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MATHEMATICAL MODELING OF A HYDROGEN PRODUCTION REACTOR FROM ALUMINUM WASTE

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Abstract. *It is known that fossil and non-renewable sources of energy are abundant and should remain in use for many years. However, the need to diversify the energy matrix and the search for renewable and environmentally more appropriate sources of energy are objectives that are necessary and even urgent. Hydrogen is a type of clean energy that can be produced in a number of sustainable ways, such as from aluminum waste. This article proposes the development of a mathematical model of a reactor with the purpose of producing hydrogen through recyclable aluminum. The mathematical model was developed based on the model proposed by Noland et al. (2020), which includes the kinetics of the balanced chemical reaction of* H_2 *production from aluminum waste. Through the results and graphs obtained, it was considered that the kinetics of the hydrogen production reaction was modeled mathematically in an adequate way. The theoretical* H_2 *production curve data coincided with the experimental data at more than one point. The consumption profile of aluminum, sodium hydroxide and water was also modeled. Consumption data show similar behavior and occur exponentially. After approximately 25 minutes of reaction, there is a 5% decrease in the radius of the aluminum particles, total consumption of moles of sodium hydroxide and 1.4 g of water.*

Keywords: *mathematical modeling, hydrogen production, reactor, renewable energy, aluminum*

1. INTRODUCTION

It is known that fossil fuels are abundant, have a large stock of raw materials and are expected to still exist and be used for many years to come. However, scientific research and policies adopted by several countries need to aim at diversifying the energy matrix through alternative energy sources, in order to reduce environmental impacts and preserve the environment (Dresselhaus and Thomas, 2001; Bengtsson, 2006). Smalley (2005) elaborated a list of the main problems that will be faced by humanity during the 21st century and chose energy as the main problem to be solved. He also states that by solving the problem involving energy, all other problems can be solved, but he emphasizes that energy with lower costs is necessary for this purpose.

Dresselhaus and Thomas (2001), already at the beginning of the 21st century, called attention to the need to develop innovative and environmentally appropriate technologies for alternative energy sources in the future to replace traditional, fossil and nuclear sources. More recently, Chen et al. (2018) reinforced that this need is current and that the main obstacles to be overcome are the generation and storage of renewable energy in a technically and economically viable way.

New processes and technologies (such as the production of hydrogen) that aim to produce alternative energy, even though they present major limitations and bottlenecks, are part of this context presented so far. The reaction of hydrogen with oxygen can be used to produce energy in fuel cells. In addition, the product originated from this reaction is water (H_2O), which does not contribute to environmental degradation and increase in temperatures through the greenhouse effect (Bolt et al., 2020).

Hydrogen can be obtained through numerous processes and techniques that are already widely used, involving biomass, water and fossil fuels (Bakenne et al., 2016). Recently an alternative method of hydrogen production has been studied. This method involves the use of aluminum for the extraction of the H_2 molecule from the water molecule (Bolt et al., 2020). The authors also state that aluminum is the third most abundant element on our planet and corresponds to 8.1% of the composition of the Earth's crust. For the production of hydrogen, aluminum waste can be used, such as beverage cans used and directed to recycling or disposal. Therefore, the whole process can become even more environmentally friendly, since it can use the metal in its waste form. It is known that there is an extensive collection network for discarded aluminum, which indicates that raw material for the process is not a problem.

The development of appropriate mathematical models is of fundamental importance in engineering projects today. Through the developed models, it is possible to optimize the system being studied, in order to achieve maximum performance with minimal energy or reagent consumption, in addition to defining the best operating parameters of the proposed process. Mathematical models are capable of simulating the process in any operating condition without the need to carry out real experiments. The inclusion of mathematical modeling processes for the production of hydrogen from aluminum waste is extremely important for the improvement of the process as a whole. This will allow the technology to gradually become more viable, as cost reductions and efficiency increases can be achieved.

Some articles found in the literature already address the production of hydrogen from aluminum (Hurtubise et al., 2018; Setiani et al., 2018; Bolt et al., 2020; Noland et al. (2020) Haller et al., 2021). This article proposes the development of a mathematical model of a reactor with the purpose of producing hydrogen through recyclable aluminum. The mathematical model was developed based on the model proposed by Noland et al. (2020), which includes the kinetics of the balanced chemical reaction of H_2 production from aluminum waste that occurs inside the reactor.

