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Thermodynamic features of metal hydride thermal sorption compressors and perspectives of their application in hydrogen liquefaction systems

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1. Introduction

Hydrogen compression is required for the majority of technologies involving storage, transportation and utilisation. Taking into account the low density of hydrogen, the process of its compression is more energy intensive as compared to other gases. High diffusivity and fluidity of hydrogen create additional difficulties in the development of mechanical facilities for its compression. Additionally, the presence of lubricants in the mechanical (piston) compressors results in contamination of the compressed gas that in some cases, particularly for hydrogen liquefaction, is intolerable. Thus, membrane compressors are commonly used; but they are characterised by low energy efficiency and a short operating lifetime that essentially increases the operation costs and makes the final product more expensive. Therefore, alternative hydrogen compression methods characterised by lower energy consumption and higher workability are in great demand \[1\].

Reversible intermetallic hydrides are able to repeatedly absorb and desorb gaseous hydrogen at different pressures, which depend on the temperature potential of the released/absorbed heat \[2–5\]. This feature forms a basis of thermo-chemical technology of hydrogen compression realised in a thermal sorption compressor (TSC) utilising metal hydrides (MHs), in which exothermic and endothermic processes of H\(_2\) absorption and desorption in the MH are similar to processes of suction and discharge in a mechanical compressor \[1, 6–13\]. As a rule, the development of an MH TSC is preceded by its modelling aimed at the determination of the number of H\(_2\) compression stages including proper selection of the MH materials to provide compression from \(p_1 = p\text{min}\) to \(p_2 = p\text{max}\) (specified by a customer) over an available temperature range, \(T_1 = T\text{min} \ldots T_2 = T\text{max}\) \[13–16\], as well as optimisation of heat transfer performance in the MH beds in MH containers for hydrogen compression (generators—sorbers) to improve the dynamic characteristics of the TSC \[14, 16–18\].

Hydrogen compression in the TSC is a thermally driven process transforming heat into potential energy of pressurised hydrogen. In doing so, the TSC is a heat engine which can be and has to be analysed from the point of view of engineering thermodynamics. Such analysis is generally scarce in the literature. Though its features were briefly presented in the review \[10\] and some original publications \[9, 12, 19, 20\], for better understanding, it makes sense to clarify some details and to apply thermodynamic analysis to real thermally driven hydrogen compression systems. This will be considered in the first part of the present work (sections 2.1–2.3).

One of the most promising fields of the TSC application is cryogenic engineering where thermally driven compression is incorporated in the processes of hydrogen liquefaction \[21–23\]. The use of TSCs in cryogenic hydrogen systems on-board spacecraft (Space Shuttle Orbiter Endeavour, 1996; Planck satellite, 2009–2013) has been proven to be successful \[10, 24–27\]. Accordingly, sections 2.4 and 2.5 of this perspective will evaluate several opportunities of integration of the TSC in the hydrogen liquefaction process.
2. Results and discussion

2.1. Theoretical aspects of thermo-chemical hydrogen compression

When utilising MH for hydrogen compression in a TSC, the following sequence of thermal and thermo-chemical processes is realised (figure 1). Hydrogen gas, whose thermodynamic state is characterised by parameters of the point 1 ($p_1 T_1$), is absorbed in a hydride-forming material in an isobaric–isothermal process accompanied by the release of heat of phase transformation of hydrogen from a free molecular state to a pseudo-condensed one in the MH matrix. At point 2, the absorption is finished, and heat is supplied to the MH. By heating to temperature $T_2$ in the polytropic process 2–3, the MH transforms to a state able to desorb hydrogen at the pressure $p_2 > p_1$. The heat supply in the isobaric–isothermal process 3–4 results in MH dissociation and hydrogen release at parameters $p_2$ and $T_2$. To compress a new portion of hydrogen in the TSC, the MH is cooled down to the starting temperature $T_1$, in the process 4–1.

