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METROLOGY, STANDARDIZATION, AND CONTROL OF NANOTECHNOLOGIES

Challenges in Regulatory, Experimental, and Theoretical Computational Maintenance of Safety in Hydrogen Power Engineering

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Abstract—The formation and development of hydrogen power engineering (HPE) as a technologically efficient and competitive part of the future with a carbon-free or low-carbon economic paradigm makes it necessary to overcome many obstacles related not only to the maturity, availability, and economic efficiency of technologies but also to a sufficient, socially acceptable level of safety in HPE. Even if most technological and economic issues are resolved, the pace of adopting scientific and engineering developments in HPE on an industrial and commercial scale may be inhibited by the level of comprehensive (analytical, theoretical and computational, experimental) scientific and engineering support for safety in HPE facilities, networks, and systems throughout their entire life cycle (from design to decommissioning) and the completeness and sufficiency of the regulatory framework for both, new reactor centers with related new technologies and infrastructural HPE safety systems. Three classes of correlated challenges in the theoretical computational, experimental, and regulatory support safety in HPE are formulated and described in brief. Their timely resolution is critical to the successful transition to the carbon-free technological paradigm.

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INTRODUCTION

The coming decade will witness a sharp increase in the demand for hydrogen as an efficient energy-producing (accumulation, transport, and utilization) material. The main drivers of this large-scale increase are transportation (maritime, railroad, automobile, aviation) and distributed combined (heat + electricity) power supply systems in industry and the housing and utilities sector.

As noted in pioneer [1] and subsequent reviews [2], HPE is applied *downstream* (down the energy stream from a source of energy), that is, in energy transport, processing, and utilization, but not *upstream* (extraction of primary energy raw materials). HPE is only complementary to oil, nuclear, or renewable (solar, wind) power engineering and is not a new source of energy per se. In other words, HPE is the way to apply available sources of energy as efficiently as possible, improve their utilization efficiency factor and ecofriendliness, or obtain other advantages (Fig. 1).

Russia plans to switch over from carbon to hydrogen power engineering on the basis of two cumulative technologies, including nuclear hydrogen power engineering technologies (nuclear power engineering plants (NPEPs) and renewable energy sources, using solar, wind, and water power.

The bicomponent approach will allow:

—the creation of a new market for the nuclear industry, industrial heating that consumes more than 40% of organic fuel;

—saving natural gas and oil, using them as raw materials in various industries with a high level of processing. Currently, large-scale processing is executed mainly by the steam reforming of natural gas (methane). This is attended by the flaring of about one half of the source gas, with the products of the combustion being released into the atmosphere. The utilization of nuclear energy can considerably improve the ecofriendliness of large-scale hydrogen production and efficiency of utilizing source raw materials, that is, natural gas or other hydrocarbons;

