HYDROGEN PRODUCTION METHODS EFFICIENCY COUPLED TO AN ADVANCED HIGH TEMPERATURE ACELERATOR DRIVEN SYSTEM

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ABSTRACT

The hydrogen economy is one of the most promising concepts for the energy future. In this scenario, oil is replaced by hydrogen as an energy carrier. This hydrogen, rather than oil, must be produced in volumes not provided by the currently employed methods. In this work two high temperature hydrogen production methods coupled to an advanced nuclear system are presented. A new design of a pebbled-bed accelerator nuclear driven system called TADSEA is chosen because of the advantages it has in matters of transmutation and safety. For the conceptual design of the high temperature electrolysis process a detailed computational fluid dynamics model was developed to analyze the solid oxide electrolytic cell that has a huge influence on the process efficiency. A detailed flowsheet of the high temperature electrolysis process coupled to TADSEA through a Brayton gas cycle was developed using chemical process simulation software: Aspen HYSYS®. The model with optimized operating conditions produces 0.1627 kg/s of hydrogen, resulting in an overall process efficiency of 34.51%, a value in the range of results reported by other authors. A conceptual design of the iodine-sulfur thermochemical water splitting cycle was also developed. The overall efficiency of the process was calculated performing an energy balance resulting in 22.56%. The values of efficiency, hydrogen production rate and energy consumption of the proposed models are in the values considered acceptable in the hydrogen economy concept, being also compatible with the TADSEA design parameters.

Keywords: nuclear hydrogen production, ADS, HTE, sulfur-iodine, efficiency.

1. INTRODUCTION

Hydrogen is the element considered as the basis of the energy system of the future; The progressive replacement of petroleum can help reduce the environmental impacts associated with the production and use of it. Hydrogen combustion does not produce greenhouse gases, but the application of hydrogen in the future will be as an energy vector rather than as a fuel. An energy vector is a substance that stores energy so that it can be later consumed in a controlled manner. The energy vectors differ from the primary energy sources in which they need to be produced, and a certain amount of energy must be invested. Fortunately the procedures for producing hydrogen are very varied
(Linares) .

Hydrogen production has developed into several branches that can be grouped into the following categories: thermochemical, electrochemical, photobiological and photoelectrochemical.

Very high temperature nuclear reactors can meet the requirements for their implementation in the production of hydrogen in this new energy scenario. The so-called generation IV of nuclear reactors and even some reactors of generation III +, present some projects of nuclear reactors that reach operating temperatures near 1000 oC. Currently the technologies of the HTR-10 and HTTR reactors are contemplated to be coupled to a hydrogen production system using a high-parameter electrolysis process or a thermochemical water dissociation cycle [1], [2].

There are also international projects that study the use of a system driven by a particle accelerator or ADS (Accelerator Driven System) capable of reaching temperatures near 900 oC, sufficient in theory for the production of hydrogen and with some promising characteristics in the transmutation Of long-lived nuclear [3].

The use of generation IV of nuclear reactors for high temperature applications is a topic of repeated reference in the scientific literature today. The high-temperature electrolysis processes and the iodine-sulfur cycle of thermochemical dissociation of water have the greatest possibilities of being used in the production of hydrogen in large volumes [4].

Currently there are several international projects trying to gather experiences in thermal applications of generation IV nuclear reactors. In 2009 the EUROPAIRS (End-User Requirements for Industrial Process Heat Applications with Innovative Nuclear Reactors for Sustainable Energy Supply) project was launched with the participation of 27 countries under the auspices of the European Community. Its main objective is to evaluate the real potential of the coupling of a very high temperature nuclear reactor (VHTR) with industrial processes. Programs such as EUROPAIRS aim to achieve results that improve the technical compatibility between nuclear systems and industrial processes, as well as the economic feasibility of linking systems [3].

Chemical Process Simulation (CPS) and CFD (Computational Fluid Dynamic) dynamics programs offer significant advantages to compensate for this difficulty. The broad database of these CPS programs in terms of chemical species, reactions and the ease of simulation of complex chemical processes make them ideal for the simulation of processes of dissociation of the thermochemical water, as the I-S.

The optimization of the main thermodynamic parameters of a complex chemical process, such as the I-S process, is a task that requires consideration of several factors. The energy consumption of the components, the efficiency of the chemical reactions, the conversion rates of the species should be considered when building an efficient model. The I-S cycle is a closed process, all the chemical components of the cycle are recycled at a theoretical yield of 100%, although in reality this value is not achieved. Theoretically, only water as the raw material for the process must be incorporated continuously [5], [6].

The use of CFD software to solve electrochemical problems is on the rise in recent times. The coupling between fluid dynamics models and electric and electrochemical field models made by commercial CFD programs has shown excellent results compared to experimental and theoretical results [7]–[9].

2. SECOND OR SUBSEQUENT MAJOR HEADING

2.1. Nuclear systems for hydrogen production.

The processes of hydrogen production using both steam reforming and thermochemical decomposition of water and high temperature electrolysis have been associated with some so-called generation IV reactors capable of providing sufficient energy and temperature for these processes [10]–[12].

At the moment, nuclear development is concentrated in the next generation of commercial reactors, some projects of this generation are called VHTR (Very High Temperature Reactor). Among its most important applications is the production of hydrogen by high temperature methods.
A ball-bed-driven throttle-driven system has been studied and designed to achieve high temperatures with the objective of cogeneration of electric energy and hydrogen [13]. The design based on this technology called TADSEA (Transmutation Advanced Device for Sustainable Energy Applications), shown in Figure 7, has the theoretical capacity to reach a maximum core exit temperature of 950 ºC.

Figure 1. TADSEA´s cross-section representation.[14]
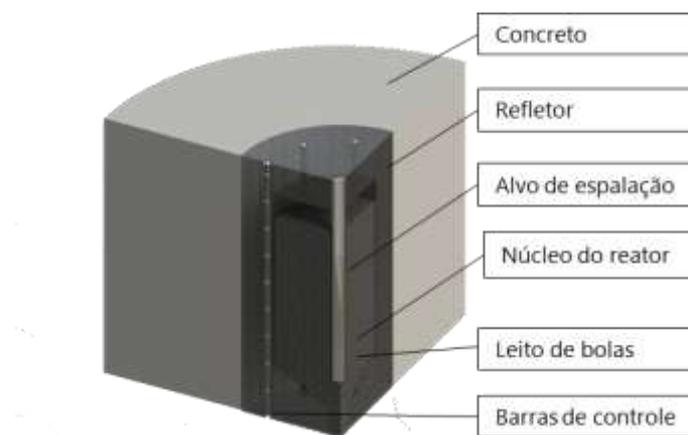
Thus, in principle it can be used for the production of hydrogen by means of high temperature electrolysis or thermochemical cycle I-S of water dissociation. Some of the most important features of TADSEA are presented in Table 1.

