks of feeding reactor with sodium	50%); Perform easks of feeding reactor with	Workforce: inexperience.		2	6	Tolerable risk	
11			Workforce: reckless, negligence	3	2	6		
12			Method: unappropriated utensils	3	1	3		
13			Materials: unappropriated PPE, equipment and utensils		1	3		
14	nydioxide		Machine: feed point is too small		1	3		

Table 6. Risk Matrix.

This same table was prepared to be able to compare the risk indices for solutions of the same concentration (12.5 M), however, one prepared with solid soda and the other with 50% liquid soda.

For this study, worksheets were prepared containing preventive actions for the causes and for the effects for all the proposed situations and the summary was as follows: automate the equipment that proceeds to the supply, both for solid soda and for liquid soda; provide PPE and apply training to users.

Subsequently, the studies are directed to the process of identifying the alternative to obtain the maximum production of hydrogen. Identifying this condition, if it is obtained with a concentration different from that established in this study, a new round of risk assessment should be carried out and followed by a study of the maximum point of hydrogen generation, until the maximum condition of production of this gas with minimum risk is obtained. Results and discussion

Noteworthy that more concentrated solutions require fewer interventions of users in the preparation of new solutions, which denotes a lower probability of accidents occurring. For this reason, more concentrated solutions are preferred.

Through the observations obtained in the tables presented, even having a higher cost, it was identified that the use of 50% liquid caustic soda has significant advantages, since it does not require dilution with water, the solution is already ready for use (one less risk, splashes); does not cause heating of the solution when dissolving with water, which the dilution of solid soda causes (avoids risk of burns in users) and does not cause the formation of strongly alkaline vapors that are generated in the reaction of solid soda with water (one less risk, burns of the user's respiratory system).

Conclusion

It is concluded that, through risk management analysis, the use of liquid caustic soda is in commercial terms a more practical option and presents a lower probability of accidents, making it the best alternative. It should be noted that the

proposed methodology for risk identification presented a more complete, consistent and devoid of weaknesses RMP, addressing the HAZOP method, and combined with the production of sustainable hydrogen for clean energy generation is an unprecedented study and not addressed so far in the literature, demonstrating its innovative and essential character in terms of safety with practical applications in the field of renewable energies that are so necessary today.

Acknowledgements

To the Brazilian National Council of Scientific and Technological Development - (CNPq) - [project 300093/2022], Renault and UFPR for the funding and the development of the project called "ROTA 2030".

References

Assumpção, L. F. J., 2022. Handbook for managing on-the-job accidents; method 11s; quick and safe response. 1st Editions. Publisher: Amazon.com.

Assumpção, L. F. J., 2018. *Manual prático para implementação de SGA e certificação ISO 14.001/2015*. Editora Juruá, 5ª edicão, Curitiba.

CETESB, 2023, Chemical Product Information Sheet, Compressed Hydrogen (in Portuguese), Companhia Ambiental do Estado de São Paulo CETESB, São Paulo, licenciamento.cetesb.sp.gov.br/produtos/ficha_completa1.asp?consulta=HIDROG%CANIO%20COMPRIMIDO. Accessed 14 July 2023.

<u>Chauhan, A. S., Nepal, B., Soni, G., Rathore, A. P. S.,</u> 2018, Examining the state of risk management research in new product development process, Eng. Management Journal, Vol. 30. pp. 85.

Cheng, Z., Ni, L., Wang, J., Jiang, J., Yao, H., Chen, Q., Cui, F., Jiang, W., Ye, S., 2021, Process hazard evaluation and exothermic mechanism for the synthesis of n-butylmagnesium bromide Grignard reagent in different solvents, Process Saf. Environ. Prot., Vol. 147, pp. 654.

De Silva, K. G. V. K., Gunasekera, M. Y., De Alwis, A. A. P., 2022, Development of a risk informed quantitative decision making framework for major accident hazards installations in Sri Lanka, Process Saf. Environ. Prot., Vol. 162, pp. 965.

Dincer, I., Aydin, M. I., 2023, New paradigms in sustainable energy systems with hydrogen, Energy Convers. Manag., Vol. 283, pp. 116950.

Dunjo, J., Fthenakis, V., Vilchez, J. A., Arnaldos, J., 2010, Hazard and operability (HAZOP) analysis. A literature review, Journal of Hazardous Materials, Vol. 173, pp. 19.

