Deflagration and Detonation Simulation in Hydrogen-Air Mixtures

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Abstract : Previously, the phrase ”hydrogen safety” was often used in terms of NPP safety. Due to the rise of interest to “green” and, particularly, hydrogen power engineering, the problem of hydrogen safety at industrial facilities has become ever more urgent. In Russia, the industrial production of hydrogen is meant to be performed by placing a chemical engineering plant near NPP, which supplies the plant with the necessary energy. In this approach, the production of hydrogen involves a wide range of combustible gases, such as methane, carbon monoxide, and hydrogen itself. Considering probable incidents, sudden combustible gas outburst into open space with further ignition is less dangerous by itself than ignition of the combustible mixture in the presence of many pipelines, reactor vessels, and any kind of fitting frames. Even ignition of 2100 cubic meters of the hydrogen-air mixture in open space gives velocity and pressure that are much lesser than velocity and pressure in Chapman-Jouguet condition and do not exceed 80 m/s and 6 kPa accordingly. However, the space blockage, the significant change of channel diameter on the way of flame propagation, and the presence of gas suspension lead to significant deflagration acceleration and to its transition into detonation or quasi-detonation. At the same time, process parameters acquired from the experiments at specific experimental facilities are not general, and their application to different facilities can only have a conventional and qualitative character. Yet, conducting deflagration and detonation experimental investigation for each specific industrial facility project in order to determine safe infrastructure unit placement does not seem feasible due to its high cost and hazard, while the conduction of numerical experiments is significantly cheaper and safer. Hence, the development of a numerical method that allows the description of reacting flows in domains with complex geometry seems promising. The base for this method is the modification of Kuropatenko method for calculating shock waves recently developed by authors, which allows using it in Eulerian coordinates. The current work contains the results of the development process. In addition, the comparison of numerical simulation results and experimental series with flame propagation in shock tubes with orifice plates is presented.

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