Table 1 – TADSEA´s main design parameters.[14]

Parameter	Valor
Interior radius	15,5 cm
External radius	125,75 cm
Height	293,94 cm
Balls in the core	94092
Inlet/Outlet temperature	590 ℃ /950 ℃
Power	100 MW
Coolant	Helium
Helium mass flow rate	53 kg/s
Coolant pressure	7 MPa

The high levels of safety, plant control and the possibilities of long life waste transmutation is one of the main advantages of the systems driven by accelerator. The TADSEA was qualitatively studied for the hydrogen production cycle through the I-S cycle [13] But the development of a thermodynamic model to perform a process efficiency calculation for this reactor is not reported. In addition, the integration of the high temperature electrolysis plant with this technology was not evaluated.

2.2. High temperature nuclear production methods coupled to an VHTR.

2.2.1 Iodine-sulfur thermochemical water splitting cycle.

The cycles of thermochemical dissociation of water offer unique advantages, making them attractive candidates for the production of hydrogen in large volumes. Direct thermal decomposition of water requires extreme temperatures above two thousand Kelvin [15], However the thermochemical cycles use substantially lower temperatures, in the order of 1173 K, combining endothermic and exothermic reactions at low temperatures where, the balance of species and chemical reactions have as a general result the dissociation of the water molecule. The I-S process is composed of three chemical reactions:
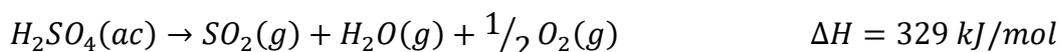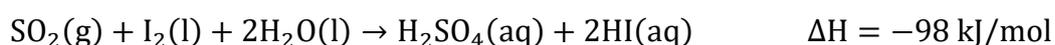
$$SO_2(g) + I_2(l) + 2H_2O(l) \rightarrow H_2SO_4(aq) + 2HI(aq) \qquad \Delta H = -98 \text{ kJ/mol}$$

$$H_2SO_4(ac) \rightarrow SO_2(g) + H_2O(g) + {}^1\!/_2\, O_2(g) \qquad \Delta H = 329\, kJ/mol$$

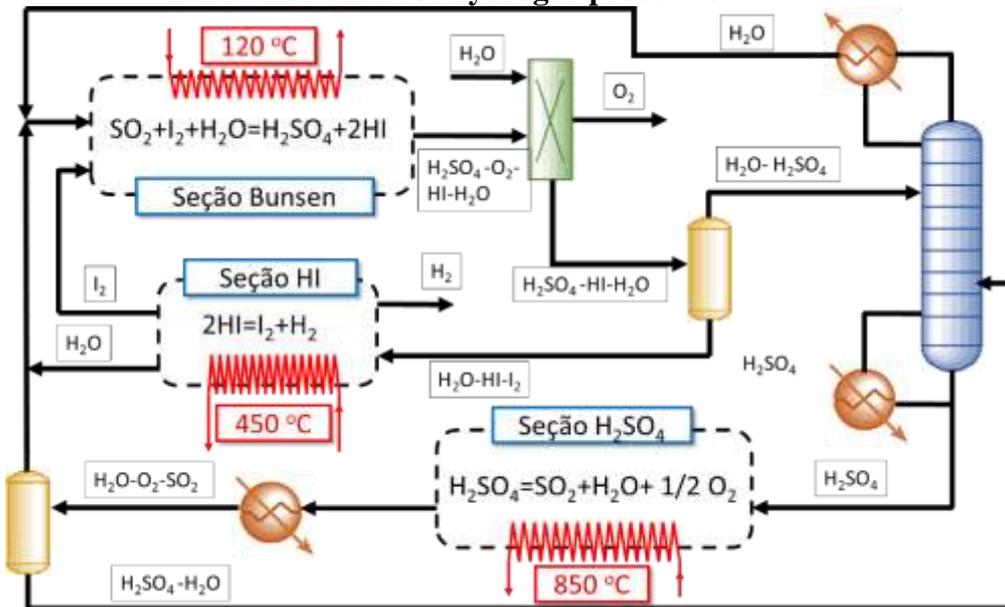$$2HI(ac) \rightarrow H_2(g) + I_2(g) \qquad \Delta H = 119\, kJ/mol$$

Figure 2. Conceptual design of the Iodine- sulfur thermochemical water-splitting cycle flowsheet for hydrogen production .

2.2.2. High temperature electrolysis

Electrolysis is a method of producing hydrogen and oxygen by the direct decomposition of water using electric energy. Conventional electrolysis has been commercially developed since 1890[15].

The electrolysis process is produced in electrolyzers which currently have a production rate ranging from a few cm3 / min to thousands of m3 / h. There are case studies of hybrid plants using renewable energy, which reduces energy costs and minimizes the emissions associated with the hydrogen produced [16].

Under normal pressure and temperature conditions, the change in Gibbs free energy (ΔG) for the water dissociation reaction is positive so it is not spontaneous and an amount of energy equivalent to the value of ΔG must be supplied. In an electrolytic cell, energy is supplied by applying a potential difference between the electrodes placed on an electrolyte. The potential difference V applied to the electrodes produces a maximum work calculated by:

$$\Delta G = nFV_{rev}$$

The V_{rev} magnitude is also known as the thermodynamically reversible potential under normal pressure and temperature conditions (25°C ,1 bar) ΔG=237,178 kJ/mol, then we can rewrite equation 4 as:

$$V_{rev} = \Delta G / nF = 1,229 \text{ V}$$

But ΔG is a parameter dependent on the temperature, the composition of the electrolyte and the gas pressure that can be calculated according to the expression:

$$\Delta G_e = \Delta G_e^0 + RT * ln \left[\frac{(\frac{f_{H_2}}{p^0}) * (\frac{f_{O_2}}{p^0})^{0.5}}{\alpha_{H2O}} \right]$$

2.3. Materials and methods

2.3.1. Chemical process simulation.

The process of thermochemical dissociation of water I-S fit in the category of chemical system, for which the use of so-called activity models is recommended. In these models those recommended to work with various fluids and acids are NRTL and NRTL-Extended developed by Renon and Prausnitz (1969). Other packages may also be used. For the thermodynamic treatment of other chemical species, gaseous components and to approach the distillation columns the Peng-Robinson package is recommended [17].