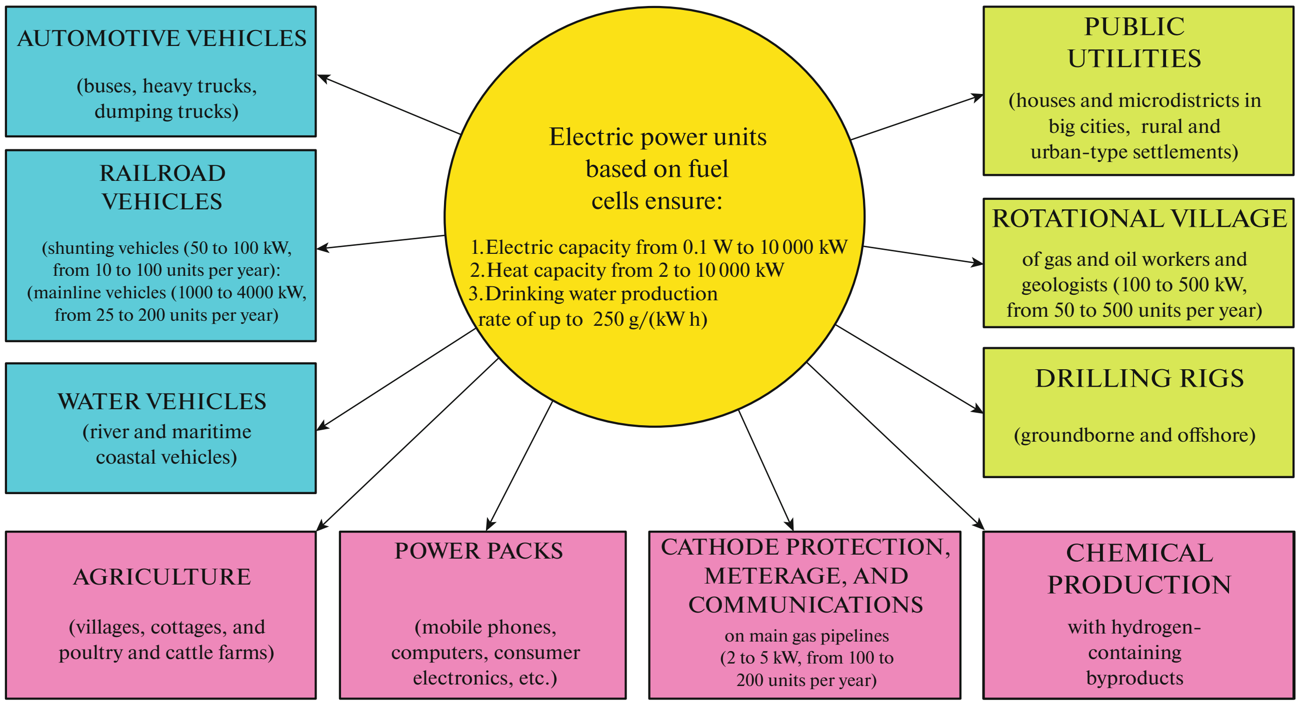

Fig. 1. (Color online) Applications of hydrogen fuel cells [2].

—the improvement of national energy and economic security by producing environmentally pristine hydrogen fuel from water. In terms of energy equivalents the demand and potential market of hydrogen are comparable with the demand and market for electricity. This is a commodity in demand in both domestic and foreign markets;

—the reduction of the emissions of noxious substances into the environment, GHG emissions included. In particular, the requirements on the quality of air have been toughened: the WHO has already reclassified diesel fuel vapors from the category potential carcinogens (group 2a), where they were put in 1989, to carcinogens (group 1);

—the establishment of Russia as the world's leader in the domain of NPE technologies.

The system-level (experimental, theoretical and computational, analytical and regulatory) scientific and engineering maintenance of the safe development, buildup, and operation of HPE is necessary for meeting Russia's economic and social demands in an efficient, socially favorable, and ecofriendly manner.

Even if all of the existing economic and technological challenges in HPE are resolved, its competitiveness and niche in the carbon-free power engineering of the future will be determined by safety levels.

The potential vulnerable hotspots are the innovative NPEP with a chemical engineering section (CHES) for producing hydrogen, the infrastructure of HPE, including transportation, distribution, and storage networks, and also the hydrogen utilization systems that are in contact with the mass consumer who does not practice the safety culture elaborated in the nuclear industry.

The safety of HPE must be:

—ensured by a system of analytical, computational, engineering, technological, regulatory, and organizational measures,

—aimed at the staged protection of engineering systems proper, personnel, and mass consumers against potential hazardous exposures,

—based on the risk-informed management of safety and durability (functional stability),

—developed considering potential actions, dangerous ones included, of people, engineering and physical systems as well as cyberdata networks, that ensure the management of HPE components and subsystems, from large-capacity and small-scale hydrogen producers through hydrogen logistics systems (localized and extended) to large-scale, small-scale, and household consumers of hydrogen.

In most industrially developed economies, HPE is currently viewed as a domain of innovation. This is why the pace of applying scientific and engineering developments on an industrial and commercial scale will be limited by the quality and level of standardizing not only in terms of the maturity of technologies and engineering systems but also in terms of maintaining safety throughout the life cycle of HPE.

This work formulates and describes in brief the three classes of correlated challenges in the theoretical computational, experimental, and regulatory maintenance of safety in HPE that are incompletely and insufficiently described in earlier reviews by European [3] and American [4] authors. Their timely resolution is critical to the successful transition to the carbon-free technological paradigm.

Despite the fact that the pioneer, intensive, and large-scale steps towards the safe utilization of hydrogen as a fuel and energy producing material have been taken in the Soviet Union and the United States since the late 1950s, 1970s, and 1980s as part of developing rocket and space technologies, nuclear and hydrogen power engineering, and effort aimed at improving the hydrogen safety of NPPs with VVER-type reactors, respectively, it has currently become necessary to reconsider and specify the accumulated expertise, technologies, and experience of utilizing engineering systems with the circulation of hydrogen. The applicability of sectoral rules and norms developed under minor resource restrictions (for aviation, spacecraft, and special applications) is significantly limited for the utilization of hydrogen on a mass scale as a commercial product.

The topics described in this work in brief are:

—key challenges the regulatory maintenance of safety in HPE that are expedient to consider for amending existing or elaborating new domestic federal and sectoral HPE safety rules and norms;

—test data necessary for substantiating by experimentation new and/or amended existing rules and standards for which the existing scientific and engineering blueprints fail to meet the modern requirements;

—analytical tools (conceptual patterns of safety analysis and design as well as models of dangerous natural, technological or managerial processes) for substantiating, evaluating, managing, and continuously improving the safety of HPE.

REGULATORY CONTROL OF HYDROGEN POWER ENGINEERING

Modern systems of regulatory safety control have two core frameworks at their basis: these are performance (goal)-based and risk-informed frameworks (PBF/GBF and RIF).

In the performance-based[1] framework [5, 6] for engineering regulation the decision making process is based on the requirements on the goal or performance parameters of an engineering system and the results of this performance.

First, the performance-based framework is focused on the results of an incident (its effects) or on the functional purpose set for the engineering system, not on the process or technique of safety provision. Since this framework deals with quantitative indicators, it allows deviations from the norm (or average) to be easily tracked and attention and resources to be focused on those elements of the system or processes that can become sources of risk.

