

Modeling of the efficiency of using sorption metal hydride technologies for the purification of gaseous hydrogen from accompanying impurities during its production, storage and transportation

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Abstract. The article analyzes the systems for generation, purification, transportation and storing of gaseous hydrogen as the alternative renewable energy source for ensuring of level of ecological safety of power plants with reciprocation internal combustion engines exploitation process. Purpose of the study is to improve the description of the process of purifying gaseous hydrogen from associated impurities during its production, storage and transportation based on the results of mathematical modeling analysis using improved mathematical apparatus based on modified thermodynamic perturbation theory. Problem of the study is the imperfection of the existing mathematical apparatus for describing the processes of purification of gaseous hydrogen as a commercial product and renewable ecological safe energy carrier using sorption metal hydride technologies based on $\text{TiMn}_{1.5}$. Idea of the study is to develop a list of recommendations and organizational and technical measures for obtaining ultra-high purity gaseous hydrogen in environmental protection technologies by improving the adequacy of the mathematical description of the processes of its sorption-desorption by intermetallic compounds based on $\text{TiMn}_{1.5}$. Task of the study is to adapt the mathematical apparatus of the modified thermodynamic perturbation theory to describe the process of selective sorption of hydrogen by metal hydrides of the type $\text{TiMn}_{1.5}$ from gas mixtures obtained during its production, storage and transportation. Object of the study is sorption processes in metal hydride technologies for the purification of gaseous hydrogen as an alternative fuel and a useful commercial product based on $\text{TiMn}_{1.5}$. Subject of the study is mathematical description of the course of hydrogen sorption processes by intermetallic compounds of the type $\text{TiMn}_{1.5}$ when purified from gas impurities. Methods of the study are literature analysis, modified thermodynamic perturbation theory, mathematical modeling. Scientific novelty of results of the study is for the first time, an apparatus for mathematically describing the processes of hydrogen sorption by intermetallic compounds of the type has been suggested $\text{TiMn}_{1.5}$ from gas mixtures during its production, storage and transportation based on the improvement of the modified thermodynamic perturbation theory. Practical value of results of the study is the improved mathematical apparatus and the results of its application which are suitable for developing a list of recommendations and organizational and technical measures for obtaining ultra-high purity gaseous hydrogen as an ecological safe renewable fuel in environmental protection technologies both during the times of armed aggression and during the post-war reconstruction of critical infrastructure and economic potential of our country. The main part of the research is devoted to the adaptation of the mathematical apparatus of the modified perturbation theory to describe the