The Peng-Robinson (PR) model is ideal for calculating densities in systems with many hydrocarbons involved, but can be used with excellent results in non-ideal systems, such as the IS cycle, and together with the NRTL or NRTL- Extended may result in a very detailed description of the cycle thermodynamics [18]. The PR model solves any one, two or three phase system with a high level of accuracy provided that the system complies with the following conditions: temperature range >-271 oC and pressure range <100.000 kPa.

These limitations are not a problem for their use in the simulation of the I-S process since the basis of the latter establishes thermodynamic parameters in this range. The state equation of the PR model employs a special treatment to the interaction of some components (He, H_2, N_2, CO_2, H_2S, H_2O). The formulation of the model equation of the model used in HYSYS® is [19]:

$$P = \frac{RT}{V-b} - \frac{a}{V(V+b)+b(V-b)} \qquad 1$$

Indicating that $Z = \frac{PV}{RT}$ is the compressibility factor the state equation can be written as:

$$Z^3 - (1-B)Z^2 + (A - 2B - 3B^2)Z - (AB - B^2 - B^3) = 0$$

Where:

$$A = \frac{aP}{(RT)^2}$$

$$B = \frac{bP}{RT}$$

$$b = \sum_{i=1}^{N} x_i \left(0,077796 \frac{RT_i}{P_i}\right)$$

$$a = \sum_{i=1}^{N} \sum_{j=1}^{N} x_i x_j \left[\left(0,457235 \frac{(RT_i)^2}{P_i}\right) a_i \left(0,457235 \frac{(RT_j)^2}{P_j}\right) a_j\right]^{0,5} (1 - k_{ij})$$

$$\frac{H - H^{ID}}{RT} = Z - 1 - \frac{1}{2^{1,5}bRT}\left[a - T\frac{da}{dt}\right] \ln\left(\frac{V + (2^{0,5} + 1)b}{V - (2^{0,5} - 1)b}\right)$$

$$\frac{S - S_o^{ID}}{R} = \ln(Z - B) - \ln\frac{P}{P^o} - \frac{A}{2^{1,5}bRT}\left[\frac{T}{a}\frac{da}{dt}\right] \ln\left(\frac{V + (2^{0,5} + 1)b}{V - (2^{0,5} - 1)b}\right)$$

$$a = \sum_{i=1}^{n} \sum_{j=1}^{n} x_i x_j \left(a_i a_j\right)^{0,5} (1 - k_{ij})$$

$$b_i = 0,077796 \frac{RT_i}{P_i}$$

$$a_i = 0,457235 \frac{(RT_i)^2}{P_i} a_j$$

$$\sqrt{a_j} = 1 + m_i \left(1 - T_i^{0,5}\right)$$

For the calculations of enthalpy and entropy parameters, the equations used are as follows:

$$m_i = 0,37464 + 1,5422w_i - 0,26992w_i^2$$

Combining the state equation for the thermodynamic variables of pressure, temperature and volume and equations for the calculation of the enthalpy and entropy of each component of the system can be obtained through the PR model a complete thermodynamic description of the process. However, this model does not include the chemical activity data of the components, so it is insufficient to describe chemical reactions and therefore must be complemented by other models that are able to simulate them.

The equations of the NRTL (Non-Random Two Liquids) model were proposed by Renon and Prausnitz in 1968 [20]. This equation uses the theory of statistical mechanics and the net cell theory to represent the structure of liquids. The equations governing the NRTL model are:

Where:

$$\ln(\gamma_i) = \frac{\sum_{j=1}^{N} \tau_{ji} G_{ji} X_j}{\sum_{k=1}^{NC} G_{ki} X_k} + \sum_{j=1}^{N} \frac{X_j G_{ij}}{\sum_{j=1}^{NC} G_{kj} X_k} \cdot \left\{ \tau - \frac{\sum_{k=1}^{N} \tau_{kj} G_{kj} X_k}{\sum_{k=1}^{N} G_{kj} X_k} \right\} \qquad 2$$

$$G_{ij} = \exp(-\alpha_{ji} \cdot \tau_{ji})$$

$$\tau_{ij} = \frac{g_{ij} - g_{ji}}{RT} \qquad\qquad \tau_{ji} = \frac{g_{ji} - g_{ij}}{RT}$$

The expressions of the NRTL model allow us to create equations capable of representing the behavior of liquid-vapor, liquid-liquid and liquid-liquid-liquid equilibria. In this way HYSYS links the thermodynamic variables calculated by the PR model with the chemical activity of the system components, obtaining chemical reactions that describe it [21].

2.4. CPS model for the HTE process coupled to the TADSEA

The SOEC simulation and optimization is one the most important task to do in this study. The SOEC included in the flowsheet developed for the HTE process was studied deeply optimizing its main operating parameters in order to maximize the hydrogen production rate [22]. In order to incorporated the model build in CFD was performed an approach of the electrolyzer cell consisting in a conversion chemical reactor reproducing the conditions obtained in the detailed CFD study as shown in Figure 3:

Figure 3 - SOEC flowsheet developed in HYSYS for HTE simulation.
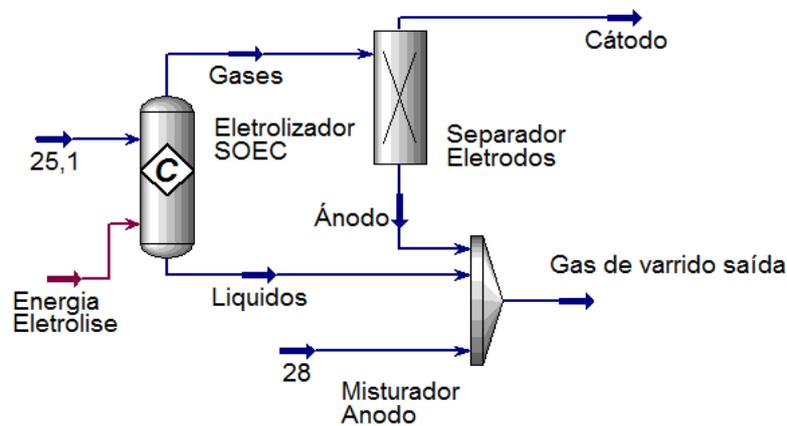
Fonte: Autor.