Haller, M. Y., Amstad, D., Dudita, M., Englert, A., Häberle, A., 2021, Combined heat and power production based on renewable aluminium-water reaction, Renewable Energy, Vol. 174, pp. 879.

Harder, R., Holmquist, H., Molander, S., Svanstrom, M., Peters, G. M., 2015, Review of environmental assessment case studies blending elements of risk assessment and life cycle assessment, Environ Sci Technol, Vol. 49, p. 13083.

Huang, X., Gao, T., Pan, X., Wei, D. L., Qin, C. L., Huang, Y., 2013, A review: Feasibility of hydrogen generation from the reaction between aluminum and water for fuel cell applications, J. Power Sources, Vol. 229, pp. 133.

Hurtubise, D. W., Klosterman, D. A., Morgan, A. B., 2018, Development and demonstration of a deployable apparatus for generating hydrogen from the hydrolysis of aluminum via sodium hydroxide, Int. J. Hydrogen Energy, Vol. 43, pp. 6777.

ISO 45001, 2018, Occupational health and safety management systems – Requirements with guidance for use.

Jiang, X., 2023, Rapid decarbonization in the Chinese electric power sector and air pollution reduction Co-benefits in the Post-COP26 Era, Resources Policy, Vol. 82, pp. 103482.

Jung, C. R., Kundu, A., Ku, B., Gil, J. H., Lee, Jang, J. H., 2008, Hydrogen from aluminum in a flow reactor for fuel cell applications, Journal of Power Sources, Vol. 175, pp. 490.

Mayer, N., Heymans, P., 2022, Design of a modeling language for information system security risk management. Luxembourg Institute of Science and Technology.

Minkowycz, W. J. E. M. Sparrow, G. E. Schneider, R. H. Pletcher., 2006. *Handbook of numerical heat transfer*. 2nd ed. Chapter 17. New York: Wiley.

Mokhtarname, R., Urbas, L., Zerafat, M., Safavi, A. A., Salimi, F., Harasi, N., *Integration of mathematical modeling with HAZOP Study of a polymerization plant: capabilities and lacunae*, 7th International Conference on Control, Instrumentation and Automation (ICCIA), 978-1-6654-0350-4/21, 2021.

Nguyen, H., Safder, U., Kim, J., Heo, S. K., Yoo, C. K., 2022, An adaptive safety-risk mitigation plan at process-level for sustainable production in chemical industries: An integrated fuzzy-HAZOP-best-worst approach, J. Clean. Prod., Vol. 339, pp. 130780.

Omrani, R.; Shabani, B., 2017, Gas diffusion layer modifications and treatments for improving the performance of proton exchange membrane fuel cells and electrolysers: A review, Int. J. Hydrogen Energy, Vol. 42, pp. 28515.

Raimundo, R. C., 2019. *Development and construction of sustainable alkaline membrane fuel cell (in Portuguese)*. Ph.D. thesis, Graduate Program in Mechanical Engineering, Federal University of Parana, Curitiba, Brazil.

Assumpcap, L.; Zeni, E.; Vargas, J.; Yaher, D.

Mathematical model of risk management in a device for generating a sustainable hydrogen production

Soler, L., Macanás, J. Münoz, M., Casado J., 2007, Aluminum and aluminum alloys as sources of hydrogen for fuel cell applications, Journal of Power Sources, Vol. 169, pp. 144.

Tohidi, H., 2011, The role of risk management in IT system of organizations. Procedia Comput. Sci., Vol. 3, pp. 881. Vargas, J. V. C., Gardolinski, J. E., Ordonez, J., Hovsapian, C., R., 2010. "Alkaline membrane fuel cell". Patent, United States Patent and Trademark Office, Registry number: US 61/363,689, Provisional filed on july 13, 2010.

Wagner, S. M., Bode, C., 2006, An empirical investigation into supply chain vulnerability. Journal of Purchasing and Supply Management, Vol. 12, pp. 301.

Yan, F., Dong, L., Wang, B., Ge, J., Wang, B., 2022, Using risk meshing to improve three-dimensional risk assessment of chemical industry, Process Saf. Environ. Prot., Vol. 168, pp. 1166.

Responsibility notice

The authors are the only responsible for the printed material included in this paper.

The proceedings of the ENCIT 2024 will be published in AdobeTM PDF format.