The performance-based framework can be implemented without *risk insights*. Even in this case it provides a big window of opportunity for compliance with preset performance criteria. Because it is not always possible to establish an objective measurable performance/operation criterion, there are several applications where this framework cannot be used.

The risk-informed framework [7, 8] is the one, where a decision, whether it be political, economical, or engineering, is made using both aspects of the problem, deterministic and probabilistic, for concentrating the attention of the parties involved in decision making on those dangerous processes and conditions that have the greatest influence on the risk magnitude.

For example, the RIF as applied to resolving NPE safety challenges is the one that uses the results of probabilistic safety analysis in combination with deterministic safety analysis so as to focus the attention of operating bodies of NPPs, organizations that provide work and services to these bodies, and also experts from Rostekhnadzor, who carry out licensing activities, or from the federal government oversight of nuclear use on safety-affecting problems. A part of the RIF is *risk-informed decision making*, defined as a decision-making technique using both aspects of the problem, deterministic and probabilistic.

The RIF of safety analysis expands the capabilities of the deterministic approach by

—explicitly considering a broader set of safety threats;

—providing concrete logical means of prioritizing on the basis of risk significance, operation experience, and/or engineering solutions;

—making it easier to consider a broader range of resources that can neutralize dangers/threats;

—explicitly identifying safety analysis uncertainties and describing them in numbers;

—improving the quality of managerial decisions by analyzing the sensitivity of results to initial assumptions and by analyzing uncertainties in source data and structural and stability calculations of buildings.

On the one hand, the indicated features of the RIF sometimes allow for the reduction of the extent of unjustified conservatism in the deterministic approach; on the other hand, they provide the methodological base for formulating additional requirements on the design of support structures that allow cutting the costs of maintaining a required safety level in an economically efficient manner.

The using of risk magnitude as a metric, that is, the measurable scale of the safety of support structures, focuses the designer's attention on those components

[1] The terms *performance-based framework* and *goal-based framework* are used hereafter as synonymous.

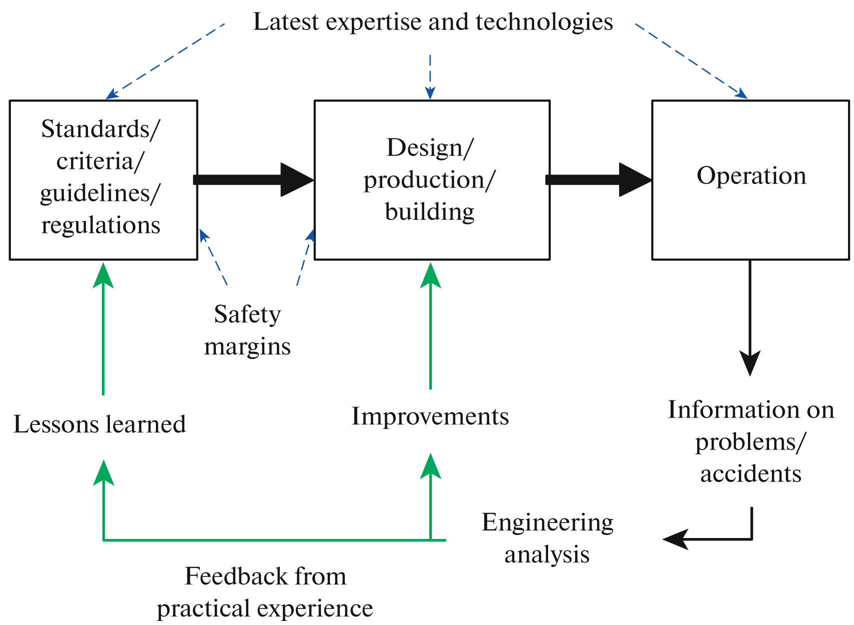

Fig. 2. (Color online) Diagram of the deterministic approach to safety provision.

of the system that make the greatest contributors to risk magnitude. This makes it possible to place available resources precisely on the critical protection components and alleviate the requirements for the members or components that make no significant contribution to the magnitude of risk.

Although the deterministic approach was successfully used to maintain the safety of complex engineering systems over a broad time range, there remains room for improvement.

The systemic and consistent application of the RIF provides opportunities for improvement by analyzing risks more explicitly and including the understanding of risks in the practice of designing and utilizing support structures as well as overseeing their safety.

For the correlation between the deterministic approach and the RIF see the diagrams in Figs. 2 and 3. Unlike the currently mainstream *directive* framework, the RIF explicitly takes into account not only engineering analysis results but also information on analyzing risks linked with a dangerous/protected facility or technology.

On the one hand, the RIF allows more realistically (as compared with the directive framework that often uses so called conservative assumptions[2] defined as assumptions about the worst-case scenario) and, on the other hand, numerically correlating a risk with the strengths of a specific engineering solution.

The concept of the regulatory maintenance of safety in HPE must be elaborated considering both the above-described trends, clearly seen in the foreign [9–11] and Russian [12, 13] practices of regulatory safety foundation and the new tendencies in the research results and best practices of and conceptual approaches to maintaining safety in complex systems, network engineering systems included.