The P power required for high temperature electrolysis includes thermal (Q_{Heat}) e a elétrica (W_{elect}) and is calculated according to the expressions:

$$V_{op} = \text{average } V_{nerst} + i \cdot ASR$$

$$W_{elect} = V_{op} \cdot i \cdot A$$

$$P = W_{elect} + Q_{Heat}$$

Where:

i : current density (A/cm^2).

ASR : área specific resistance (Ωcm^2).

V_{op} : voltage (V).

A : electrolitic cell area (cm^2).

averageV$_{nerst}$: average Nernst potential.

For the generation of electrical energy required for the HTE process, a Gas Brayton cycle connected to TADSEA is used. The model consists of a gas turbine and an electric generator connected to it, two compressors (one low pressure and the other high) with an IHX intermediate heat exchanger, heat recovery unit and another heat exchanger at the entrance of the Low pressure compressor. The helium flow from the TADSEA is separated into two streams by a valve, thereby controlling the gas turbine dedicated mass flow and the HTE process. This last mass flow will vary depending on the power demand of the components of the proposed model for the HTE process.

The proposed model for the Brayton gas cycle built in HYSYS is presented below:

Figure 4 – Brayton gas cycle flowsheet coupled to TADSEA.

Considering an electric generator efficiency of 98% [23] Then the available electrical energy for the HTE process is WSOEC = 38.29 MWe. The calculation of the efficiency of the energy conversion cycle (ηPCS) is done by the expression:

$$\eta_{PCS} = \frac{W_{elect}/\eta - W_{Comp} - W_{Cir}}{Q_{TADSEA}} = 44{,}03\ \%$$

Where:

W_{elect}: Electric power produced by the generator.

W_{Comp}: Electric power consumed in compression.

W_{Cir}: Electric power consumed in circulation.

The power obtained in the gas turbine (W$_{turb}$= 68,97 MWe) And the other powers involved in the Brayton cycle (W$_{comp}$= 32,09 MWe, W$_{cir}$= 0,2085 MWe) Were obtained from the energy balance of the proposed model. For the initial conditions an efficiency for the energy

conversion cycle is η_PCS = 44.03%. The thermal efficiency of the energy conversion cycle can be calculated according to [23] :

$$\eta_{ter} = \frac{W_{SOEC}}{Q_{TADSEA}} = 38{,}29 \ \%$$

The efficiency value obtained for the proposed model of the Brayton cycle is in the order of those reported for other Brayton cycle models, considering that realistic values were used for the components of the cycle.

The electric energy obtained from the conversion cycle and the mass flow of helium from TADSEA will be used for the components of the hydrogen production process by HTE and the gas sweeping system. To connect the Brayton cycle and the flow diagram for the HTE process, an IHX type heat exchanger with the characteristics reported in other works [11]

Figure 5 – HYSYS HTE flowsheet proposed for the electrolysis section.
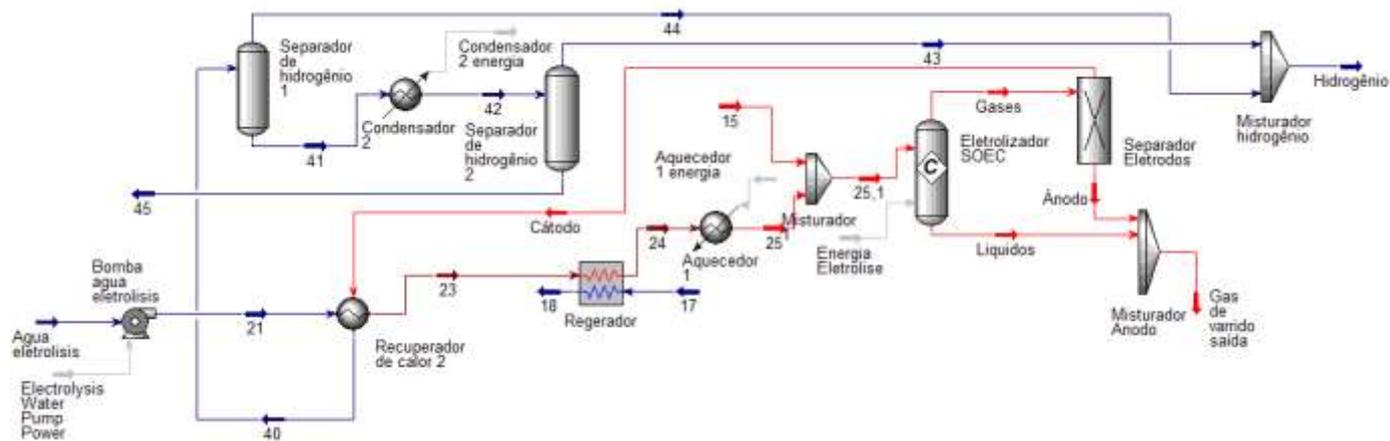
The electric energy obtained from the Brayton cycle is used for the electrolysis reaction in the SOEC Electrolyzer considering that an optimized unit cell consumes 48 kW and the energy consumptions of the components were estimated the initial flows that the SOEC can process with the energy supplied to the model.
Thus, with the available electrical energy can be fed 770833 unit cells with a total electrical consumption of 38.2 MWe, this being the maximum number of cells that can compose the stack of SOEC. Also the incoming mass flow in the SOEC (25.1) is calculated considering the mass flow of the unit cell optimized in the study made in CFD, obtaining 9.25 kg / s for the model in HYSYS, always keeping the mass fractions calculated in the model in FLUENT.
A sweep gas system is used for separate the gases after the electrolysis subsection. This system can be used for syngas production, but this was not considered in this work.