2. MATERIALS AND METHODS

2.1 Mathematical modeling

The mathematical modeling and the mass balance of the parameters analyzed for the reactor were performed using the MATLAB software. The model proposed by Noland et al. (2020) was used as basis. The authors proposed a model that considers the kinetics of the balanced chemical reaction of hydrogen production from aluminum waste (Al) and sodium hydroxide (NaOH). The experimental data used were also obtained from the same article. It was considered a perfectly stirred reactor and the aluminum particles were represented by spheres.

2.2 Equations used in the mathematical model

The balanced chemical reaction of hydrogen production in the presence of sodium hydroxide, according to Hurtubise et al., (2018), is described in Eq. (1):

$$2Al + 2NaOH + 6H_2O \rightarrow 2NaAl(OH)_4 + 3H_2 \quad (1)$$

The general equation of the reactions involved in the hydrogen production process can be seen in Eq.(2):

$$r = k_0 S_{Al}^{bs} [NaOH]^{bc} \exp\left(\frac{E_a}{RT_r}\right) \quad (2)$$

For the consumption of the reagents (aluminium, sodium hydroxide and water) Eq. (3), Eq. (4) and Eq. (5) were determined. Aluminum consumption was measured according to the decrease in the radius of its particles and, consequently, in their surface area. The calculation of the area of aluminum particles can be observed through Eq. (6). Finally, the Eq. (7) refers to the molar concentration of sodium hydroxide:

$$\frac{dRAl}{dt} = -\frac{Y_{Al} r}{S} \quad (3)$$

$$\frac{dNaOH}{dt} = -Y_{NaOH} r \quad (4)$$

$$\frac{dH_2O}{dt} = -Y_{H_2O} r \quad (5)$$

$$\frac{dRAl}{dt} = -\frac{Y_{Al} r}{S} \quad (6)$$

$$[NaOH] = \frac{NaOH}{H_2O} \quad (7)$$

All the hydrogen produced in the process, inside the reactor, is represented by equation 8:

$$\frac{dH_2}{dt} = r \quad (8)$$

2.3 Initial conditions used in the development of the mathematical model

The initial parameters that were considered and used for the simulations through the mathematical model can be checked in Tab. 1:

Table 1. Initial parameters used in the development of the mathematical model

Parameter	Symbol	Value	Unit
Frequency factor	k_0	$72004.899.10^6$	$mLH_2.s^{-1}.cm^{-2bs}mol\ NaOH^{-bc}kgH_2O^{bc}$
Reaction order (Al)	bs	1	-
Reaction order (NaOH)	bc	0.55	-
Activation energy	E_a	65000	$J.mol^{-1}$
Universal gas constant	R	8.314	$J.mol^{-1}.K^{-1}$
Reaction temperature	Tr	305	K
Aluminum area	S	1265.12	cm^2
Aluminum sphere radius	R_{Al}	0.000615	cm
Number of particles	N	$266,312.10^6$	Number of particles
Constant of stoichiometric proportionality	Y_{Al}	$4.15948.10^{-5}$	-
Constant of stoichiometric proportionality	Y_{NaOH}	$2.77299.10^{-5}$	-
Constant of stoichiometric proportionality	Y_{H2O}	$1.49741.10^{-6}$	-
Number of moles of NaOH	NaOH	0.03	moles

3. RESULTS AND DISCUSSION

Through Fig.1 it can be seen that the mathematical model developed and proposed fit well to the experimental data of hydrogen production reported by Noland et al. (2020). At more than one point the theoretical curve data touches the experimental data points. The production of hydrogen in the reactor occurs exponentially, tending to reach the steady state (900 mL) after 25 minutes of reaction.