The papers MUST be formatted strictly according to these instructions. The present file can be used as a template for Microsoft WordTM. Also, it could be used as a formatting guide to users of others text processing software.

The papers are limited to a maximum of 8 pages, including tables and figures.

(single space line, size 10)

2. TEXT FORMAT

(single space line, size 10)

The manuscripts should be written in English, typed in A4 size pages, using font Times New Roman, size 10, except for the title, authors affiliation, abstract and keywords, for which particular formatting instructions are indicated above. Single space between lines is to be used throughout the text.

The text block that contains the title, the authors' names and affiliation, the abstract and the keywords must be indented 0.1 cm from the left margin and marked by a leftmost black line border of width $2\frac{1}{4}$ pt.

The first page must have a top margin of 3 cm and all the other margins (left, right and bottom) must have 2 cm. All the other pages must be set with all margins equal to 2 cm.

PAGES **SHOULD NOT** BE NUMBERED

The body of the text must be justified. The first line of each paragraph must be indented by 0.5 cm. Sufficient information must be provided directly in the text, or by reference to widely available published work. Footnotes should be avoided.

All the symbols and notation must be defined in the text. Physical quantities must be expressed in the SI (metric) units. Mathematical symbols appearing in the text must be typed in *italic* style.

Bibliographic references should be cited in the text by giving the last name of the author(s) and the year of publication, according to the following examples: "Recent work (Bandarra Filho and Jabardo, 2011)..." or "Recently, Bandarra Filho and Jabardo (2011)..." In the case of three or more authors, the form "(Cavalini Junior et al., 2015)" should be used. Two or more references having the same authors and publication year must be distinguished by appending "a", "b", etc., to the year of publication. For example: "In papers (Santos et al., 2013a) and (Santos et al., 2013b)...".

Acceptable references include journal articles (MLA, 2004), numbered papers, dissertations, theses (Cavalini Junior, 2013), published conference proceedings, preprints from conferences, books (McConnell and Varoto, 2008), submitted articles (if the journal is identified).

References should be listed at the end of the paper according to instructions provided in Section 4.

(single space line, size 10)

2.1 Section titles and subtitles

(single space line, size 10)

The section headers and sub headers must be aligned at left, typed with Times New Roman, size 10, bold style font. They must be numbered using Arabic numerals separated by points. No more than 3 sublevels should be used. One single line size 10 must be included above and below each section title/subtitle.

(single space line, size 10)

2.2 Mathematical equations

(single space line, size 10)

The mathematical equations must be indented by 0.5 cm from the left margin. They must be typed using Times New Roman, italic, size 10 pt. font. Arabic numerals must be used as equation numbers, enclosed between parentheses, rightaligned, as shown in the examples below. Equations should be referred to either as "Eq. (1)" in the middle of a phrase or as "Equation (1)" in the beginning of a sentence. Matrix and vector quantities can be indicated either by brackets and braces, as in Eq. (1), or in bold style, as in Eq. (2). Symbols used in the equations must be defined immediately before or after their first appearance.

One blank line must be included above and below each equation.

(single space line, size 10)

$$[M]\{\ddot{x}\}+[C]\{\dot{x}(t)\}+[K]\{x(t)\}=f(t) \tag{1}$$

(single space line, size 10)

$$\mathbf{M}\ddot{\mathbf{x}}(t) + \mathbf{C}\dot{\mathbf{x}}(t) + \mathbf{K}\mathbf{x}(t) = \mathbf{f}(t)$$
(2)

(single space line, size 10)

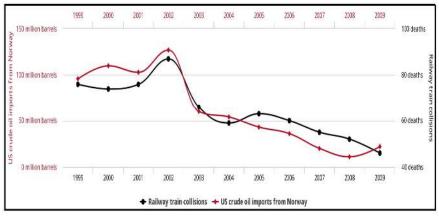
2.3 Figures and tables

(single space line, size 10)

Figures and tables should be placed in the text as close as possible to the point they are first mentioned and must be numbered consecutively in Arabic numerals. Figures must be referred to either as "Fig. 1" in the middle of a phrase or as "Figure 1" in the beginning of a sentence. The figures themselves as well as their captions must be centered in the breadthwise direction. The captions of the figures should not be longer than 3 lines, centered and use Times New Roman size 10.