Figure 6 – Complete process flow diagram for the HTE process coupled to TADSEA through a Brayton gas cycle.
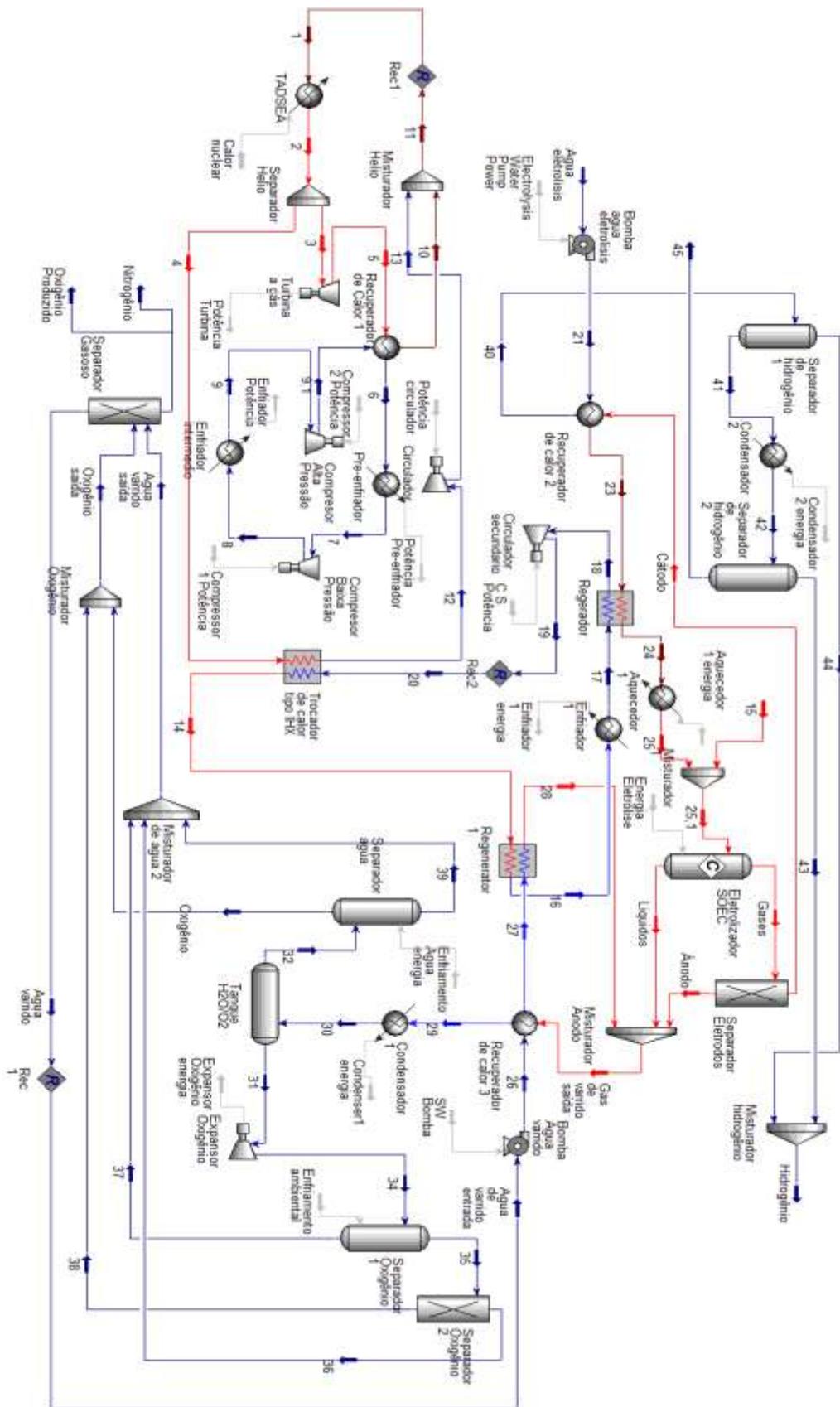
The efficiency of the proposed model for the hydrogen production process by the HTE high temperature electrolytic connected to the TADSEA is calculated using the ratio of the energy contained in the hydrogen produced HHV (High Heating Value) and the energy consumed during the production process according to the Published by Havergo in 2009 [24]:

$$\eta_{H_2} = \frac{HHV}{\sum_i Q_i} = 34{,}51\%$$

The denominator of the equation is calculated after making an energy balance in the proposed model, quantifying the thermal energy consumed as well as the electric consumption of the components of the flow diagram (Q_i). The obtained efficiency value is in the range of values reported in the literature for HTE systems connected to other reactors and semiempirical studies for the TADSEA operating temperature range [25].

2.4.1. Parametric studies for the HTE proposed flowsheet.

The electrical power of the SOEC and other parameters of the flow diagram will also depend on the operating voltage, which will result in a change in the efficiency of the complete process. Therefore, a parametric analysis was made of the influence of the operating voltage of the SOEC on the efficiency of the process.

**Figure 7 – Effect of the SOEC operating voltage in the HTE process efficiency**.
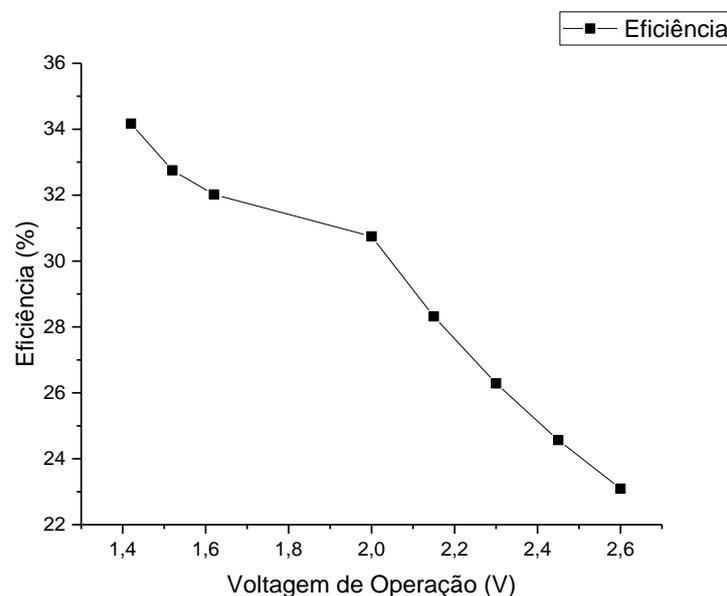
Increasing the operating voltage of the electrolytic cell produces a decrease in the overall efficiency of the high temperature electrolyzing process as shown in Figure. This behavior has several causes: the first is the considerable increase in the electrical energy required for the electrolysis in the SOEC that is not compensated by the increase of the hydrogen production as it is reported in some works [25], [26].
 Additionally, increasing the operating voltage of the electrolyzer increases the power consumption of other components of the model, especially the capacitors.