As applied to the policy management of hydrogen and nuclear power engineering, it should be noted that, according to the concept of the development of HPE in Russia, hydrogen and nuclear power engineering facilities for the large-scale production and consumption of hydrogen will include a reactor plant (with a high-temperature gas-cooled reactor as one of the options) and a hydrogen-production CHES, combined in an NPEP plant.

According to clause 3 of the Federal Law 170-FZ on Nuclear Energy Use, NPEPs are nuclear power use facilities; according to clause 6, the requirements on maintaining safety at these facilities must be established by the federal rules and regulations in the domain of nuclear power use.

This is why the policy management documents for NPEPs must set the requirements not only on ensuring explosion prevention at the facility but also on the safety of this facility and activities in the domain of nuclear energy use (nuclear and radiation safety).

The safety of using nuclear energy at NPEPs, high-temperature gas-based reactors, CHESs, and their joint operation have not been subject to any legal regulation in Russia so far. The situation that may be caused by the design features of NPEPs is that some of the current requirements on maintaining safety at NPPs will not apply to these plants. This is why, to set

[2] This term is borrowed from the theory of maintaining safety of high-responsibility systems, such as nuclear power engineering, fuel (oil, gas) power generation, and airspace industry.

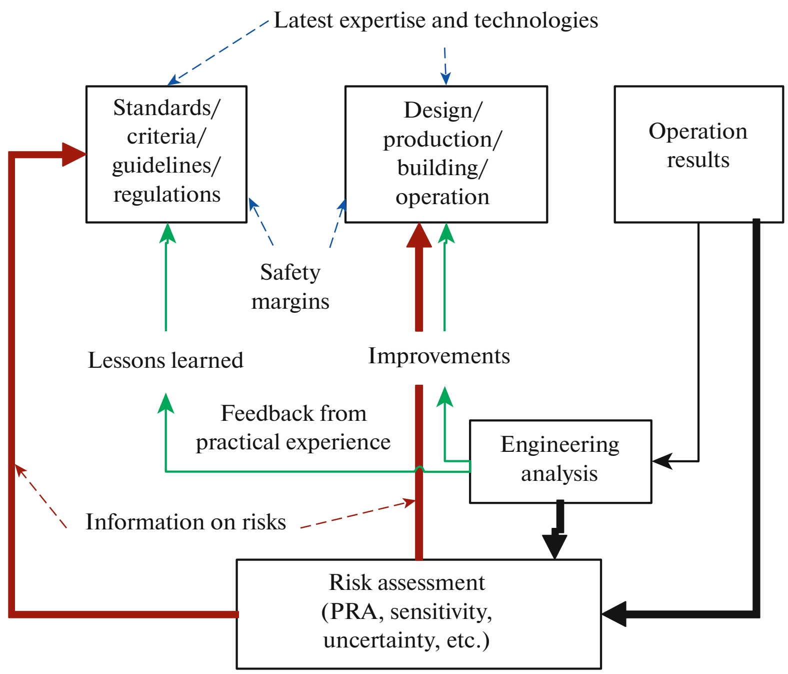

Fig. 3. (Color online) Diagram of the risk-informed approach to safety provision.

the purposes and main criteria of maintaining safety at NPEPs and the main principles of and general requirements on the engineering and organizational steps aimed at achieving this safety, and also efficiently regulate the safety conditions at these facilities, it may be needed to elaborate and adopt a whole set of federal rules and regulations in the domain of nuclear energy use.

The elaboration of the operation and safety rules and regulations for hydrogen nuclear power engineering (HNPE) must include the following phases:

—forming a list of regulatory permits that will cover and be analyzed with regard to HNPE for the large-scale production and consumption of hydrogen;

—analyzing the current federal norms and regulations with regard to HNPE for the large-scale production and consumption of hydrogen;

—forming a list of individual nuclear safety provisions and general safety provisions for NPP reactor systems that are to be included in documents for HNPE.

The tasks expedient to consider in the first place are the following phases of regulatory activity:

—assessing the legal framework for fullness and sufficiency and prepare projects of amending the current laws and regulations of Russia; elaborating, where relevant, new requirements on ensuring safety at new reactor facilities and respective new HNPE technologies;

—elaborating the concept of main safety maintenance provisions for the production, storage, and transportation of hydrogen to NPEPs;

—elaborating the concept of safe and functionally sustainable HPE;

—elaborating and adopt the federal code of rules and regulations Main Provisions of Safety Maintenance for Production, Storage, and Transportation of Hydrogen at Nuclear Power Engineering Plants.

To elaborate and specify the domestic rules and standards of safety maintenance for HPE, it is necessary to prepare:

—primary scientific and engineering data that include the test data on dangerous factors of hydrogen combustion and explosion in emergency conditions and the best hydrogen safety maintenance practices;

—risk and durability analysis tools, including procedures and software for deterministic and probabilistic safety analysis;

—functional (working) models of engineering systems of hydrogen fire and explosion protection, including the explosive mixture monitoring system; flameless hydrogen removal system (passive catalytic hydrogen recoils); systems of inerting devices and facilities with inert gases, chemical deterrents, water steam; ventilation systems, etc. These systems must be designed considering the peculiarities of the propagation and combustion of hydrogen and the distinctness of HPE facilities and engineering items and devices intended for the safe production, storage, distribution, and use of hydrogen as an energy-producing material and a product of mass consumption.