Therefore, when the temperature difference between the source ($T_2 = T_{\text{max}}$) and sink ($T_1 = T_{\text{min}}$) of the heat is available, it is possible to realise a closed cycle, in which the compression of a working medium is carried out thermo-chemically, with the help of reversible MHs. To close the cycle, it is necessary to add to the processes considered above the isobaric hydrogen cooling (process 4–5) followed by its isothermal expansion at $T_1$ to the starting pressure $p_1$ (process 5–1). The processes, in which hydrogen is in the free molecular state and the starting hydride-forming material does not contain hydrogen, are shown in figure 1 in different planes. The overlay of the $T$–$S$ diagrams for the systems ‘metal hydride–hydrogen’ ($S_{\text{MH}}$, shown in blue) and ‘free molecular hydrogen’ ($S_{\text{H}_2}$, shown in violet) was done on the temperatures of points 1 and 2 which are common for both MH and hydrogen; the $T$–$S$ diagrams of the ‘metal hydride–intermetallic’ systems ($S_{\text{M–H}_2}$, shown in green) were overlaid on the temperatures of points 4 and 1. As a result of the realisation of the sequence of processes described above, the system returns to its initial state thus enabling us to repeat the compression cycle.

In the considered case, a direct transformation of heat into potential energy of compressed hydrogen, bypassing the intermediate stages of the energy transformation sequence ‘heat—electricity—mechanical compression—compressed hydrogen’, which are conventional for mechanical gas compression technology, is realised.

It has been shown in [28] that thermo-chemical hydrogen compression, when the heat of the processes is completely recovered, is optimal from a thermodynamic point of view, i.e. the energy supplied in the form of heat is transformed to the compression work with an efficiency equal to the efficiency of the reversible Carnot cycle realised in the same temperature range.
In the thermal sorption compressor, the ratio of discharge and suction pressures \( \frac{p_1}{p_2} \) is a function of the temperatures of absorption \( T_1 \) and desorption \( T_2 \) processes, as well as the heat of formation of the MH \( (q_f) \):

\[
\frac{p_1}{p_2} = \exp \left[ \left( \frac{T_2 - T_1}{T_2} - \frac{\Delta T_2}{T_2} - \frac{\Delta T_1}{T_1 + \Delta T_1} \right) \cdot \frac{q_f}{R T} \right]
\]

(1)

where \( \Delta T \) [K] are the temperature gradients in the processes of heat supply (2) and removal (1), and \( R = 8.3145 \text{ J/(mol K)}^{-1} \) is a universal gas constant.

Derivation of equation 1, together with analysis of the influence of the temperature gradients on the compression ratio and efficiency of hydrogen compression, is presented in section 1 of the supplementary information, which can be found online at stacks.iop.org/JPENERGY/2/021007/mmedia.

To analyse the influence of the initial and final pressures on the efficiency of hydrogen compression in the TSC, let us express the temperatures of the thermal sorption processes via the corresponding hydrogen equilibrium pressures. Then the efficiency \( (\eta_{TSC}) \) of the theoretical cycle for the TSC will be written as:

\[
\eta_{TSC} = \frac{\ln p_2 - \ln p_1}{\Delta S(\text{f})/R - \ln p_1}
\]

(2)

Analysis of data on \( p = f(1/T) \) shows that these dependencies coincide at \( T \to \infty \) confirming the equality of the entropy increments in thermal sorption processes for these MHs:

\[
\lim_{T \to \infty} \ln p = \Delta S/R = \text{Const.}
\]

(3)

Taking equation (3) into account, from equation (2) the dependencies exhibiting influence of the ‘boundary’ pressures on the compression efficiency at a constant compression ratio can be found. By taking partial derivatives of the function and replacing differentials with finite increments, we obtain relations for the estimation of the changes of the system efficiency depending on the deviation of the real pressures from the equilibrium values in the corresponding processes:

\[
\Delta \eta_{TSC}^p = \frac{1}{p_1(\Delta S/R - \ln p_2)} \Delta p_1.
\]

(4)

It follows from equation (4) that in the whole pressure range \( 0 < p < \infty \), at \( p_2 > p_1 \) \( |\eta_{TSC}^p| < |\eta_{TSC}^p| \).

Assuming \( \Delta p_1 = \Delta p_2 \), the hydrogen compression efficiency in the TSC will be influenced by the pressure deviation from the equilibrium value at a much higher extent for the absorption process than for the desorption one.

Derivation of equation (4) and consideration of its effect are presented in section 2 of the supplementary information. The data analysis shows that at the fixed value of the temperature of heat removal, even a small change in hydrogen absorption pressure significantly affects the thermodynamic efficiency of the compression; this effect becomes more pronounced when the compression ratio increases. This finding is important from an application point of view, because it pays attention to the fact that during development of a TSC, the absorption parameters should be set as close as possible to their equilibrium values as it is possible.

