Modelling of Aluminium-fuelled Power Plant with Gas Turbine

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Abstract. Presented work is devoted to the modeling of aluminum-fuelled power plant based on aluminum-water reactor, steam-hydrogen turbine, condenser and air-hydrogen fuel cell battery. Parameters of aluminum-water reactor were the following: pressure – 15 MPa, temperature – 600 K, steam to hydrogen mass ratio – 40. It was shown that without gas turbine the plant’s electrical and total efficiencies are 12 % and 72 % respectively. If gas turbine with internal efficiency of 80 % is used the electrical efficiency of plant increases up to 25 ÷ 30 %. Total efficiency of power plant in this case can reach 80 %.

1. Introduction
Aluminum has been proposed for the role of perspective non-organic energy storage mater by a number of researchers [1]-[5]. Potentially high level of aluminum integration in future energy economy is bounded with high content of aluminum in the earth's crust, safety and moderate cost of aluminum storage and transportation [6], as well as possible regeneration of such energy carrier. One of promising ways to convert the chemical energy of aluminum into useful forms of energy is aluminum oxidation in water or water steam with heat and hydrogen production [7]. When aluminum reacts with water, 15-16 MJ of heat, 0.111 kg of H₂ and more than 1.9 kg of aluminum oxide are produced per a kg of aluminum. Oxidation products (aluminum oxide or hydroxide) can be returned to the cycle of aluminum production or used for the production of adsorbents, catalysts, insulators, high-purity aluminas and other [8]-[10].

Aluminum oxidation in water under standard conditions is impossible due to formation on its surface of an oxide film. The search of ways of aluminum surface activation or oxide film destruction for fast and complete aluminum oxidation is an actual tusk today [7]. A number of methods of aluminum activation have been already proposed. These methods include the mechanochemical preparation of highly reactive aluminum powder alloyed with gallams of various compositions including Ga, In, Sn, Zn and other additions [11]-[12]. Enhanced aluminum oxidation in water is observed after aluminum co-milling with graphite [13] and silicon [14]. Aluminum particle surface is activated by milling with different metal oxides such as Al₂O₃, TiO₂, Co₃O₄, Cr₂O₃, Fe₂O₃, MnO₂, NiO, CuO, ZnO, MoO₃, Bi₂O₃ and other [15]-[17]. Milling with salts was also proposed as perspective way of aluminum activation [18]-[20]; new aluminum surface created by milling is covered by salt during the storage of aluminum preventing its oxidation, such surface is revealed by salt dissolution in aqueous medium. Aluminum oxidation can be accelerated in alkaline aqueous solutions [21]. There is also incalculable quantity of methods which assume the use of additional chemicals that help to realize fast and complete aluminum oxidation in aqueous media. Recently developed method of aluminum micron powder oxidation in high-temperature steam [22]-[24] allowed applying pure (without alkali and any other chemical activators) water as oxidant.
Kinetics of aluminum micron powders oxidation in high-temperature boiling water was studied in [25-26]. It was established that aluminum powders with average particle size from 4 to 70 μm, which are produced in industrial scale, were intensively oxidized within the special reactor under about 300 °C and 10 MPa water steam; the reaction time was several tens of seconds.

Further development of power plant based on “aluminum-water” reactor as high-pressure steam-hydrogen generator was based on the results of kinetic experiments and a number of designing investigations. One of such calculations was presented in [23]. It was devoted for thermodynamics of nonstop reactor operation. Reactor’s thermo- and gas-dynamic parameters estimation and optimization was carried out in that work, an optimum parameter field (composed of reactor temperature, pressure, volume and others) in the view of thermodynamic effectiveness was determined.