Another parameter that influences efficiency is the mass water flow that is supplied to the system. While this should result in an increase in the amount of hydrogen produced does not mean that the efficiency of the process increases. The initial value of 8.325 kg / s defined for the initial model was established after calculating it to obtain the greatest use of the energy from the TADSEA and the gas sweeping system.

Figure 8 – Effect of the initial water mass flow in the HTE process efficiency.
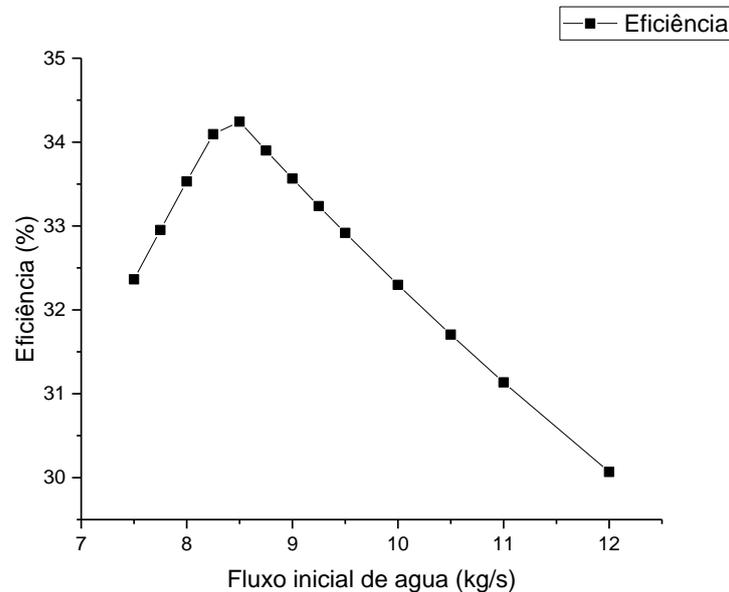
At rates ranging from 7.5 kg / s to 8,325 kg / s, although the efficiency of the process is less than optimal, it grows with increased flow because the additional power that is consumed is offset by an increase in hydrogen production In SOEC. For values above 8,325 kg / s the process efficiency decreases when the flow increases, firstly because as it was obtained in the detailed analysis of the SOEC the mass fraction of hydrogen decreases with the increase of the water flow. In addition there is an increase in the energy required in the SOEC that exceeds the energy that TADSEA can provide, thus requiring additional electrical energy for the SOEC.

The other study carried out is the calculation of the efficiency depending on the temperature and the power of the TADSEA. This study was done by varying the temperature at the exit of the TADSEA that influences the efficiency of the process due to the variation of the parameters of the Brayton cycle and the gas sweep system and the HTE process. Increasing the temperature at the TADSEA outlet decreases the amount of helium required to produce the same electrical power in the gas turbine and simultaneously increases the amount of helium available to heat the gases in the HTE system, both of which have positive effects on the efficiency of the process as Is shown in Figure 9.

**Figure 9 – Effect of the outlet coolant temperature in the HTE process efficiency.**
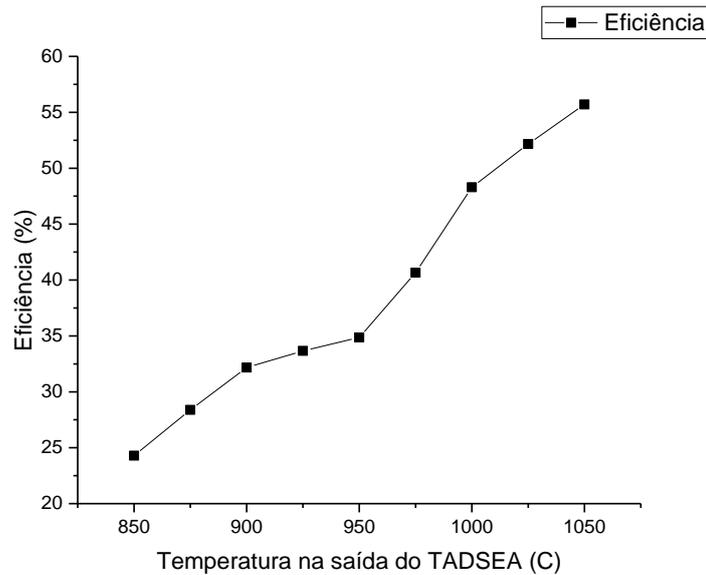
The results presented above show that the efficiency of the complete cycle considering a detailed flow diagram model and realistic values for the component definitions can reach values above 55%, values reported by Yildiz and Kasimi and other authors for nuclear systems with these temperatures in the exit . [27].

2.5. CPS model for the IS cycle coupled to the TADSEA.

The IS process can be divided in 3 main sections: Bunsen section, H2SO4 decomposition section and HI decomposition section. In this study was performed the optimization of the section operating parameters separately. Then the complete model was analyzed with the improved conditions and results. For Bunsen section was obtained the optimal water molar flow feed into the process Taking into account the results obtained, the values of the initial flow $SO_2=2,813e-2$ kgmole/s, $I_2=0,25$ kgmole/s e $H_2O= 0,45$ kgmole/s, respecting the previously defined stoichiometry.

Figure 10 – Effect of the water mass flow to Bunsen section in the conversion rate.
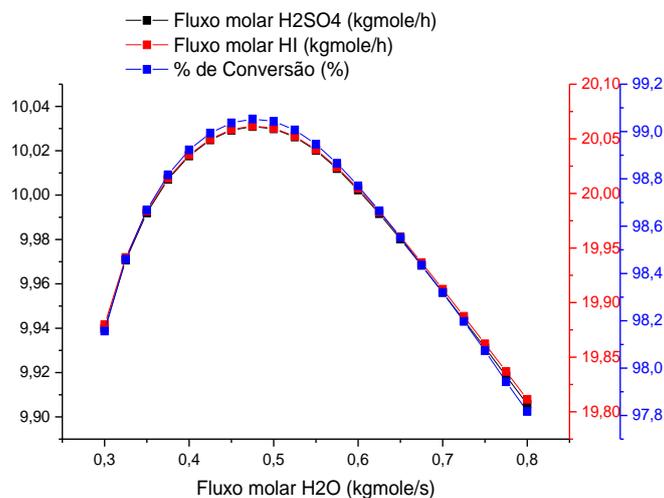
Another important analysis that must be realized by the importance of the process efficiency is the influence of the power dedicated to the heating of the Bunsen reactor in the production of acids, as it also influences the production of hydrogen. A variation of the thermal power consumed (energy flow E4) is made in the reactor to ensure the homogeneity of the temperature in the reaction volume. Figure 11 shows the results obtained for this analysis.