The increase of discharge pressure requires the increase of temperature potential of the supplied heat. This results in significant heat losses during the cooling of MHs from the desorption temperature to the absorption one. To increase the efficiency of thermo-chemical hydrogen compression, it makes sense to introduce heat recovery, which is characterised by the parameter \( \sigma \) equal to the fraction of heat re-distributed between generators–sorbers during the time between absorption and desorption processes.

Using experimental data on the \( p = f(T) \) dependence for absorption and desorption processes [29] and the van’t Hoff equation, we obtain:

\[
q_s = R \cdot B,
\]

(5)

where \( B \) is a tangent of the slope of \( \ln p - \frac{1}{T} \) dependence (isostere).

Substituting the value of the phase transition energy, we obtain:

\[
\eta_{TSC} = \frac{T_{\text{min}}}{B} \ln \left( \frac{p_{\text{max}}}{p_{\text{min}}} \right).
\]

(6)
So, at a pre-defined value of $p_{\text{max}}/p_{\text{min}}$ and a fixed lower temperature $T_{\text{min}}$, which is determined by the parameters of environment where the heat is dissipated to, the cycle efficiency increases when the value of $B$ decreases. Accordingly, it is recommended to use MHs characterised by a flat dependence $\ln p = f(\frac{1}{T})$ for the thermo-chemical hydrogen compression. It will allow us to use a wider temperature range in the TSC and, therefore, achieve higher efficiency at a pre-defined compression ratio. This information is necessary for the selection of MHs used in TSCs for specific applications, as well as for the development of technology for the preparation of hydride-forming materials with pre-defined properties [30–32].

The theoretically achievable value of the maximum pressure generated by the thermo-chemical compression can be estimated on the basis of interrelations between thermodynamic parameters of the first-order phase transition applied to thermal sorption processes in MHs. Considering the thermodynamic state of the 'metal hydride–hydrogen' system in the critical point [29] where specific volumes of hydrogen in a pseudo-condensed ($v_{H}^{\text{h}}$) and gaseous ($v_{H}^{\text{g}}$) states are equal, and taking into account the compressibility coefficient of the gas, $\gamma$, we get:

$$p_{\text{max}} = \frac{R \cdot T_{\text{c}}}{v_{H}^{\text{g}} \cdot \gamma}. \tag{7}$$

The value of $v_{H}^{\text{h}}$ can be determined from the data on hydrogen packing density in the crystal lattice of an MH. From the known values of the amount of interstitial atoms, $N$, in the unit volume of the MH and the mass of a hydrogen atom, $m_{H}$, we can determine it as:

$$v_{H}^{\text{h}} = \frac{V_{H}^{\text{h}}}{N \cdot m_{H} \cdot V_{g}}. \tag{8}$$

Then, under condition $v_{H}^{\text{h}} = v_{H}^{\text{g}}$, we get:

$$p_{\text{max}} = \frac{R \cdot T_{\text{c}} \cdot N \cdot m_{H}}{\gamma}. \tag{9}$$

It follows from equation (9) that the higher maximum pressure during thermo-chemical hydrogen compression can be provided when using MHs with a higher volumetric density of hydrogen in the crystal lattice.

### 2.2. The influence of real factors on hydrogen compression efficiency

Thermodynamic efficiency of the existing TSCs is lower than the theoretical limit due to the external and internal irreversibility caused by the real conditions of heat exchange and interaction of hydrogen with MHs, as well as specific design features of main parts of the compressors.

The discrete structure of MHs and presence of voids in the generators–sorbers and gas distributing system result in the formation of 'dead space', which negatively influences the performance of the TSC. The value of coefficient, $k_{v}$, which takes into account the influence of the dead space, is equal to the ratio of hydrogen mass in the dead space at the desorption parameters to the total mass of hydrogen in the system.

When compressing hydrogen to high pressures, $p_{2} \gg p_{1}$, the value of $k_{v}$ can be calculated as follows:

$$k_{v} = \frac{p_{2} \cdot (1/\rho_{h} - 1/\rho)}{T_{2} \cdot R}, \tag{10}$$

where $\psi$ is a mass fraction of hydrogen in MH; $\rho_{h}$ is the bulk density of MHs; $\rho$ is the compact MH density.