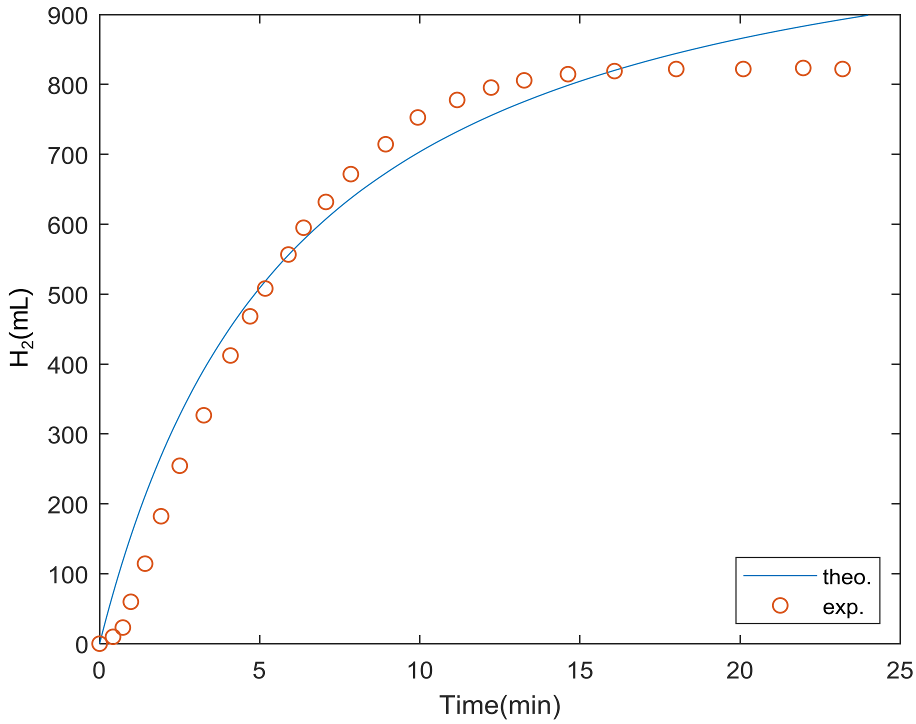

Figure 1. Experimental data and theoretical curve of the mathematical model of hydrogen production, in mL, over time

Figure 2 demonstrates the consumption of aluminum for the production of hydrogen by decreasing the radius, in micrometers, of the metal particles. As the radius decreases, there is also a decrease in the total aluminum surface available for the reaction. Consumption also occurs exponentially and after 25 minutes of reaction there is a decrease of approximately 5% of all aluminum in the reaction medium.

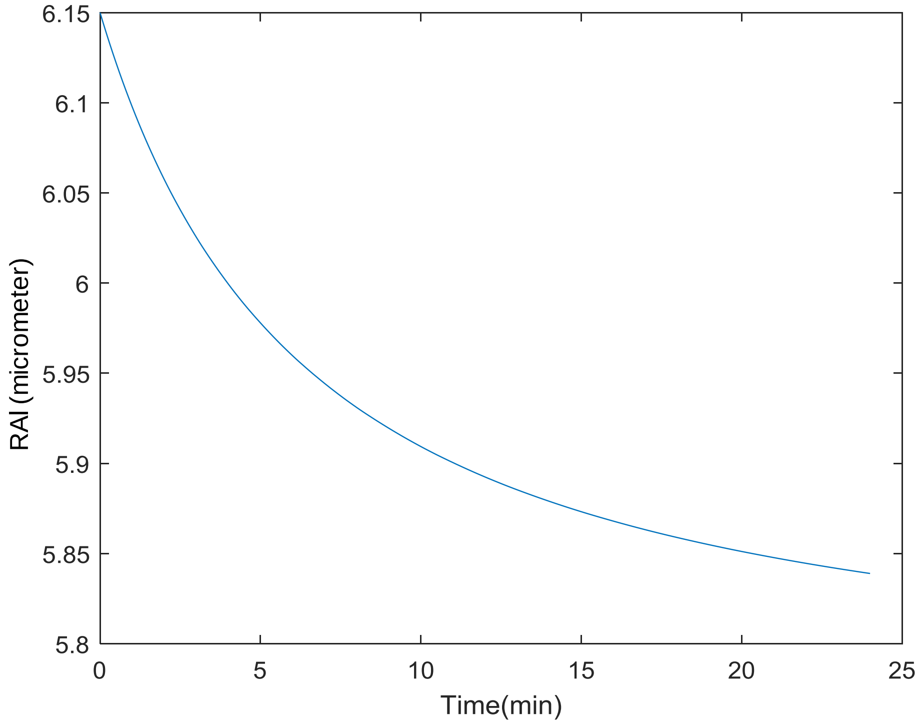

Figure 2. Theoretical curve of aluminum consumption (decreased particle radius) in the hydrogen production reaction over time

