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RESULTS OF APPLICATION OF THE MATHEMATICAL APPARATUS FOR THE STUDY OF THE PURIFICATION OF GASEOUS HYDROGEN FROM ACCOMPANYING IMPURITIES BY USING OF SORPTION METAL HYDRIDE TECHNOLOGIES

Production, storage, transportation and use of hydrogen as the most environmentally safe and energy-efficient motor fuel is a very relevant and promising innovation environment protection technology. The study analyzes the systems for generation, purification, transportation and storing of gaseous hydrogen as the alternative renewable energy source for ensuring the level of ecological safety of power plants with reciprocation internal combustion engines exploitation process on the example of units of firefighting and emergency rescue equipment of institutions of the SES of Ukraine [1]. The 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 processes based on the results of mathematical modeling analysis using improved mathematical apparatus based on modified thermodynamic perturbation theory. The main part of the research is devoted to the adaptation of the mathematical apparatus of the modified perturbation theory to describe the sorption processes of the interaction of hydrogen, which is in the state of a gas mixture, and intermetallic compounds of the $TiMn_{1,5}$ type. It is shown that based on sorption metal hydride technologies of the $TiMn_{1,5}$ type it is possible to achieve ultra-high purity of gaseous hydrogen as a commercial product when using it as an ecologically safe, renewable type of motor fuel. Mathematical modeling of hydrogen sorption by intermetallic compounds, performed on the basis of the mathematical apparatus of the thermodynamic perturbation theory improved in the study and on the example of the intermetallic hydride $TiMn_{1,5}$, based on the application of the lattice gas model for metal hydrides.

A list of recommendations and organizational and technical measures has been developed to implement this type of environmental protection technologies in the practice of the institutions of the SES of Ukraine, in particular the operation of firefighting and emergency rescue equipment units with reciprocating internal combustion engines, both during times of armed aggression and during the post-war reconstruction of critical infrastructure and economic potential of our country and ensuring compliance with the requirements contained in the Order of the SES of Ukraine No. 618 (on the main activities) dated September 20, 2013 «On approval of the Regulations on the organization of ecological support of the State Emergency Service of Ukraine» and in the historical perspective of achieving the sustainable development goals contained in the Decree of the President of Ukraine No. 722/2019 dated September 30, 2019 «On the Sustainable Development Goals of Ukraine for the period up to 2030» [2-5]. The results of computational studies using the mathematical apparatus suggested by the authors are shown in Figure 1. This study has been carried out as part of the scientific and research work of the Department of Environmental Protection Technologies of the Educational and Scientific Institute of Management and Population Safety of the National University of Civil Protection of Ukraine of SES of Ukraine «Development of a methodology for complex assessment of the impact of exploitation and application of special equipment on the environment in conditions of military aggression»

(State Registration № 0124U000374, 01.2024–12.2026).

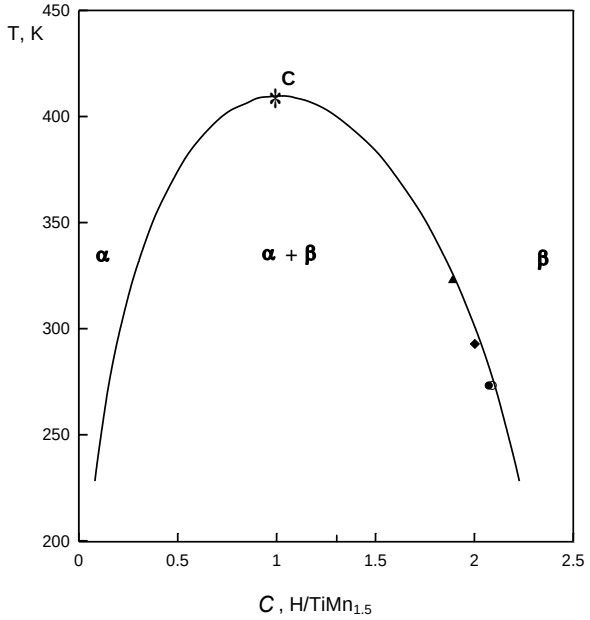

Figure 1 – Decomposition curve of homogeneous phases of the $TiMn_{1.5}$–H_2 system into disordered α-, β-phases: ——— calculation results; *C – critical point of α–β-equilibria (calculation); ○ and ●,♦,▲ – experimental results on H_2 desorption

At the same time, materials from the VCU library system have been used, including electronic versions of journals and other materials, databases, interlibrary subscription as part of participation in Non-Resident Academic Associates program co-sponsored by the College of Humanities and Sciences at Virginia Commonwealth University (VCU) and the Davis Center for Eurasian Studies at Harvard University in 2024–2025 academic year.

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