The equation for the determination of the TSC efficiency, $\eta_{\text{eff}}$, which takes into account the influence of factors related to practical realisation of the thermo-chemical compression, has the following form:

$$\eta_{\text{eff}} = \frac{q_{c} (1 - k_{v}) \left( T_{2} - T_{1} - \frac{\Delta T_{2}}{T_{2}} \cdot \frac{\Delta T_{1}}{T_{1} + \Delta T_{1}} \right)}{q_{c} (1 - k_{v}) + (1 - \sigma) \left( \frac{1}{\tau} \cdot k_{m} \cdot (T_{2} - \Delta T_{2} + \Delta T_{2} - T_{1} + \Delta T_{1} - \Delta T_{1}) + q_{c} k_{v} \right)}, \tag{11}$$

where $\Delta T_{1}^{\prime}$ and $\Delta T_{2}^{\prime}$ relate to temperature hysteresis in the sorption processes; $c_{h}$ is the heat capacity of the material of high-temperature parts of the TSC (metalware); $k_{m}$ is a coefficient accounting the mass ratio of the MH and the metalware.

The results of thermodynamic (exergy) analysis of hydrogen compression in the TSC are presented in figure 2, which shows performance losses in separate system components as a percentage of the available exergy of heat at a high temperature level [33].
Figure 2, which shows the change of exergy flows in the processes of the cycle of thermo-chemical hydrogen compression (figure 1), was built on the basis of test results of prototype TSCs (see the next section for the details). The known values of temperature potentials of the heat in the processes involved allowed us to determine exergy losses in each process/system element.

The work losses, $\Delta L_i$, in a thermodynamic system where irreversible processes take place were determined as:

$$\sum_{i=1}^{n} \Delta L_i = T_0 \sum_{i=1}^{n} \Delta S_i,$$

where $\Delta S_i$ are entropy changes in separate system elements at the reference temperature $T_0$, and $n$ is the number of elements in the object under investigation.

The data of the exergy analysis is the basis of information for the advancement of design and performance of MH compressors [34]. Analysis of the data shows that for the increase of thermodynamic perfection of the compression cycle it is necessary, first of all, to realise heat recovery in the transient processes and to decrease temperature-driving forces during realisation of the thermal sorption processes.

In many ways, the TSC productivity is determined by the rate of heat transfer, which provides the running of the thermo-chemical processes of hydrogen interaction with a hydride-forming material. Intensification of these processes is achieved by the increase of temperature difference between the heat source and the heat sink. Undoubtedly, it accelerates the heat exchange process and increases the amount of hydrogen compressed per a unit of time (productivity of the installation). At the same time, it results in the decrease of thermodynamic efficiency of utilisation of heat consumed for hydrogen compression. The factor of external thermodynamic irreversibility, which causes exergy losses in the system, can be accounted for by the introduction of an additional parameter related to temperature gradient in heat exchange processes when determining the TSC compression ratio (equation (1) and estimating its efficiency (equation (11)).

Selection of operation parameters of the TSC is carried out starting from specific operation conditions, which determine the priority of one of a number of performance characteristics. In the more general case, it is necessary to make an optimisation (when selecting the specific price of compressed hydrogen as a target value), by looking for a compromise between the productivity, efficiency and capital costs of the TSC.

2.3. Characteristics of the existing TSCs

The developed theory of thermo-chemical hydrogen compression has allowed us to analyse the performance of a number of prototype MH TSCs [10, 35–38]. Typical analysis is presented in figure 3 as an indicator diagram of gas compression at different pressures, where $k_s = m_H/m_g$ is a coefficient that reflects the dynamics of the specific mass content of hydrogen in MHs in sorption processes.

To build a real indicator diagram, it is necessary to operate with the actual values of pressure in the TSC and hydrogen content in the MH—both were taken from experiments. Analysis of the processes taking place in the experimental TSCs (figure 3) shows that, when increasing the pressure at the same desorption temperature and the duration of the compression cycle, the useable hydrogen sorption capacity of the MH decreases. Therefore, to maintain the specified compressor productivity, it is necessary to improve the design and operational features by the intensifying heat exchange processes in the MH. It will improve the compressor’s efficiency and productivity by the shortening duration of the compression cycle. This result can be achieved by the placing of a heat conductive matrix (copper, aluminium) in the MH bed.