The priorities for experimental and theoretical computational studies needed for creating a full-fledged code of regulatory documents on HPE infrastructure safety are described in brief below.

NEW AND REVAMPED EXPERIMENTAL DATA

For the various industries where hydrogen is handled or can form (gas, oil chemical, chemical, metallurgical, glass, and alimentary), the hydrocarbon fuel and energy industry, nuclear power engineering, and the airspace industry have accumulated a significant bulk of devices, knowledge, tools, and technologies for hydrogen safety maintenance. In all of the enumerated cases, however, the circulation of hydrogen took place inside industrial systems that were distinguished by certain achievements in safety culture on the part of trained personnel and for which sectoral or corporate industrial safety management systems had been elaborated and adopted.

New and revamped experimental data are needed to minimize the number of regulatory obstacles for reconciling the elaborated set of regulations and standards on hydrogen safety with the relevant and emerging international regulatory systems of safety maintenance for HPE infrastructure and hydrogen transportation.

The integrated safety maintenance of HPE, including NPEPs with a high-temperature gas-cooled reactor and a hydrogen-production CHES as well as the infrastructure for transporting, storing, distributing, and using hydrogen, requires the use of primary scientific and engineering data, including the experimental data on the dangerous factors of hydrogen combustion and explosion in emergency conditions and the best empirical and analytical practices of hydrogen safety (*best practices*) maintenance, including data for verifying and validating computer codes intended for the design validation of fire and explosion safety.

The most relevant current areas of experimental research are described below.

Combustion of Ultralean Hydrogen-Containing Gas Mixtures

Switching from ball-like to deflagration flames. Air–hydrogen gas mixtures burn in an essentially different manner from hydrocarbon fuels, and this depends on the initial concentration of hydrogen in the mixture. In ultralean mixtures with an H_2 content of below 10 vol %, a flame cannot burn as a continuous front (as in deflagration flames in nearly stoichiometric and rich mixtures) and splits on its own into small, bubble- or ball-like sets of fire that emerge upwards due to buoyancy effects [14].

Despite the significant effort made to determine the combustion peculiarities of ultralean air-hydrogen mixtures, their essence and dangerous features are still understudied. The lack of knowledge about the ultralean combustion of hydrogen shows in the current absence of agreement in the answer to the question at what minimal concentration a mixture can ignite or explode. The concentrations of H_2 that are currently being used as the respective criteria are 2, 4, 8, and 10 vol %. To provide a justified answer to the specified and other similar questions about the danger of combustion of ultralean air-hydrogen mixtures, it is necessary to conduct additional tests aimed at studying the characteristics of emerging ball-like flames and their conversion to deflagration flames (Fig. 4).

Propagation of air-hydrogen flames in narrow passages. There is no consistent and scientifically valid definition of the bottom concentration limit for air–hydrogen mixture explosions that can produce dangerous baric effects. Research, design, engineering, and regulatory literature makes use of several hydrogen concentration values that characterize concentration limits for various physico-chemical processes (ignition, flame boost, explosion).

The experimental study of near-critical combustion processes under the Earth's gravity is inhibited by buoyancy effects of air–hydrogen mixtures.

The specialized Hele–Shaw cell [17] was constructed and patented for minimizing the effect of gravitation on flame propagation [16]: on the one hand, the gas mixture convection in this cell is inhibited; on the other hand, the heat losses from the flame front allow studying the free propagation of combustion fronts almost in the entire combustibility range of air–hydrogen mixtures.

These experiments are aimed at visually examining the main global (at the characteristic volume scale) morphological features of 2D free propagation of combustion waves in a closed Hele–Shaw horizontal cell in ultralean (from 4 to 12 vol % of H_2) air-hydrogen gas mixtures.

The three morphotypes of 2D free flame boost discovered (Fig. 5) in the tested range of chemical compounds are quasi-continuous, dendritic, and radiating.

Two intermittent transitions were registered for the global morphology of the combustion front at a gradual reduction in the hydrogen concentration in the mixture. The first morphological transition (continuous-dendritic combustion) occurs at H_2 concentrations from 8 to 9 vol %. The second transition (dendritic-beamlike combustion) occurs at H_2 concentrations from 7 to 7.1 vol %. In the series of the tests conducted the global morphology (shape and standard sizes) of the combustion front is retained within each of the three discovered ranges for a fixed concentration of hydrogen in the mixture, whereas the course of the main branches or beams is stochastically variable.