Based on the results of [22]-[26] and other designing investigations an experimental co-generation aluminum-fuelled power plant was developed [27]. It consumes aluminum micron powder as primary fuel and pure water as primary oxidant. Hydrogen, which is produced within aluminum-water reactor, is used as secondary fuel for electrical energy generation via air-hydrogen fuel cell battery. Nominal hydrogen generation rate of the plant is 10 m³/hour. Developed and created power plant outputs useful electrical energy and heat, and also it can produce hydrogen as end product. From 1 kg of aluminum the power plant produces 1 kWh of electrical energy and 5–7 kWh of heat. Plant’s electrical and total efficiencies are 12 % and 72 % respectively.

Main reason of low electrical efficiency of created aluminum-fueled power plant is that only chemical energy of hydrogen is converted into useful electrical energy and the heat of aluminum-water reaction doesn’t used. At the same time the heat of aluminum-water reaction per a kg of Al is about 15-16 MJ and it is comparable with the chemical energy of 0.111 g of hydrogen produced from a kg of Al. So it is profitable to convert the heat of aluminum-water reaction into useful electrical energy as well.

One of possible way to convert the heat of aluminum-water reaction into useful electrical energy is the use of gas turbine after aluminum-water reactor and before a fuel cell. In this case steam-hydrogen mixture generated in aluminum-water reactor expands in steam-hydrogen turbine, then water is condensed in a condenser and then hydrogen is consumed by air-hydrogen fuel cell battery (figure 1). Presented work is devoted to the modeling of aluminum-fuelled power plant with gas turbine shown in figure 1. Parameters of aluminum-water reactor are imported from our previous research [27]. The main aims of presented work are the development of calculation method and calculation of thermodynamic parameters of proposed plant.

2. Modeling methods

2.1. Input data for calculation

In this paper, we will consider the calculation of scheme of power plant based on the reactor of hydrothermal oxidation of aluminum described in our previous research work [22-27]. To oxidize micron fractions of aluminum powder with high rates and completeness of reaction in such reactor, a high temperature of 570 to 630 K and a pressure of 10 to 20 MPa is created. Aluminum is fed to the reactor in an aqueous suspension by means of a high-pressure pump. Aluminum hydroxide and hydrogen formed within the reactor are withdrawn from the bottom and the top of reactor correspondingly. During the continuous operation of reactor, the temperature and pressure are kept constant in it.

The composition of the steam-hydrogen mixture at the outlet from the reactor depends on the water excess ratio with respect to aluminum in the suspension entering the reactor [23]. The ratio of the mass of steam to the mass of hydrogen can be from 30 to 40 [24]. In this case, the thermal energy of the steam-hydrogen stream reaches 60 ± 80 % of the thermal energy released in the reactor (15-16 MJ per kg of Al), and taking into account the chemical energy of hydrogen, the steam-hydrogen mixture contains from 80 to 90 % of the chemical energy of aluminum (30.97 MJ/kg).

In present work we will consider the following parameters of aluminum-water reactor: pressure – 15 MPa, temperature – 600 K, steam to hydrogen mass ratio – 40. We assume that hydrogen output rate is 1 g/s that corresponds to aluminum consumption rate of 9 g/s (in case of full oxidation of aluminum). Taking into account the calorific value of aluminum (30.97 kJ/g), the input heat power is 278.7 kW.
2.2. Modelling of steam-hydrogen turbine

The main calculation element of the scheme shown in figure 1 is steam-hydrogen turbine (or steam-gas turbine in common case). The process of expansion of the steam-hydrogen mixture in the steam-hydrogen turbine includes both the expansion of both components and the process of heat exchange between them. To calculate the process of steam-hydrogen expansion we will use two databases: Industrial Formulation for the Thermodynamic properties of Water and Steam (IAPWS-1997) and IVTAN THERMO [28] for other individual substances (like H2).