The analysis of the diagrams shows that the investigated operation regimes of the TSC are characterised by almost vertical lines corresponding to the transient processes 2–3 and 4–1. It confirms the relatively low
influence of the dead space in specially developed generators–sorbers with increased MH density. In turn, the specific productivity of the TSC increases by 27%, with a simultaneous increase of efficiency by 8.5%. The detrimental effect of the dead space, however, becomes significant at high, above 30 MPa, discharge pressures [6, 10].

We shall compare now thermodynamic characteristics of hydrogen compression in mechanical and thermal sorption compressors. In the TSC utilising intermetallic hydride LaNi$_{4.8}$Al$_{0.2}$H$_x$, when compressing hydrogen from 0.1 to 15.0 MPa, it is necessary to have a heat source with a temperature potential of 500 K and a heat sink with temperature potential of 293 K [39]. The estimation of efficiency of the conversion of energy produced by fuel combustion at a thermal power plant into work of hydrogen compression when using an electrically actuated mechanical compressor is characterised by an exergy efficiency of 0.183. For the TSC operating at the parameters specified above the exergy efficiency of the thermo-chemical heat transformation into the energy of compressed hydrogen will be equal to 0.575, or almost three times higher than for the mechanical compression. This significant improvement is due to the absence of intermediate energy transformation steps required by the mechanical compression.

Combined experimental and computational-theoretical studies allow one to forecast the energy performance of TSCs. Examples are presented in figure 4.

To produce mechanical work, $L$, which drives a mechanical compressor, it is necessary to consume heat in the amount of $Q = L/\eta_H$ where $\eta_H$ is the efficiency of a power plant transforming the heat into the work.

During the analysis, it was assumed that $\eta_H = 0.35$ corresponds to the existent level of efficiency for thermal power plants. Hydrogen compression in a mechanical compressor was assumed to be polytropic, at the polytropic index of $n = 1.2$ and starting gas temperature of $T_0 = 303$ K. Figure 4 compares consumption of the heat for hydrogen compression, depending on the compression ratio, $p_2/p_1$, for the mechanical compressor (1) and TSCs utilising LaNi$_3$H$_x$ (2) and FeTiH$_x$ (3).

The graphs presented in figure 4 show that the heat consumption for the compression in the TSC (2, 3) exhibits much less pronounced dependence on the compression ratio than for the mechanical compression.
(1). It can be considered as an advantage for the use of TSCs for the achievement of high compression ratio. Conversely, in the mechanical compressor the increase of \( p_2/p_1 \) requires more intensive consumption of electricity and, in turn, very high consumption of heat for the electricity generation at a thermal power plant.

When comparing the dependencies presented in figure 4, we can identify two characteristic ranges of compression ratio. At \( p_2/p_1 > 25 \), the hydrogen compression using the TSC is less energy intensive than that for the mechanical compressor while in the range \( p_2/p_1 \leq 25 \), it becomes more energy intensive. However, the quantitative loss is compensated by the quality of the consumed heat, which depends on its temperature potential.

The quality of consumed energy can be defined via dimensionless exergetic temperature (or heat qualification coefficient), \( \tau \), equal to the efficiency of the Carnot cycle realised between ambient \( (T_0) \) and operating \( (T_r) \) temperatures [40]:

\[
\tau = 1 - T_0/T_r, \tag{13}
\]

For the majority of reversible MHs, hydrogen compression to 100–150 atm can be achieved using a temperature potential up to \( T_r \sim 450 \text{ K} \) that corresponds to \( \tau = 0.37 \) at \( T_0 = 300 \text{ K} \) while generation of electricity via combustion of fuel at \( T_r \sim 1300 \text{ K} \) yields \( \tau = 0.77 \), and conventionally the heat qualification coefficient of electricity is assumed to be \( \tau = 1 \) [41]. Thus hydrogen compression using the TSC allows us to use primary energy with 2–3 times lower quality than conventional hydrogen compression methods consuming electricity.