The legend for the data symbols as well as the labels for each curve should be included into the figure. Lettering should be large enough for ease reading. All units must be expressed in the S.I. (metric) system. One blank line must be left before and after each figure.

(single space line, size 10)



(single space line, size 10) Figure 1. United States crude oil imports from Norway versus number of drivers killed in collision with railway train. Available from: http://tylervigen.com/spurious-correlations

(single space line, size 10)

Color figures and high-quality photographs can be included in the paper. To reduce the file size and preserve the graphic resolution, figures must be saved into GIF (figures with less than 16 colors) or JPEG (for higher color density) files before being inserted in the manuscript.

Tables must be referred to either as "Tab. 1" in the middle of a phrase or as "Table 1" in the beginning of a sentence. The tables themselves as well as their titles must be centered in the breadth-wise direction. The titles of the tables should not be longer than 3 lines. The font style and size used in the tables must be similar (both in size and style) to those used in the text body. Units must be expressed in the S.I. (metric) system. Explanations, if any, should be given at the foot of the tables, not within the tables themselves.

One blank line must be left before and after each table.

The style of table borders is left free. An example is given in Tab. 1.

(single space line, size 10)

Table 1. Experimental results for flexural properties of CFRC-4HS and CFRC-TWILL composites. Span/depth ratio = 35:1. Average results of 7 specimens.

(single space line size 10)

(Single space	c inic, bize io	
Composite Properties	CFRC-TWILL	CFRC-4HS
Flexural Strength (MPa) ⁽¹⁾	209 ± 10	180 ± 15
Flexural Modulus (GPa) ⁽¹⁾	57.0 ± 2.8	18.0 ± 1.3
Mid-span deflection at the failure stress (mm)	2.15 ± 1.90	6.40 ± 0.25

⁽¹⁾ measured at 25°C

Mathematical model of risk management in a device for generating a sustainable hydrogen production

(single space line, size 10)

3. ACKNOWLEDGEMENTS

(single space line, size 10)

This optional section must be placed before the list of references.

(single space line, size 10)

4. REFERENCES

(single space line, size 10)

The list of references must be introduced as a new section, located at the end of the paper. The first line of each reference must be aligned at left. All the other lines must be indented by 0.5 cm from the left margin. All references included in the reference list must have been mentioned in the text.

References must be listed in alphabetical order, according to the last name of the first author. See the following examples:

- Bandarra Filho, E.P. and Jabardo, J.M.S., 2011. "Convective boiling performance of refrigerant R-134a in herringbone and microfin copper tubes". *International Journal of Refrigeration*, Vol. 29, No. 1, pp. 81–91.
- Cavalini Junior, A.A., 2013. Detecção e identificação de trincas transversais incipientes em eixos horizontais flexíveis de máquinas rotativas. Ph.D. thesis, Universidade Federal de Uberlândia, Uberlândia, Brasil.
- Cavalini Junior, A.A., Lara-Molina, F.A., Sales, T.P., Koroishi, E.H. and Steffen, V., 2015. "Uncertainty analysis of a flexible rotor supported by fluid film bearings". *Latin American Journal of Solids and Structures*, Vol. 12, pp. 1487–1504.
- McConnell, K.G. and Varoto, P.S., 2008. Vibration Testing: Theory and Practice. John Wiley & Sons, New Jersey, 2nd edition.
- MLA, 2004. "How do I document sources from the web in my works-cited list?" Modern Language Association. 22 Feb. 2007 http://www.mla.org.
- Santos, D.D., Furtado, G.M., Frey, S.L., Naccache, M.F. and de Souza Mendes, P.R., 2013a. "Flow of elasto-viscoplastic fluids inside a cavity". In *Proceedings of the 22nd International Congress of Mechanical Engineering COBEM 2013*. Ribeirão Preto, Brazil.
- Santos, D.D., Furtado, G.M., Frey, S.L., Naccache, M.F. and de Souza Mendes, P.R., 2013b. "Numerical investigation of elastic and viscous effects on inertial viscoplastic fluid flows". *In Proceedings of the 22nd International Congress of Mechanical Engineering COBEM 2013*. Ribeirão Preto, Brazil. (single space, size 10)

5. RESPONSIBILITY NOTICE

(single space, size 10)

The following text, properly adapted to the number of authors, must be included in the last section of the paper: The author(s) is (are) the only responsible for the printed material included in this paper.