

# **Thermodynamic analysis of closed explosion of hexane-air mixtures**

**WALDEMAR A. TRZCIŃSKI**

Military University of Technology  
Kaliskiego 2, 00-908 Warsaw, Poland

**PIOTR WOLAŃSKI**

Warsaw University of Technology  
Nowowiejska 25, 00-665 Warsaw, Poland

**ALLEN KUHLMAN**

Lawrence Livermore National Laboratory  
Livermore, CA USA

## **Abstract**

In Ref. [1] fundamental hexane droplets/vapour–air explosion data were obtained by measuring the explosion overpressure variation in closed chambers. Tests in the chambers of volumes of 5.6, 40, 150 and 1250 dm<sup>3</sup> were performed. The experimental overpressure histories can be applied to analyse the combustion of hexane-air mixtures. However, the theoretical model of the combustion process is also required.

The purpose of this work is to apply the thermodynamic model of closed combustion for describing the rapid combustion of aerosol/vapour hexane – air mixtures. The relations between thermodynamic parameters and hexane (air) consumption are determined. These relations and experimental overpressure histories enable us to estimate the rate of combustion and fuel burned. Moreover, the law of combustion of hexane particles in rich hexane-air mixtures is proposed.

To determine the rate of combustion of hexane vapour and hexane droplets dispersed in air closed inside a chamber, the theoretical model proposed in Refs. [2-4] is applied. In this model, the analysis of the combustion and determination of combustion characteristics on the basis on the pressure history are possible.

Fuel (hexane vapour),  $\Phi$ , and oxidizer (air),  $\Omega$ , take part in reactions. In a closed combustion system they form non-stoichiometric mixture – charge, C. Therefore, the system, S, consisting of fuel, oxidizer and combustion products, is a multicomponent medium, in which the distribution of components in space is not taken into account. The exothermic processes take place as a result of transformation of reagents, R, into products, P. Let us assume that the reaction proceeds in two-steps. During the first stage, liquid fuel (hexane) evaporates and, in the second one, it reacts with oxygen from air. A rate of chemical reactions is so fast, that the transition from R to P, if fuel evaporates, is instant.

Thermodynamic properties of the components are presented on the so-called Le Chatelier diagram. The Le Chatelier diagrams for mixtures tested are obtained by the use of the CHEETAH code [5]. We assumed that the thermochemical properties of gaseous components are characterised by the equation of state for the ideal gas. The thermochemical data for hexane and hexane vapour are taken from Ref. [6].

In the case of combustion of hexane droplets in confined air we assume that if hexane evaporates it reacts with air immediately. Le Chatelier diagram for mixture of high hexane concentration of  $1 \text{ kg}_{\text{hexane}}/\text{m}^3$  is presented in Fig. 1.

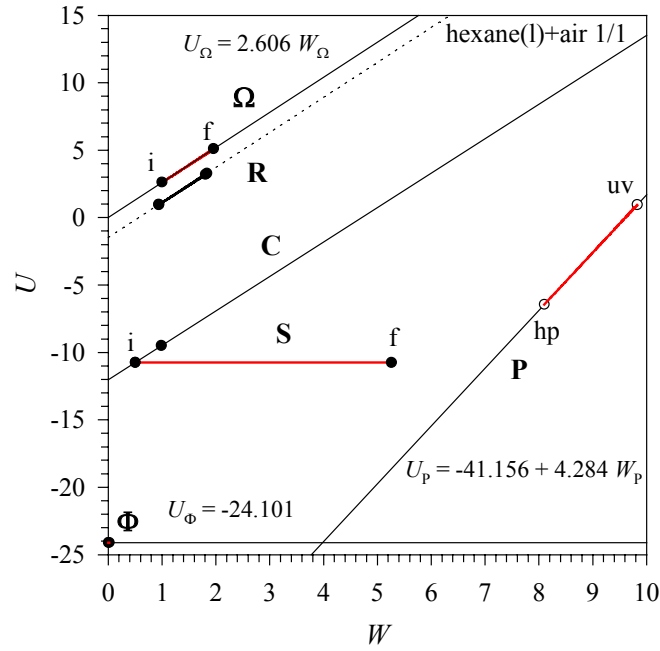


Fig. 1: Le Chatelier diagram for confined combustion of hexane in air (hexane concentration -  $1 \text{ kg}_{\text{hexane}}/\text{m}^3$ )