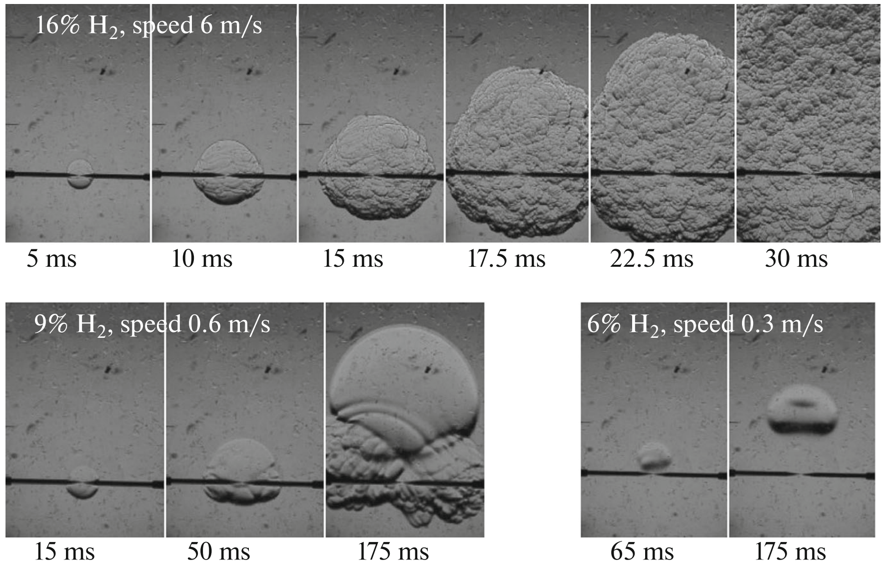

Fig. 4. Characteristic view of low-speed flames in ultralean (from 4 to 16 vol % of H_2) hydrogen-air mixtures [15].

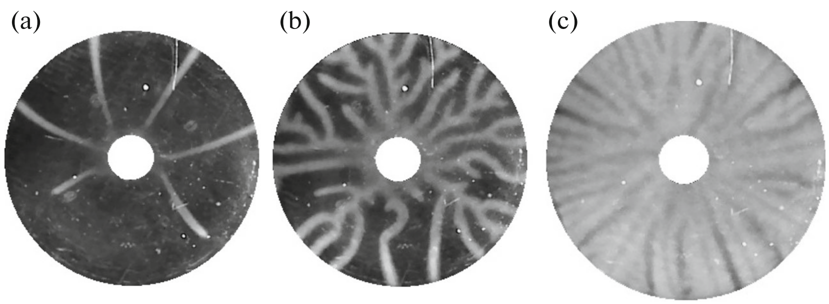

Fig. 5. Three characteristic morphotypes for the 2D propagation of ultralean hydrogen-air flame along narrow flat horizontal passages: (a) the radiated, (b) dendritic, and (c) quasi-homogeneous type, respectively [16].

It is necessary to develop this area of research for producing primary test data on the explosion safety of hydrogen fuel cells that consist from a lot of flat electrodes, that form narrow channels, and for identifying the patterns of transition from quasi-isobaric ball-like to deflagration flames capable of efficiently boosting and switching to quasi-detonation combustion mode.

Propagation and Boost of Deflagration Flames in Stratified Air-Hydrogen Gas Mixtures

The classical approach to the regulatory maintenance of hydrogen safety is based on the following assumptions:

—the source mixture is agitated and characterized by a spatially homogeneous chemical composition (local concentrations coincide in all the points and can have a single value (average across the measured volume));

—the properties of a combustible unreacted mixture are invariant (do not change in time), that is, the pace of changes in the gradients of a spatially heterogeneous concentration field is not taken into account.

As shown by multiple experimental and theoretical computational studies of combustion processes as well as by analyzing the Fukushima Daiichi nuclear disaster:

—in emergency conditions the air-hydrogen mixture can be heavily stratified and significantly affect the combustion pattern;

—the use of mixture concentration limits (Shapiro–Moffette diagram) alone does not allow taking into account the properties of a limiting or a closing space;

—currently, all of the measurable indicators and criteria of explosion safety are established only for premixed hydrogen vapor-air mixtures with a spatial homogeneous chemical composition [18];

—as shown by the results of independent experimental investigations [19, 20] of the conditions in which combustion converts to detonation in closed passages, where the unidimensional stratified distribution of hydrogen was formed;

—the known criteria of flame boost that are derived for spatially homogeneous mixtures ignore the effect of heterogeneity and do not ensure conservatism for explosivity estimates;

—concentration gradients cause a significant flame boost in noncongested passages;

—in congested passages, concentration gradients can both, accelerate and decelerate the transition to detonation, which depends on the average concentration of hydrogen.

The experimental and theoretical computation studies of the influence of stratification on the transition from combustion to detonation are in their initial phase. Their development is needed for the valid analysis, assessment, and maintenance of hydrogen explosion safety.

Formation of Explosive Clouds at Emergency Leaks of Liquid Hydrogen

In the large-scale production and transportation of hydrogen, its handling in liquid cryogenic form has several advantages [21, 22]. Despite the large amount of knowledge on the safety of liquid hydrogen, accumulated in airspace applications in Russia [23] and the United States [24], the safe designing and operation of the part of HPE infrastructure, where liquid hydrogen will be handled, require additional experimental and theoretical computation studies of hazards typical for cryogenic hydrogen.

