SIMULATION OF DETONATION AFTER AN ACCIDENTAL HYDROGEN RELEASE IN ENCLOSED ENVIRONMENTS

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SESSION: 1.3 Consequences

Abstract

The risk of detonation subsequent to some failure resulting in a hydrogen leak is analyzed numerically for two different scenarios. The first scenario corresponds to a pipe failure in an electrolyzer, resulting in a leak of approximately 42 g of hydrogen. The second scenario considers a leak of 84 g in a reformer. In both cases, the simulation considers a dispersion pattern obtained by numerical simulation of dispersion. Ignition is modeled by artificially depositing energy at some location where the mixture is detonable. Further dispersion is neglected since dispersion is very slow compared to shock motion. The equipment inside the enclosure was ignored; congestion enhances the risk of DDT by providing obstacles, but in the current simulations, detonation was artificially induced. The enclosure walls were taken to be solid. The simulation is two-dimensional, in the vertical release plane. A single step kinetic scheme was used. The simulation uses a well-validated code based upon an ENO scheme, parallelized using MPI. For the electrolyzer, ignition 500 ms after the beginning of the release appears to be close to the worst case scenario; that was the single scenario that was modeled. Results show a detonation failure in vertical directions, upward and downward, but that propagates for a while in the horizontal direction until eventually failing also. Average impulse on the enclosure walls is 500 Ns/m$^2$. For the reformer, three different dispersion patterns were modeled, since which of the three might result in the worst scenario was not so obvious. In one scenario, the detonation does not fail on the front end of the cloud, but it rapidly propagates until reaching the end wall. In the other two cases however, the detonation initially fails, but subsequently, deflagration-to-detonation transition takes place in the shocked mixture, and then the wave proceeds rapidly toward the side wall.