The parts of rising overpressures histories measured in chambers of 5.6, 40, 150 and 1250  $\text{dm}^3$  volume are taken from Ref. [1]. The time dependence of the degree of air consumed is presented in Fig. 2 for droplets of 0.5 mm diameter.

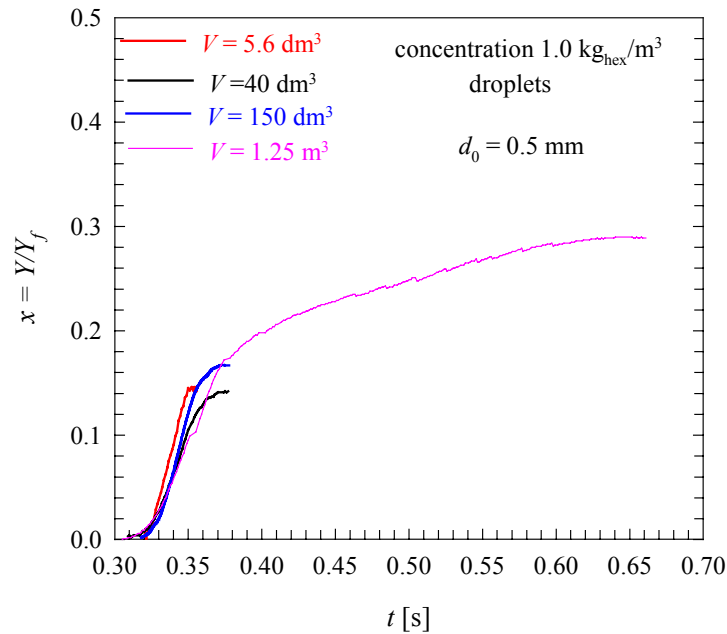


Fig. 2. Calculated degree of consumed air as a function of time for air-hexane 0.5 mm droplets mixtures in 5.6, 40, 150 and 1250  $\text{dm}^3$  chamber

The maximal rates of hexane combustion in chambers of different volumes are close each other. This fact is be taken into account in the method proposed for estimation of the rate of droplet combustion.

To described the process of hexane droplets combustion we will modify an empirical quasi-steady burning law of metal particles [7]:

$$\frac{d d_p}{d t} = -\frac{d_p}{t_b} \quad (1)$$

with

$$t_b = K d_{p0}^2 / \varphi^n \quad (2)$$

where  $d_p$  is a particle diameter,  $t_b$  the burning time of the particle,  $K$  and  $n$  empirical constants determined experimentally in quiescent oxidizing atmosphere. In (1),  $\varphi$  is the volume fraction of oxidizing species in the gaseous phase.

We assume that hexane droplets burn according to the law (1). However, due to the fact, that rich fuel mixtures are considered, the following equation is assumed of combustion of a single hexane droplet:

$$\frac{d d}{d t} = -\frac{d}{t_b} \quad (3)$$

with

$$t_b = K d_0^2 / \Phi^n \quad (4)$$

where  $\Phi = Y_{\Omega i} / Y_{\Phi i}$ .  $Y_{\Omega i}$  and  $Y_{\Phi i}$ , are the initial mass fraction of hexane and air, respectively. Hereafter the index  $i$  will be omitted.

To determine constants  $K$  and  $n$ , the experimental results from chamber tests will be used.

First, we will determine the rate of fuel mass consumption of a single droplet

$$\frac{d m}{d t} = \frac{\pi \rho_{\Phi} d}{2 K} \Phi^n \quad (5)$$

where  $\rho_{\Phi}$  is the density of hexane.

