

Using an unsaturated hydrocarbon as mitigator of developed detonation in hydrogen/syngas/air

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Detonation is a complex phenomenon due to a three-dimensional wave structure with an inhomogeneous dynamic wavefront [1-4]. The inhomogeneous front contains pressure triple points moving along it. If the triple points move in the vicinity of a soot-covered detonation tube surface, shear forces from them mark a fishnet-like pattern on the inner walls of the tube. This pattern is known as a detonation cell. As the leading shock front propagates downstream, the triple points alternate. Simultaneously, the transverse waves oscillate perpendicular to the direction of propagation [5]. Sizes of these detonation cells have been found to be one of the most important parameters in detonation research. The paper considers the influence of a hydrocarbon inhibitor on the developed detonation in a hydrogen-air or syngas-air mixture, on the destruction of the detonation front and subsequent decay of detonation cells.

The chemical reaction of hydrogen with air is a classic example of a branching chain reaction. In chain reactions, radicals play an important role as intermediate products of elementary stages. Without the mediation of radicals, the final product is not formed. The most mobile and active radical is atomic hydrogen H which plays an important role in nearly all combustion mechanisms involving hydrogen or its compounds. If its activity is reduced with a help of some chemical additive, the reaction will slow down. A slowdown in the reaction does not diminish its energy: the additive could be flammable itself. A decrease in the hydrogen atom activity can be achieved in many ways, one of which is using an unsaturated hydrocarbon; its reaction with H eliminates the double bond between the carbon atoms. The resulting alkane radical is much less active than atomic hydrogen. The amount of inhibitor could be several per cents by volume.

In the work, propylene C₃H₆ acts as an inhibitor; addition of atomic hydrogen to it gives the propyl radical C₃H₇. The self-sustaining properties of detonation are largely determined by the heat release delay time, which is determined by the development time of the chain process. Partial removal of atomic hydrogen from the chain process slows down the reaction and leads to the transition of the initially developed overdriven detonation into the combustion mode.

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References

1. V.N. Gamezo, A.A. Vasil'ev, A.M. Khokhlov, E.S. Oran *Proceedings of the Combustion Institute* **2000** Vol. 28(1), p. 611-617.
2. J.Lee, R. Knystautas, A. Freiman, *Combustion and Flame*, **1984** Vol. 56.
3. K. Kuo., *Principles of Combustion*, McGraw-Hill, Boston, **2005**.
4. V.A. Levin, I.S. Manuylovich, V.V. Markov. *Papers of the Academy of Sciences*, **2015**, 460 (1): 35–38.
5. A. Gavrikov, A. Efimenko, S. Dorofeev, *Combustion and Flame*, 2000, Vol. 120, p. 19-33. (in Russian)