SAFETY ANALYSIS AND DESIGN TOOLS FOR HYDROGEN POWER ENGINEERING

To ensure the integrated safety maintenance of the HPE in development, the earlier achieved technological advances must be used, considering the following factors:

—the building of new HPE infrastructure facilities in densely developed areas or places with a high density of population (the main consumer of hydrogen) must be performed considering the risks known from the practice of industrial safety management at dangerous HPE infrastructure facilities (pipelines, cryogenic tanks and HP vessels for storing hydrogen in various industries) usually situated at significant (safe) distances from population conurbation places,

—HPE infrastructure must be far safer and more reliable and durable (functionally stable) than the current respective levels in industry and power engineering, so as to protect the mass consumer without sufficient expertise in safety culture against potential hydrogen-induced incidents and faults and prevent him from being a source of unacceptable risks,

—in NHPE, where the nuclear reactor and the CHES as two dangerous facilities will be engaged in direct production, process, and control interaction, it is necessary to take into account underinvestigated risks of the reciprocal influence of nuclear/radiation and dangerous chemical processes as well as availability of fire-hazardous and explosive mixtures of hydrogen, methane, and carbon monoxide in the range of conditions typical for CHES plants.

The analytical tools it is currently important to develop as a matter of priority for adequately taking into account the above-enumerated features of the integrated safety maintenance of the HPE in development are expounded below.

Cascade Fault Risk Analysis Procedures

As a rule, the technogenic faults with the gravest effects occur according to cascade scenarios when a dangerous natural phenomenon, an accident at, and/or the failure of one element results in failures of and/or accidents at other elements in the system [25–27].

Natural disasters are also often attended by cascade-evolving technogenic faults. One of the most telling cases of cascade events was the heavy earthquake that occurred in Japan in 2011 and caused a tsunami wave that became the main cause of the major accident with the release of radioactive substances into the environment at the Fukushima Daiichi Nuclear Power Plant. In various research and engineering works these accidents are called cascade faults, faults with escalating effects, or domino effects.

A cascade fault caused by a natural disaster or a technogenic incident is the most complicated scenario of events in terms of system safety assessment, emergency planning, and response. This is why, we see a constantly growing interest in the problems related to the domino effect, cascade fault evolution, etc. in specialized scientific literature.

According to international and Russian statutory practices, the safety assessment of dangerous production facilities currently requires evolution analyses of cascade faults to be made [28–31]. The enumerated documents and procedures mainly declare the need for considering interconnections among the units of the facility that linked with the influence of casualty producers in the faulty unit on the neighboring units and facilities with hazardous materials. However, there are no cascade fault risk analysis procedures that are suitable for direct practical use, as this area of research is in the nascent phase and has been characterized by rapid development over the last decade [32–35].

Nonlinear Accident Models

The reduction of cascade faults and system blackout risks is one of the most promising techniques of integrated safety maintenance in complex sociotech-

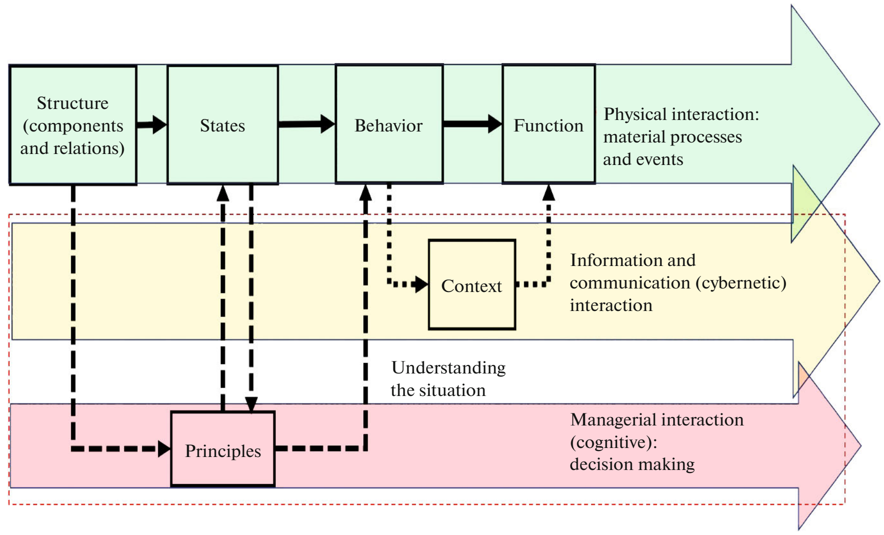

Fig. 6. (Color online) General accident model considering the three basic (physical, informational, cognitive) interactions in complex socioengineering systems [39].

nical systems. Hydrogen power engineering is undoubtedly an example of complex sociotechnical systems. Realistic models of cascade faults are needed for analyzing cascade fault risks and using this data for the durability analysis of complex sociotechnical systems.

Nowadays, the maintenance of integrated safety (various aspects of nuclear, radiation, fire, explosion, chemical, biological, and environmental safety) while analyzing major accident risks (which includes writing safety data sheets and making safety assessment of industrial sites and facilities) and elaborating administrative and technical measures for managing technogenic and natural risks (evacuation planning, etc.) involves implicitly using the so called *linear accident model* in which an accident is a chain (plot) of events, extending from a *hazard/threat to damage* through an *initiating event*.