We assume that the combustion of droplets in a chamber starts at the same time. A number of droplets in a unit volume is equal:

$$N = \frac{6 Y_{\Phi} \rho_0}{\rho_{\Phi} \pi d_0^3} \quad (6)$$

where  $\rho_0$  is the density of the droplets-air mixture.

Then, for a unit volume we obtain

$$\frac{d M}{d t} = \frac{3 \rho_{\Omega}}{K d_0^2} \Phi^{n-1} \quad (7)$$

To determined constants  $K$  and  $n$ , we compare the relation  $dM/dt = f(\Phi)$  (7) with similar function obtained from the chamber experiments. From thermochemical calculations one can obtain the relation between the degree of fuel combustion (consumed air)  $x$  and the overpressure  $\Delta p$  in the chamber. This relation can be approximated by the line  $\Delta p = a x$ . It can be used to determined the rate of fuel mass burned on the basis of experimental rate of overpressure increase.

Finally, taking into account the relation between  $\Delta p$  and  $x$ , we can write

$$\frac{d M}{d t} = \frac{\rho_0 F_R Y_f}{a} \frac{d \Delta p}{d t} \quad (8)$$

From Fig. 2 it follows that the rates of fuel burning of the same droplet diameter are similar for four tested chambers. So, the data obtained for the 150 dm<sup>3</sup> chamber will be taken into

considerations. The experimental relations  $dM/dt = f(\Phi)$ , obtained from the dependence of the rate of overpressure increase on the hexane concentration, are presented by filled circles in Fig. 3 for three droplet diameters. The experimental points in Fig. 3 were approximated by the relation (7). The following values of constants were determined:

$K = 9.1 \times 10^7 \text{ s/m}^2$  and  $n = 2.7$  for  $d_0 = 0.25 \text{ mm}$

$K = 3.4 \times 10^7 \text{ s/m}^2$  and  $n = 2.6$  for  $d_0 = 0.5 \text{ mm}$

$K = 1.8 \times 10^7 \text{ s/m}^2$  and  $n = 1.8$  for  $d_0 = 0.7 \text{ mm}$

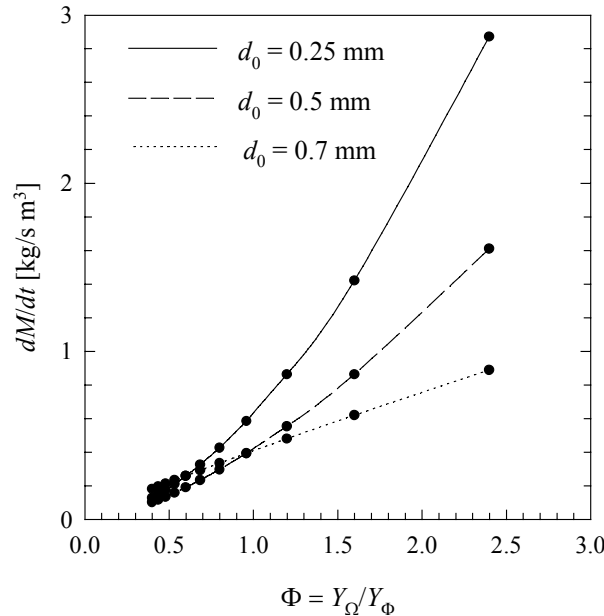


Fig. 3. Experimental relation between initial value  $\Phi$  in the mixture and the rate of fuel mass consumption

The mean values of the parameters are  $K = 5 \times 10^7 \text{ s/m}^2$  and  $n = 2.4$ . It must be underlined that the constants were determined on the grounds of the data obtained for fuel rich mixtures. For such mixtures only small part of fuel burns when air in the chamber is fully consumed. For example, for the mixtures with the hexane concentration  $1 \text{ kg/m}^3$  only 7.5 % of fuel is burned if air is fully consumed.

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