The sodium hydroxide consumption profile in the reaction occurs in a similar and exponential way. This information can be observed through the analysis of Fig.3. After approximately 25 minutes of reaction, the sodium hydroxide is consumed in its entirety, with its number of moles being reduced from 0.03 to 0.

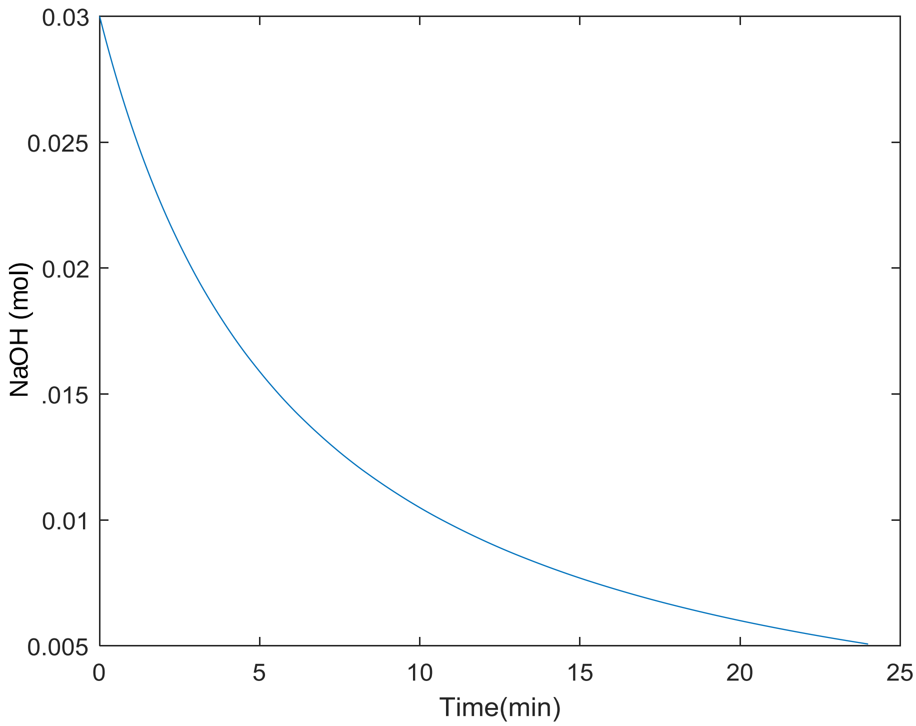

Figure 3. Theoretical curve of sodium hydroxide consumption, in moles, in the hydrogen production reaction over time

Finally, Fig. 4 depicts the consumption behavior of the last parameter modeled and considered in the hydrogen production reaction. Water is also consumed exponentially and, after approximately 25 minutes of reaction, almost 1.4 g of H_2O is consumed.