The input variable parameters in the modeling of steam-hydrogen turbine are total pressure \( P_0 \) and temperature \( T_0 \) of steam-hydrogen mixture at the input of turbine, contents of steam and hydrogen in steam-hydrogen mixture – \( \frac{m_{H_2O}}{m_{H_2O} + m_{H_2}} \) and \( \frac{m_{H_2}}{m_{H_2O} + m_{H_2}} \) respectively, pressure of the mixture at the output of turbine – \( P \), and the internal efficiency of turbine - \( \eta \). The parameter \( \eta \) characterizes the degree of irreversibility of the expansion process and depends mainly on the type of turbine and the flow characteristics of the working media. Parameters that are determined during the calculation are the initial and final partial pressures of steam and hydrogen, density of steam, final temperature, power of turbine and other parameters.

The process of isentropic expansion of steam-hydrogen mixture (\( \eta = 1 \)) is conveniently represented as successive isentropic processes of expansion of its components from its initial partial pressures (\( P_{H_2O}^0 \) and \( P_{H_2}^0 \)) and temperature \( T_0 \) to final partial pressures (\( P_{H_2O}^f \) and \( P_{H_2}^f \)) and the process of heat exchange between the components of the mixture without changing their pressures. The determination of the parameters of steam-hydrogen mixture after the isentropic expansion is flown from the solving of the following system of equations:

\[
\left\{ \begin{align*}
P &= P_{H_2O}^0 + P_{H_2}^f \\
\nu &= \frac{m_{H_2}}{m_{H_2O}} \times \frac{1}{\frac{P_0 - P_{H_2O}^0}{P_{H_2O}^0}} \\
\nu &= \nu(P_{H_2O}^0, T) \\
h_{H_2O} = f(P_{H_2O}^0, T, \nu) \\
T_{H_2}^S &= T_0 \times \left( \frac{P_{H_2}}{P_{H_2}^0} \right)^{\frac{k-1}{k}} \\
h_{H_2O}^S &= \psi(P_{H_2O}^0) \\
h_{H_2} &= C_{PH_2} \times T \\
m_{H_2O} \times \left( h_{H_2O} - h_{H_2O}^S \right) = m_{H_2} \times C_{PH_2} \times (T_{H_2}^S - T)
\end{align*} \right. \tag{1}
\]

where \( \nu(P_{H_2O}^0, T) \) – the dependence of the specific volume on pressure and temperature (it is known from IAPWS-1997); \( h_{H_2O} = f(P_{H_2O}^0, T, \nu) \) – the dependence of the specific enthalpy of steam on pressure, temperature and specific volume (it is known from IAPWS-1997); \( h_{H_2O}^S \) – the specific enthalpy of steam after isentropic expansion of steam from \( P_{H_2O}^0 \) to \( P_{H_2O}^0 \); \( T_{H_2}^S \) – hydrogen temperature after isentropic expansion from \( P_{H_2}^0 \), \( T_0 \) to \( P_{H_2}^f \); \( k \) – isentropic index of hydrogen (the dependence of \( k \) on \( T \) is not taken into account); \( h_{H_2}^S = \psi(P_{H_2O}^0) \) – the dependence of the specific enthalpy of steam on pressure and specific entropy, that in the case of known initial entropy is a function of one variable parameter (it is known from IAPWS-1997); \( h_{H_2} \) – final specific enthalpy of steam; \( h_{H_2} \), \( C_{PH_2} \) – final specific enthalpy and heat capacity of hydrogen.
**Figure 1.** Scheme of aluminum-fuelled power plant with gas turbine: 1 – aluminum-water reactor, 2 – steam-hydrogen turbine, 3 – condenser, 4 – air-hydrogen fuel cell battery.

The initial partial pressures of steam $P_{H_2O}^0$ and hydrogen $P_{H_2}^0$, as well as the specific volume of steam $v_0$, are determined using known input calculation parameters: $P_0$, $T_0$ and $\frac{m_{H_2O}}{m_{H_2}}$. Solving the system of equations (1), we determine the final temperature ($T$), the partial pressures of steam and hydrogen ($P_{H_2O}$ and $P_{H_2}$), the specific volume of steam ($v$), the specific enthalpies of steam ($h_{H_2O}$) and hydrogen ($h_{H_2}$) after isentropic expansion of the steam-hydrogen mixture.