Figure 11 – Effect of the Bunsen reactor heating power in the conversion rate.
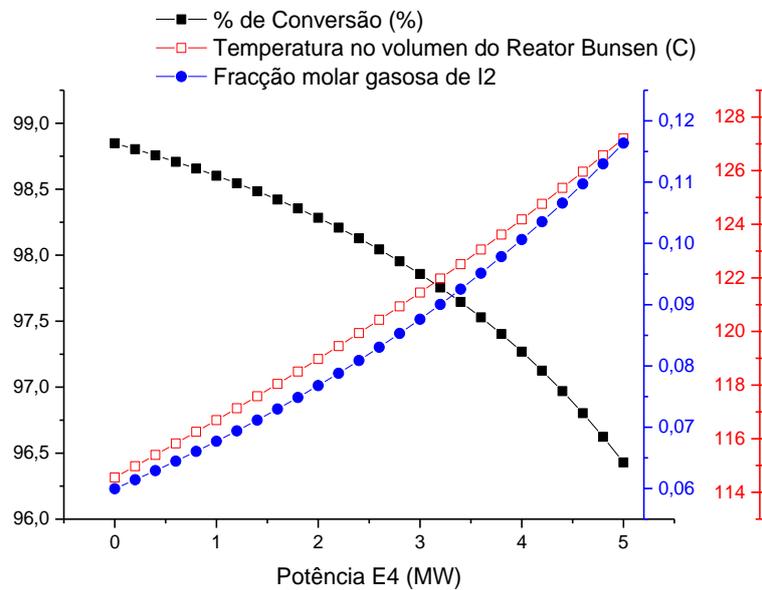
The reduction of the conversion coefficient of the reaction is justified due to the increase of the molar fraction of I_2 present in the mixture of reagents which does not favor the occurrence of the reaction on the surface of the liquid or solid iodine. This result is in correspondence with that reported by other experimental studies [28] [29].

For the sulfuric acid decomposition sections the most important analysis to do is the thermal stability by varying the operating temperature and obtaining an independent conversion factor for the whole section [30].

Figure 12 – Thermal stability of proposed sulfuric acid decomposition section.
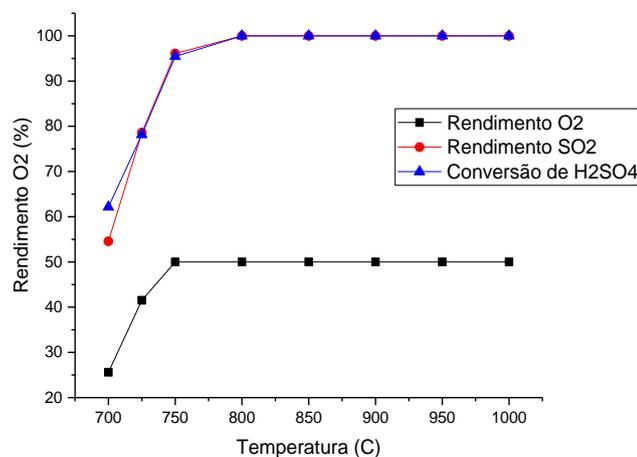
The thermal stability of the section shows an independence of obtaining oxygen at temperatures above 800 ºC which is an important result because it maximizes section efficiency for these parameters [31].

One of the most important parameters in the iodidric acid decomposition section is the purity of the acid before entering the plug flow reactor, so was employed a distillation column to concentrate the acid obtaining the results showed below.

Figure 13 – Variation of the chemical species in the HI section distillation column.
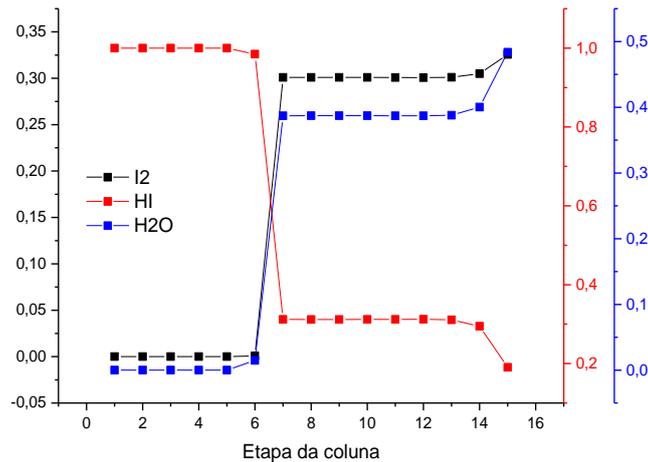
The almost 1 grade purity of the HI at the column distillation stage 1 will guaranteed the maximum conversion percent in the subsequent decomposition.

In the same way as for the HTE model, a Brayton gas cycle is used to provide the necessary electrical energy for the components of the I-S cycle and to have the opportunity of cogeneration of electrical energy, which increases the efficiency of the process. The Brayton cycle employed for the I-S model has the same characteristics as those summarized in Table X employed for the HTE process model. Figure 14 shows the complete model proposed for the I-S cycle of thermochemical dissociation of the water connected to the TADSEA by means of a Brayton gas cycle.