The conceptual insufficiency of the linear model was indicated for the first time in a classic work [36], where the methodological development of realistic, nonlinear accident models was begun, and those models were intended to consider not only the material but also organizational and social factors that determined or facilitated the occurrence of major accidents [37, 38].

Work [39] proposes expanding the Rasmussen–Lewison–Johansson nonlinear model for cascade faults; in addition to the structural and functional aspects of systems interactions, this expansion explicitly considers their behavior (process) characteristics (Fig. 6).

In addition to standard structure-function models, the proposed model includes two new elements for realistically modeling the initiation, escalation, propagation, and fading of cascade faults and points at the need for developing four extra models called *state*, *process*, *principles*, and *context* and explicitly considering three basic (physical, information, and logical) principles of intersystem interaction.

Nonlinear accident models allow improving both, the accuracy of identifying vulnerabilities in the integrated maintenance of safety in HPE and the predictive ability of risk analysis.

Nonempirical Models of Concentration Limits of Dangerous Processes

There have been various half-empirical correlations proposed over the past three decades for numerically estimate flame boost concentration limits [40, 41]. These correlations use physico-chemical characteristics of gas mixtures (expansion coefficient, Zeldovich and Lewis numbers) and geometrical characteristics for approximating available test data sets. As with any methodology, the empirical approach to estimating concentration limits has internal limitations and contradictions, in particular, in terms of minimal vapor concentrations that can prevent flame boost in severe emergency conditions.

To better the understanding of the essence of concentration limits and narrow the range of uncertainties for the hydrogen-vapor-air mixture, where efficient flame boost is possible, work [42] proposes an alternative approach to estimating concentration limits for flame boost, that is based on nonempirical kinetic thermodynamic (ab initio) modeling. The dependence of the threshold concentration of vapor on the initial gas mixture temperature (373–813 K) at a normal pressure of 100 kPa, at which flame boost is fully suppressed, was calculated (Fig. 7) using only the

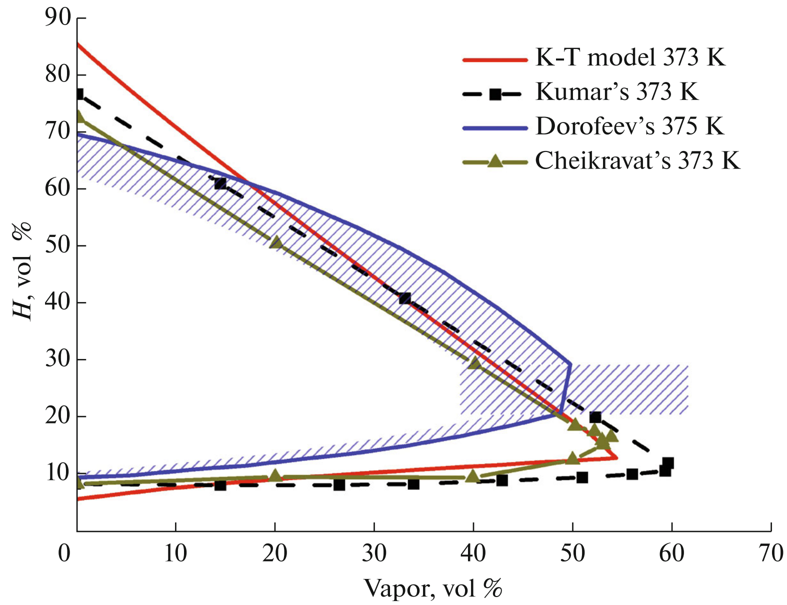

Fig. 7. (Color online) Empirical concentrational limits to the downward propagation of flames (Kumar, Cheikhravat) and accelerated flame propagation (Dorofeev). The fundamental concentration limits to the propagation of flat deflagration flames (nonempirical kinetic thermal dynamic model). Hydrogen—air—steam, 1 atm, 373 K [42].

basic kinetic and thermodynamic parameters of the hydrogen-vapor-air mixture.

The comparison of the derived dependence with the test results allowed detecting contradictions between the empirical approach to evaluating flame boost limits and the test data on the concentration limits of downward flame propagation and formulating new experimental and theoretical tasks aimed to clarify the physical essence of the transition from baric deflagrational flames to nearly isobaric ball-like flames.

The development of nonempirical models of concentration limits of other dangerous processes, for example, detonation limits or limits of the catalytic ignition of the air-hydrogen mixture by passive catalytic hydrogen recombinants, will allow understanding deeper hazard occurrence patterns, specifying safety operation limits of engineering tools, and elaborating more efficient hydrogen techniques of improving hydrogen safety.

CONCLUSIONS

We have shown the need to use two basic frameworks for the regulatory maintenance of safety in hydrogen power engineering; these are the performance-based framework and the goal-based framework.

We have also highlighted and described in brief the priorities for the experimental and theoretical computational studies necessary for creating a comprehensive modern body of regulatory documents on the safety of hydrogen power engineering as the system of systems, including both nuclear power engineering plants for the large-scale reliable production of hydrogen, independent from seasonal or daily environmental variations, and the infrastructure for storing, transporting, and distributing hydrogen as an energy producing material.

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