

# Limits of heterogeneous detonation

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New air-breathing propulsion systems operating on propagating detonations have recently become a topic of intense research and development. The most challenging problem relevant to such propulsion systems is to provide the conditions and techniques to repeatedly initiate detonation waves in a two-phase flow comprising air and liquid fuel drops (heterogeneous detonation).

According to the current understanding, chemical energy deposition in a heterogeneous detonation wave is preceded by mixture formation. The explosive mixture forms due to aerodynamic drop breakup behind the lead shock wave followed by partial vaporization of drop fragments and molecular mixing of the fuel vapor with air. Chemical energy deposition starts from localized auto-ignition events in a partially premixed medium. Further spreading of chemical reaction fronts in the space is controlled by local mixture composition. Here, all known mechanisms of reaction front propagation seem to be possible: laminar and turbulent flames, premixed, partially premixed and nonpremixed flames, as well as transient flames with secondary shock waves and “spontaneous” flames. At partial prevaporization of fuel drops in front of the detonation wave, shock-induced auto-ignition starts earlier and the contribution of the auto-ignition stage to the total energy release increases. In the limit when all liquid fuel is prevaporized in front of the detonation wave, the heterogeneous detonation behaves like the gaseous detonation.

Despite the differences in the mechanism of energy release in gaseous and heterogeneous detonations, thermodynamically such waves are very similar to each other. At similar initial conditions they have nearly similar propagation velocities, in particular at a small fuel mass fraction in the mixture. Moreover, even the propagation mechanisms of such waves are very similar. Both gaseous and heterogeneous detonations propagate due to a strong coupling between the lead shock wave and chemical energy deposition. In suspensions of very fine hydrocarbon drops in oxygen the observed structure of a heterogeneous detonation resembles the structure of the corresponding gaseous detonation. The necessity of ensuring the stability of the “shock wave – reaction zone” complex implies that the reaction zone lengths in gaseous and heterogeneous detonations should not differ considerably. Otherwise the strong feedback between the lead shock wave and the reaction zone in the heterogeneous detonation would hardly exist. Some differences in the reaction zone lengths could however be possible due to various stabilizing effects of shock reflections from particles in the post-shock flow.

The existing models of the heterogeneous detonation are based on considering the average flow behind the lead shock wave. It is assumed that the heat release rate is controlled either by drop vaporization (fine drops) or aerodynamic drop breakup (large drops). Finite-rate chemical reactions are usually not taken into account in such models. In some cases, empirical correlations for ignition delays are used which are based on the average temperature in the post-shock flow. As the use of averaged parameters in the two-phase post-shock flow does not account for complex local phenomena it is worth to consider auto-ignition and combustion of fuel drop suspensions in the heterogeneous detonation wave. Based on the solution of such a problem one can estimate the characteristic rate of chemical energy release and compare it with that relevant to the gaseous detonation. Using the thermodynamic similarity of gaseous and heterogeneous detonation, it is possible then to determine the limiting conditions for the heterogeneous detonation in terms of drop size and prevaporization degree.

The objective of this work is to estimate the minimal drop size and the minimal drop prevaporization degree required for the rate of energy release to be equal to that typical for the near-limit gaseous detonation. At the limit of gaseous detonation the characteristic reaction time is on the order of 100  $\mu$ s. This fact can serve as the approximate criterion for drop suspension detonability: once the drop burnout time is less than or about 100  $\mu$ s, heterogeneous detonation of such a suspension is possible. Only very fine drops are considered herein (less than 10  $\mu$ m in diameter) to avoid consideration of drop breakup. The auto-ignition and combustion of fuel drop suspensions is considered within the frame of the mathematical model accounting for the screening effect of neighboring drops (“spray” effects).