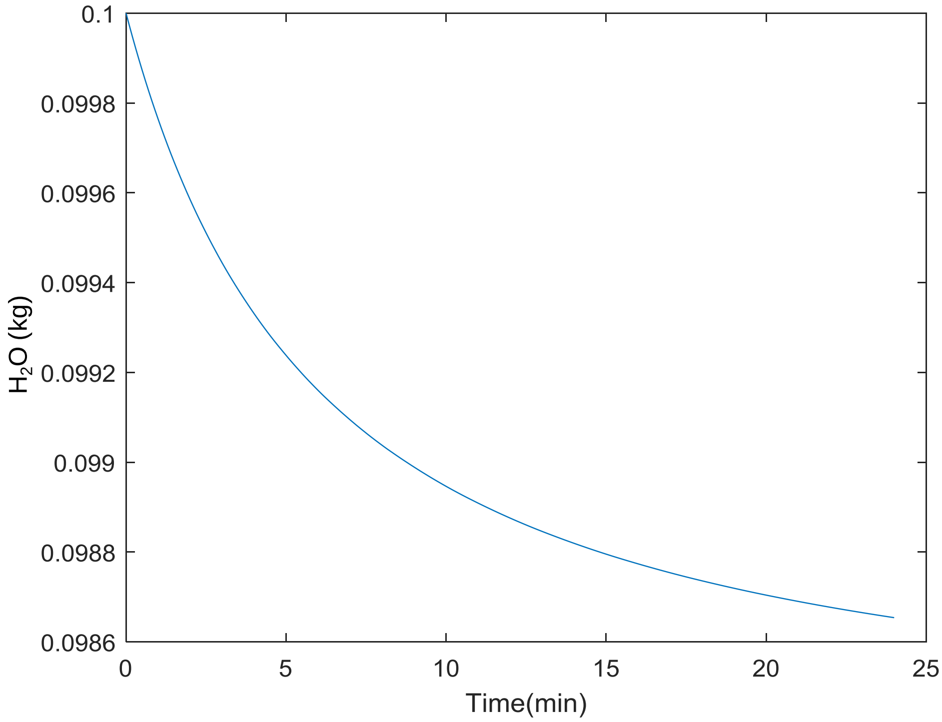

Figure 4. Theoretical curve of water consumption, in kg, in the hydrogen production reaction over time

4. CONCLUSIONS

Energy consumption nowadays has increased considerably. The process of economic growth that countries are going through causes the demand for energy to increase proportionally. The search for alternative, renewable and environmentally more appropriate energy sources and the diversification of the energy matrix have always been objectives of the scientific community. The context in which the world is inserted today makes this an even more urgent need. There are several examples of new energy sources. Hydrogen from the most diverse raw materials has recently emerged as a promising alternative to traditional fuels and even to other renewable energy sources.

The objective of this article was to develop a mathematical model that describes the production of hydrogen from aluminum scrap. The proposed model fitted well to the experimental data, describing in a general way the H_2 production process. The development and improvement of mathematical models for this purpose are necessary to make the proposed technology viable and feasible, increasing the performance of the reactions and reducing costs with energy, reagents and time. The next steps of this work will involve other variables involved in the process, in order to make the model even more refined and able to predict hydrogen production even more correctly.

5. ACKNOWLEDGEMENTS

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6. REFERENCES

Bakenne, A., Nuttall, W., Kazantzis, N., 2016. “Sankey-Diagram-based insights into the hydrogen economy of today”. International Journal of Hydrogen Energy. Vol. 41, No. 19, pp. 7744-7753.

Bengtsson, L., 2006. “The global energy problem”. Energy & environment. Vol. 17, No. 5, pp. 755-765.

Bolt, A., Dincer, I., Agelin-Chaab, M., 2020. “Experimental study of hydrogen production process with aluminum and water”. International Journal of Hydrogen Energy. Vol. 45, No. 28, pp. 14232-14244, 2020.

Chen, L., De Angelis, F., Jin, S., Sun, Y. K., Kamat, P. V., 2018. “Energy research outlook. What to look for in 2018”. ACS Energy Letters. Vol. 3, No. 1, pp. 261-263.

Dresselhaus, M. S. and Thomas, I. L., 2001. “Alternative Energy Technologies”. Nature. Vol. 414, No. 6861, pp. 332-337.

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. 879-893.

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”. International Journal of Hydrogen Energy. Vol. 43, No. 14, pp. 6777-6788.

Noland, B. M. and Erickson, P. A., 2020. “Apparent kinetics of hydrogen production with water-slurried aluminum delivery in aqueous sodium hydroxide solutions”. International Journal of Hydrogen Energy. Vol. 45, No. 46, pp. 24285-24299.

Smalley, R. E., 2005. “Future global energy prosperity: the terawatt challenge”. Mrs Bulletin. Vol 30, No. 6, pp. 412-417.

Setiani, P., Watanabe, N., Sondari, R. R., Tsuchiya, N., 2018. “Mechanisms and kinetic model of hydrogen production in the hydrothermal treatment of waste aluminum”. Materials for Renewable and Sustainable Energy. Vol. 7, No. 2, pp. 1-13.

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