The performance of isentropic expansion of steam-hydrogen mixture is:

$$L = (m_{H_2O} + m_{H_2}) \times (h_0 - h) \quad (2)$$

where $h_0$ is the specific enthalpy of the steam-hydrogen mixture before expansion, and $h$ is the specific enthalpy of the steam-hydrogen mixture after expansion. The initial and final specific enthalpies of the steam-hydrogen mixture are composed of the corresponding enthalpies of steam and hydrogen:

$$h_0 = \frac{m_{H_2O} \times h_{H_2O}^0 + m_{H_2} \times h_{H_2}^0}{m_{H_2O} + m_{H_2}} \quad (3)$$

$$h = \frac{m_{H_2O} \times h_{H_2O} + m_{H_2} \times h_{H_2}}{m_{H_2O} + m_{H_2}} \quad (4)$$

where $h_{H_2O}^0$, $h_{H_2}^0$ - specific enthalpies of steam and hydrogen before expansion, $h_{H_2O}$, $h_{H_2}$ - after expansion. By substituting the values of specific enthalpies found in equation (1) into equations (2)-(4) we find the performance of steam-hydrogen mixture in isentropic expansion.

In case of irreversible adiabatic expansion of steam-hydrogen mixture ($\eta < 1$), the enthalpy of steam-hydrogen mixture after the expansion ($h'$) will be greater than the final enthalpy of the isentropic process, and the performance of turbine will decrease in comparison with $L$ by:

$$Q = (m_{H_2O} + m_{H_2}) \times (h' - h) = (m_{H_2O} + m_{H_2}) \times (h^0 - h) \times (1 - \eta) \quad (5)$$

The performance of the process of irreversible expansion is equal to:

$$L' = (m_{H_2O} + m_{H_2}) \times (h^0 - h) \times \eta \quad (6)$$

Irreversible expansion of steam-hydrogen mixture can be represented in the form of two successive processes: isentropic expansion of steam-hydrogen mixture and heat input ($\Delta Q$) to the mixture. As the temperature of the mixture increases as a result of the heat input, the ratio of the partial pressures of steam and hydrogen generally changes. Heating of steam-hydrogen mixture at constant pressure is described by the equation:

$$\Delta Q = m_{H_2O} \times (h'_{H_2O} - h_{H_2O}) + m_{H_2} \times C_{p,H_2} \times (T' - T) = (m_{H_2O} + m_{H_2}) \times (h^0 - h) \times (1 - \eta) \quad (7)$$

where $h'_{H_2O}$ is the specific enthalpy of steam, $T'$ is the final temperature of the mixture after irreversible expansion.
The determination of the parameters of steam-hydrogen mixture after the irreversible adiabatic expansion is realized through the following system of equations:

\[
\begin{align*}
\frac{\partial p}{\partial T} &= \frac{\partial p'}{\partial T'} \\
\frac{\partial v}{\partial T} &= \frac{\partial v'}{\partial T'} \\
\frac{\partial h}{\partial T} &= \frac{\partial h'}{\partial T'} \\
\frac{\partial m_{H_2} (h'_{H_2} - h_{H_2}) + m_{H_2} C_{P_{H_2}} (T' - T)}{\partial (m_{H_2} + m_{H_2})} &= (h^0 - h) (1 - \eta)
\end{align*}
\]

From system of equations (8) we find the temperature of steam-hydrogen mixture after irreversible expansion \(T\), the final partial pressures of steam and hydrogen \(P'_{H_2O}\) and \(P'_{H_2}\), the specific volume of steam \(v'\), the specific enthalpies of steam \(h'_{H_2O}\) and hydrogen \(h'_{H_2}\). Thus, the modeling of stem-hydrogen turbine is a successive solution of the systems of equations (1) and (8). It determines the final temperature of steam-hydrogen mixture after adiabatic expansion, the partial pressures of steam and hydrogen, the specific volume of steam and the specific enthalpies of steam and hydrogen.