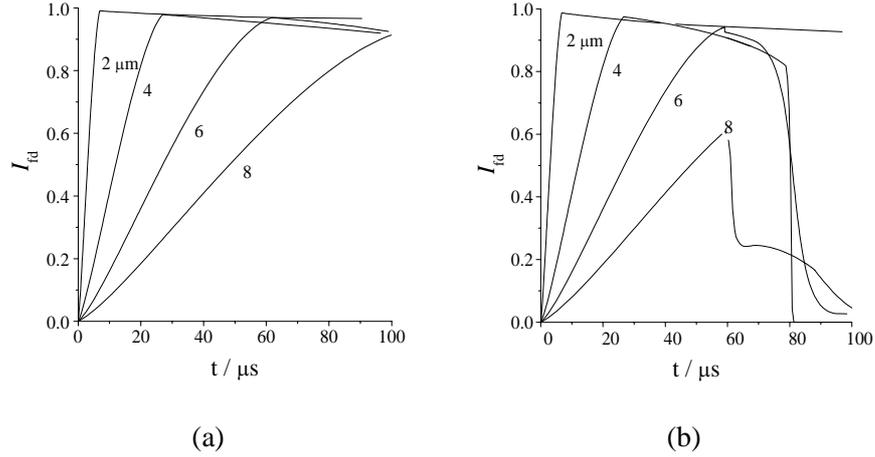


Figure 1. Time histories of the fuel vapor content  $I_{fd}$  in the stoichiometric n-heptane suspensions of drops of different initial size at the fuel prevaporization degree  $I_{fg} = 0$  (a) and  $I_{fg} = 0.25$  (b).

The kinetic mechanism applied consists of 8 reactions with 8 species (Fuel,  $O_2$ ,  $N_2$ ,  $H_2O$ ,  $CO_2$ ,  $CO$ ,  $H_2$ , and generalized radical R). Let us introduce the normalized fuel vapor content in the drop suspension as

$$I_{fd}(t) = M_0^{-1} \int_{r(t)}^R 4\pi\xi^2 Y_f(\xi, t) d\xi$$

where  $M_0$  is the initial drop mass,  $t$  is time,  $Y_f$  is the partial fuel vapor density in the gas phase,  $r$  is the drop radius, and  $R$  is the characteristic size of the elementary sphere in the uniform drop suspension depending on the two-phase mixture equivalence ratio  $\Phi$  as

$$R \approx 1.211r_0 [\rho_l / (\rho_g \Phi \phi_{st})]^{1/3}$$

Here,  $\rho_l$  and  $\rho_g$  are the gas and liquid densities and  $\phi_{st}$  is the stoichiometric fuel-air ratio. The parameter  $I_{fd}$  corresponds to the instantaneous amount of fuel vapor in the drop suspension caused by drop vaporization behind the lead shock wave. For the case of partial liquid prevaporization in front of the shock wave, the prevaporization degree,  $I_{fg}$ , is introduced as the ratio of the fuel mass in the gas and condensed phases. Figure 1 shows the predicted time histories of  $I_{fd}$  in the stoichiometric n-heptane suspensions of drops of different initial size at  $I_{fg} = 0$  (a) and  $I_{fg} = 0.25$  (b) behind a shock wave with the post-shock pressure of 30 bar and temperature of 1500 K typical of the von Neumann spike conditions. The condition  $I_{fd} = 1$  corresponds to complete drop evaporation, while  $I_{fd} = 0$  stands for complete burnout of the fuel vapor. Clearly, at zero prevaporization degree n-heptane drops 2, 4, 6, and 8  $\mu m$  in diameter cannot support heterogeneous detonations because their burning time is much larger than 100  $\mu s$ . This finding contradicts to the common opinion that fine drop suspensions are readily detonable due to fast drop vaporization. As a matter of fact “spray” effects in such suspensions result in a considerable cooling of the gas and longer reaction times. Frequently used single-drop approximations neglecting the “spray” effects are therefore inadequate for the detonability analyses. Partial prevaporization of liquid fuel is the way to control the detonability of drop suspensions. For example, at 25-percent prevaporization, n-heptane drops 4, 6, and 8  $\mu m$  in diameter are capable of supporting the heterogeneous detonation as the drop burning time becomes less or about 100  $\mu s$ . Again, 2-micrometer drops in the stoichiometric n-heptane–air suspension cannot support detonation due to long reaction time.

Thus, the detonability of liquid suspensions is mainly determined by the fuel prevaporization degree. The sensitivity of heterogeneous detonation to the drop size is less pronounced. Note that the characteristic time of aerodynamic drop breakup behind the lead shock wave is on the order of 10  $\mu s$  or less. Therefore the findings reported herein seem to be also applicable to larger drops as the breakup fragments are very fine. The approximate “100-microsecond” criterion used herein could be replaced by a more sophisticated one, however qualitatively the main conclusions are expected to remain valid.