### 2.4. Application of TSC in hydrogen liquefaction installations

The work required to liquefy a gas significantly increases with the decrease of temperature of gas–liquid phase transition. So, because of the low temperature of hydrogen condensation \( (T_c = 20 \text{ K}) \), theoretical mechanical work required for its liquefactions is 43 times higher than for the liquefaction of Freon-22 \( (T_c = 233 \text{ K}) \) [42]. Due to the low inversion temperature for hydrogen, the use of liquefaction methods based on gas throttling is possible only at temperatures below 200 K. Taking it into account, the commonly used hydrogen liquefaction systems include hydrogen pre-cooling with liquid nitrogen carried out in special heat exchangers. The existence of two modifications of molecular hydrogen, ortho- \((\text{oH}_2)\) and para- \((\text{pH}_2)\), introduces additional features into liquefaction schemes requiring elimination of spontaneous exothermic \( \text{oH}_2\text{–pH}_2 \) conversion. In practice, before hydrogen liquefaction it is necessary to increase the content of \( \text{pH}_2 \) from 75% (equilibrium concentration at the room temperature) to >95% (equilibrium concentration of \( \text{pH}_2 \) is equal to 99.79% at \( T = 20.4 \text{ K} \) [43].

The minimum theoretical work necessary to liquefy hydrogen in a reversible process is equal to its exergy in the liquefied state:

\[
L_{\text{min}} = (H_i - H_f) - T_0 (S_i - S_f), \tag{14}
\]

where indexes ‘\( i \)’ and ‘\( f \)’ correspond to the initial and final states, and \( T_0 \) is the ambient temperature.

It is known that the hydrogen compression process makes the greatest contribution in the energy consumption of liquefaction of gases. Taking into account the high thermodynamic efficiency of thermo-chemical compression, introducing the MH TSC in the layout of a hydrogen liquefaction installation seems to be reasonable. The MH TSC can serve not only as a base component of a liquefaction or refrigeration installation but also can be used in an additional refrigeration circuit. It allows us to eliminate cooling with liquid nitrogen that significantly complicates the operation.

Figure 5 shows schematics of hydrogen liquefaction installation on the basis of the TSC [44]. Realisation of a two-circuit scheme, in which the first circuit provides a closed expander cooling cycle providing necessary temperature before throttling hydrogen flow in the second circuit, allows us to increase efficiency of the liquefaction when the pressure in the installation \((\sim 10.0 \text{ MPa})\) remains technically acceptable. Theoretical consumption of energy in the form of heat for the liquefaction of 1 kg of hydrogen in the installation on the basis of the TSC is not higher than 320 kJ. Moreover, the additional cooling agent, liquid nitrogen, is not required for this layout.

Previous studies [45] showed that MHs are efficient catalysts of the ortho–para conversion process. In this case, complex use of MH technologies in systems for hydrogen liquefaction and its re-liquefaction during transportation and long-term storage of the liquid hydrogen is a very promising extension of functionality of the MH systems.
2.5. Hydrogen turbo-expander converters

Realisation of the advanced hydrogen liquefaction process (figure 5), where the MH TSC of the cooling circuit (1) is characterised by the high range of the operating pressures (~0.3 and ~10 MPa in the suction and discharge lines, respectively), requires a special approach to the development of a rotor-type expansion engine [39].

A high hydrogen compression ratio and, as a result, low specific volumes, put certain conditions on both selection of a running-flow part and also the number of stages.

In this case, formula for the determination of the number of stages in a turbine, \( Z_T \), has the following type:

\[
Z_T = \frac{L_T}{L_{st}} = \frac{c_p \Delta T}{T_{av}} R_{H2} A^2 \mu \text{Eu,}
\]

where \( L_T \) is the heat difference triggered in a turbo-expander; \( L_{st} \) is the heat difference triggered in one stage of a turbo-expander; \( c_p \) is the heat capacity of hydrogen; \( \Delta T \) is the temperature difference at the inlet and outlet of the stage; \( T_{av} \) is the average temperature in a step; \( A \) is the ratio of flow velocity to sound velocity; \( R_{H2} \) is the gas constant for hydrogen; \( \mu \) is the stage load factor; \( \text{Eu} \) is the Euler number.

A feature of use of hydrogen in a turbo-expander provides an opportunity to increase the ratio of the pressure drop per one stage to the total pressure drop, as compared to other gases, because velocity of sound in hydrogen is higher. It allows us to provide a minimum level of gas-dynamic losses by the increase of velocity of the working flow.