Figure 14 - Proposed model for the complete I-S cycle.
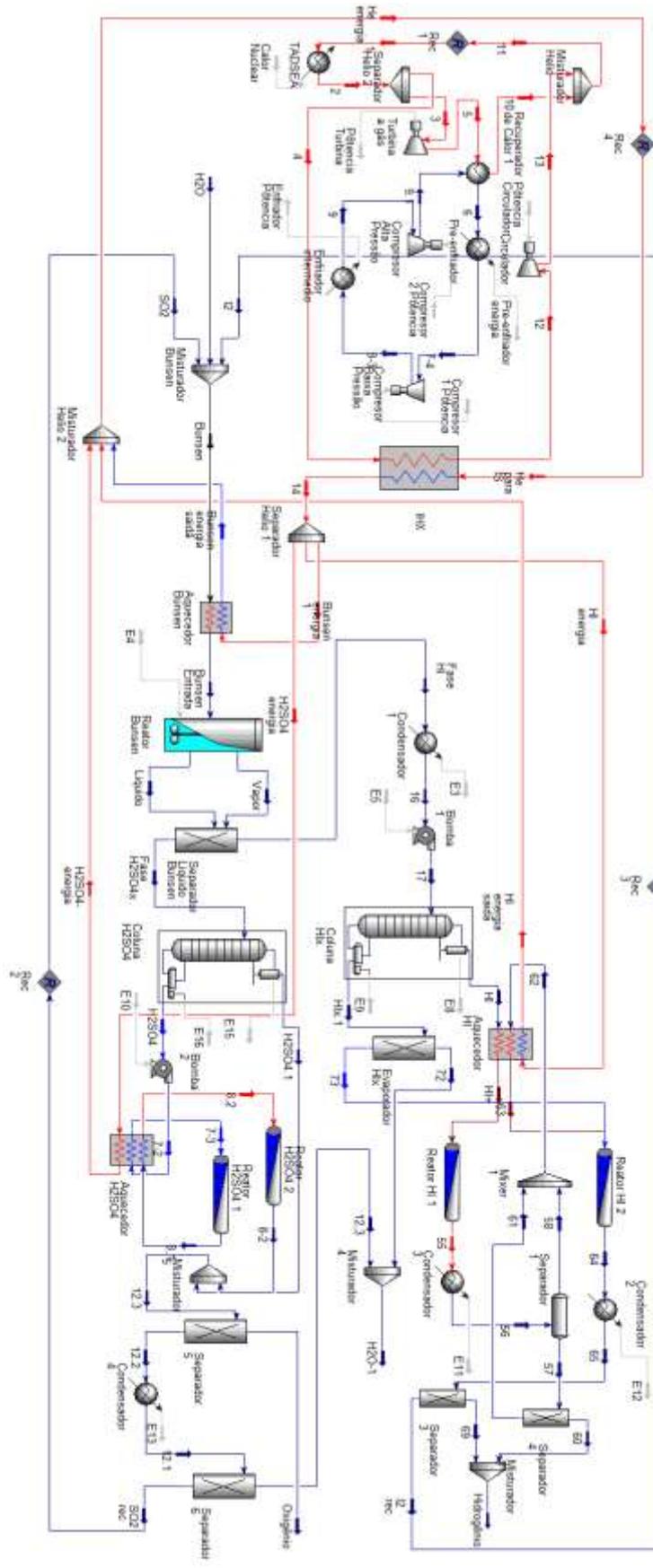
In the case of the I-S cycle model 33.01 kg / s of helium are used for the Brayton cycle, producing an electric power W_elect = 47.66 MWe considering the same polytropic efficiency of the turbine. The energy consumed in the Brayton cycle in compression and circulation is W_Comp = 18.14 MW and W_Cir = 0.9349 MW. Considering that the helium flow that was dedicated to the Brayton cycle has a power of Q_TADSEA = 62.26 MW then the efficiency of the energy conversion cycle can be calculated as:

$$\eta_{PCS} = \frac{W_{elect} - W_{Comp} - W_{Cir}}{Q_{TADSEA}} = 45,92 \text{ \%}$$

This obtained efficiency value is in the range of values reported by other authors for theoretical and semiempirical calculations [11], [32]. The proposed model is flexible because the fraction of the helium flow of TADSEA that is dedicated to the production of electric energy can be modified, also modifying the capacity of hydrogen production.

The total efficiency of the IS process is determined as the ratio between the energy contained in the produced hydrogen (Q_{H2}) and the amount of energy that was consumed in both thermal and electrical [33].

$$\eta_{I-S} = \frac{Q_{H_2}}{H_{heat} + H_{elect}} = 22,56 \text{ \%}$$

The value obtained for the proposed model is in the range of values reported by some of the most complete works of the main research groups dedicated to the theme [34]–[36].

3. CONCLUSIONS

The model for the HTE process was developed using the parameters obtained in the CFD study for a unit cell of the SOEC. Finally, a stack of these unit cells composed of 770,833 cells operating at a current density of 0.6135 A / cm2 can be supplied by TADSEA. It was calculated the water mass flow rate that can process the model (8.325 kg / s), guaranteeing the maximum efficiency of the HTE process. The flow diagram for optimized conditions produces 0.164 kg/s of hydrogen.
The efficiency of the complete model was calculated by performing an energy balance on the components of the flow diagram and considering the energy contained in the hydrogen produced using HHV. The overall efficiency of the process is 34.51%, acceptable value is coincident with the data reported by other authors.

A model is also developed that represents a detailed approximation of a process flow diagram for the IS cycle that allows obtaining the compositions and operating conditions of the material flows and model components. This represents a powerful tool for evaluating the integration of the I-S cycle with several energy sources, such as a very high temperature nuclear system.

It is proposed a model for the complete and closed I-S cycle connected to the TADSEA with a thermal power of 100 MW employing a Brayton gas cycle for the generation of energy. The proposed model has the possibility of cogeneration of electric energy to improve the efficiency of the process. The connection of the TADSEA with the model for obtaining hydrogen is done

by employing an IHX type heat exchanger achieving an energy conversion cycle efficiency of η_PCS = 53.27%.

The total efficiency of the iodine-sulfur water dissociation process is calculated by making an energy balance in the proposed model and calculating the energy contained in the hydrogen produced using HHV resulting in an overall efficiency of 22,56 %.

The efficiency, production rate and power consumption values of the models developed for the HTE and I-S cycles allow us to conclude that both methods are compatible with TADSEA, and that this nuclear system can be used as a primary source of energy. Although the design for the I-S cycle presents lower values of efficiency, this presents the advantage of the cogeneration of electric energy. However, the model for the high-temperature electrolysis process does not allow this cogeneration, besides having higher efficiency values, it has the possibility of being used for cogeneration of syngas.

In relation to the future work that will be done are a technical and economic evaluation of the models considering the costs of both methods, so that economic elements can be incorporated to evaluate the feasibility of their employment linked to TADSEA. In the case of the HTE process model, it is possible to analyze the possibility of producing syngas in the gas scan subsystem as a by-product of the model. In addition, the models will be made in dynamic mode to evaluate other operating parameters of the processes and their influence on efficiency. Process safety assessments can also be made based on the models developed and the results obtained in this work.

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