3. Results and discussion

Table 1 and table 2 shows the power of steam-hydrogen turbine, the final temperature \(T\), the final partial pressures of steam and hydrogen \(P_{H_2O}\) and \(P_{H_2}\), and the dryness of steam \(X\) and the thermal power of condenser (from steam condensation), depending on the final expansion pressure \(P\) of steam-hydrogen mixture. In table 1 the internal efficiency was \(\eta = 1\), i.e. isentropic expansion. In table 2 \(\eta = 0.8\).

Increasing of final pressure leads to decrease of work of steam-hydrogen turbine. On the other hand, the temperature of condenser increases with practically constant value of heat produced in the condenser. From the comparison of table 1 and table 2 it follows that with an increase in the irreversibility of the process of expanding, the performance of turbine decreases, the dryness of steam \(X\) at the outlet from it increases and, accordingly, the heat of condensation increases.

The development of turbine for steam-hydrogen mixture should take into account the degree of dryness of the steam, which affects the wear rate (erosion) of the working parts of turbine. When steam-hydrogen mixture is expanded in turbine with \(\eta = 0.8\), the dryness of steam at the outlet of turbine changes from 0.75 to 0.8 for final pressures of 0.1 and 1 MPa respectively. It should be noted that such dryness may not be acceptable for some standard turbines.

The efficiency of a fuel cell depends on the specific power per a surface unit of its electrodes. Usually, with power increasing, the efficiency becomes less. So, if we use fuel cells with low power density, we have high efficiency (it can be up to 70-80 %). In this case, it is necessary to use fuel cell batteries with big total area of the active surface of electrodes. But, due to the relatively high cost of installed capacity of fuel cell batteries (over $ 2000), this approach becomes economically inexpedient. The operating mode of fuel cell is usually selected near the maximum power point. The efficiency of modern air-hydrogen fuel cells in operating mode lies in the range of 35-55 %.

If hydrogen output rate is 1 g/s and efficiency of fuel cell is about 50 %, we get about 50 kW of electricity and 50 kW of heat from fuel cell. Total power of considered plant is composed from power of steam-hydrogen turbine (that is in the range of 20-30 kW) and power of fuel cell (50 kW). The efficiency of plant represents the ratio, where the numerator is the sum of turbine power and fuel cell power, and the denominator is the input heat power of aluminum (with aluminum consumption rate of 9 g/s) – 278.7 kW. Neglecting mechanical and electrical losses in turbine, the overall electrical efficiency of the plant is about 25 ± 30 %. Therefore, the use of only gas turbine after aluminum-water reactor can potentially increase the efficiency of aluminum-fuelled power plant more than twice (from 12 % [27]). Total efficiency of power plant in this case reaches 70 ± 80 %.
Presented work is devoted to the modeling of aluminum-fuelled power plant based on aluminum-water reactor, steam-hydrogen turbine, condenser and air-hydrogen fuel cell battery. Parameters of aluminum-water reactor were the following: pressure – 15 MPa, temperature – 600 K, steam to hydrogen mass ratio – 40. It was shown that without gas turbine the plant’s electrical and total efficiencies are 12 % and 72 % respectively. The results of the study confirmed that the efficiency of aluminum-fuelled power plant can be increased by using the gas turbine for steam-hydrogen mixture generated in aluminum-water reactor. It was shown that turbine with internal efficiency of 80 % allow increasing the overall electrical efficiency of the plant up to 25 ÷ 30 %. At the same time the scheme of plant considered in presented work is a simple and non-optimized example, and it is certainly can be improved by such standard operations like regeneration of heat or heat transfer to secondary
contour. So this work may be continued and the model developed for calculation of the parameters of steam-hydrogen turbine can be used for that.

5. References
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