For the development of the design of main components of the turbo-expander, we carried out studies of gas-dynamic processes within a model of 3D viscous gas flow using FlowER software formed on the basis of Reynolds averaging of non-stationary Navier—Stokes equations supplemented by two-parametric differential Menter’s SST model of turbulence, with the application of implicit quasi-monotonic ENO scheme of improved accuracy [46, 47].

When selecting the geometric shape of the channels of a running-flow part of the turbo-expander, the blade profiles were described by fourth-order curves. In the aggregate, it provided the modelling of the structure of 3D flow, which was similar to the real nature of gas motion in a blade apparatus.

To provide high aerodynamic cleanliness, a design option with an alternating on height blade profile has been suggested, and the main geometric parameters of the blade have been determined. It was found that the total number of stages in the expansion engine necessary to provide a pressure drop from 10.0 MPa to 0.3 MPa is equal to nine.

Figure 6 presents views of the first (a—radial-axis type) and the last (b—axial type) stages, which were developed for the hydrogen turbo-expander.

Table 1 presents integral gas-dynamic characteristics of the turbo-expander stages, which have high aerodynamic performances regarding both the level of losses of kinetic energy and internal efficiency, as well as the high degree of the total pressure decrease.
Figure 6. Views of the studied turbine stages: (a) first stage of radial-axis type; (b) last stage of axial type.

Table 1. Integral gas-dynamic characteristics of the stages of the turbo-expander.

| Parameter                                      | First stage | Last stage |
|------------------------------------------------|-------------|------------|
| Mass flow rate, kg s\(^{-1}\)                  | 1.075       | 1.067      | 1.048      |
| Absolute angle of flow exit (from axial direction), ° | 2.25        | –0.2       | –2.59      |
| Kinetic energy losses                           | 9.3%        | 11.46%     | 8.01%      |
| Kinetic energy losses with exit velocity        | 2.3%        | 3.35%      | 4.33%      |
| Internal efficiency                             | 90.7%       | 88.34%     | 91.99%     |
| Stage power, kW                                 | 970.062     | 417.863    | 451.376    |

The theoretical-computational analysis of the thermal-and-gas dynamic parameters of the hydrogen turbo-expander allowed us to determine the range of rotating frequency changes for the rotor, to calculate design and geometry characteristics of the nozzle and working blades, which showed thermodynamic preference of the radial-axis type design of the expansion engine.

The obtained data allowed us to form a design view of a high pressure turbo-expander with an overall internal efficiency of 90%.

3. Conclusions

(a) On the basis of thermodynamic analysis, the theoretically achievable maximum discharge pressure of a thermal sorption compressor was estimated. It was shown that the maximum pressure depends on the packing density of hydrogen in the metal hydride crystal lattice.

(b) It was shown that the degree of thermodynamic perfection (exergy efficiency) of the thermo-chemical conversion of primary energy in the form of heat to the energy of compressed hydrogen surpasses the efficiency of mechanical compression; the advantage of the TSC becomes higher when the compression ratio increases.

(c) On the basis of analysis of the influence of ‘boundary’ pressures on the efficiency of thermo-chemical hydrogen compression in the TSC, the major influence of the absorption pressure was shown; this influence increases with the increase of the compression ratio, \(p_2/p_1\).

(d) The influence of design and operational parameters on the compression efficiency was considered. Exergy losses in the parts of the TSC were estimated.

(e) Performances of TSCs promising their use in technological schemes of hydrogen liquefaction installations were forecasted.

(f) It was found that the introduction of TSCs in the hydrogen liquefaction schemes provides, apart from the energy preferences, some engineering advantages (high purity of the discharged hydrogen, noiselessness and absence of vibration during the operation), as compared to the mechanical compression systems.

(g) The use of the developed procedure of calculation of gas-dynamic processes in 3D flows allowed us to optimise design features of turbo-expander engines for hydrogen liquefaction systems.

(h) Research results showed that the application of metal hydride energy-technological processing of hydrogen including thermo-chemical compression and partial ortho–para-conversion, allows us to improve the techno-economic and energy performance of hydrogen liquefaction systems and to practically utilise heat of relatively low temperature potential, which is available in industries that are specialised in hydrogen production for energy and technological purposes.
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