## Lecture 9. Types of flames. Normal burning rate. Detonation

The purpose of the lecture: consideration of the types of flames, the rate of normal combustion, the detonation process and its differences from the combustion process.

**Expected results:** students mastering knowledge about the types of flames, the possibilities of determining the burning rate and the differences between the detonation process and the combustion process.

From a chemical point of view, any well-mixed mixture of fuel with an oxidizing agent contains everything necessary for combustion. Imagine that these conditions are not implemented in the entire vessel, but somewhere in one place - local heating with the formation of a sufficient number of active centers. After local initiation, a reaction wave will occur that gradually encompasses the entire reactive mixture. Two propagation modes are known, with supersonic and subsonic speeds.

The first mode - detonation - is due to the rapid compression of the substance in the shock wave, which provides the necessary heating of the substance in order for the reaction to proceed at a significant speed. In turn, heat generation in a chemical reaction maintains a constant intensity of the shock wave and thereby ensures its propagation over long distances.

The second mode - subsonic - is associated with thermal conductivity and diffusion - this is the flame propagation mode. With the thermal mechanism of flame propagation, the heat released during a chemical reaction is transferred by heat conduction to neighboring sections of unreacted gas, heats them and initiates an active chemical reaction. With a chain mechanism, the distribution of the reaction site occurs through the diffusion of active centers. Perhaps and most likely the combined effect of diffusion and thermal conductivity.

The combustion process, starting in one place, spreads in the volume where the combustible mixture is. Distinguish between normal flame propagation and detonation. Normal flame propagation occurs due to thermal conductivity or diffusion of active centers. During detonation, the combustible mixture is ignited by a shock wave.

Combustion without preliminary mixing of gases:

1) laminar diffusion flame - mixing of gases occurs only by molecular diffusion.

2) turbulent diffusion flame - the gas is mixed both due to diffusion and due to turbulent motion.

3) highly rarefied flame - mixing diffusion or Knudsen molecular flow. Typically, a highly rarefied flame is a cold flame.

Combustion in pre-cooked mixtures:

1) rarefied flame - burns at a pressure below atmospheric.

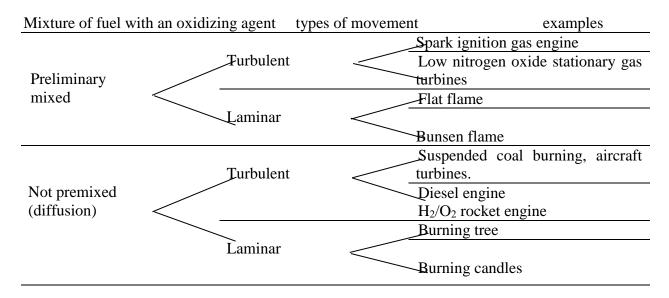
2) hot flame - occurs at  $p \ge 10^5$  Pa, T = 1000-3000 K.

3) a cold flame with T = 500-600 K occurs under certain conditions of combustion of hydrocarbons and is associated with the formation of excited molecules.

An important characteristic of the flame is the normal burning rate;  $u_0$  is the velocity of the flame front in the direction perpendicular to the flame front. For explosive decomposition of ozone, for example,  $u_0 = 1.60 \text{ ms}^{-1}$  ( $p_0 = 1 \text{ kPa}$ ,  $T_0 = 302 \text{ K}$ ,  $T_c = 1922 \text{ K}$ ).

The value  $\omega_0$  is determined by the kinetics of the combustion reaction and the thermal conductivity of the mixture (if the nature of the propagation of the flame is thermal) or by the diffusion of active centers (cold flame). In various models (theories) of flame propagation, a relationship is established between u0 and the reaction rate v in the flame zone and the processes of heat or substance transfer based on the heat conduction or diffusion equation.

## The main types of flames



In the Table 9.1 presents a number of fuel molecules involved in combustion processes. The composition of the flame can be stoichiometric - with complete combustion of the fuel with the formation of  $H_2O$  and  $CO_2$ , rich and poor in fuel relative to the stoichiometric mixture.

 $2H_2+O_2 \rightarrow 2H_2O$  - stoichiometric

 $3H_2 + O_2 \rightarrow 2H_2O + H_2 - rich in fuel$ 

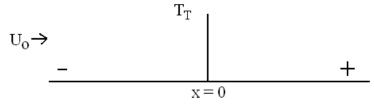
 $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$  - stoichiometric

 $CH_4 + 3O_2 \rightarrow CO_2 + 2H_2O + O_2 - fuel poor$ 

Define the order of the heating zone. Even Hertz solved the problem of a heat wave periodically heating a new one moving at a constant speed. This solution was first applied to the flame by V.A.Michelson, who considered the reaction zone as a surface x = 0 with a fixed temperature  $T_B$ ,

$$T = T_0 + (T_B - T_0) e^{Un \bullet x/\aleph}$$
(1)

where  $T_0$  is the temperature of the undisturbed substance,  $u_n$  is the flame velocity,  $\aleph = \lambda/\rho c$  is the thermal diffusivity, the ratio of temperature to density and heat capacity at constant pressure. The heat wave propagates here in the coordinate system associated with the flame front,

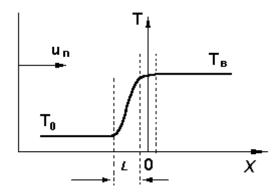


For simplicity, the material constants  $\rho$ , $\aleph$ , c are considered to be constant, independent of temperature. When burning, this assumption is strongly violated, for example,  $\aleph$  changes by 10-300 times. Distribution (1) is a solution of the heat equation

$$\frac{dT}{dx} = \lambda \frac{d^2 T}{dx^2} \qquad (\lambda, c = \text{const}) \quad (2)$$

satisfying boundary conditions T ( $-\infty = T_0$ , T(0) = T<sub>0</sub>).

The solution of equation (1) is applicable only to the region x<0, in which  $T_B$  is absent, for x>0, there are combustion products of constant temperature  $T_B$ .



In accordance with equation (1), we take as the scale of the width of the heating zone the distance at which the heating increases e times.

$$l = \frac{\aleph}{U_n} = \frac{\lambda}{\rho c U_n} \tag{3}$$

Let us calculate this value for a slowly burning mixture (6% methane with air) for which  $U_n=5$  cm/s and a rapidly burning explosive mixture of stoichiometric composition  $U_n=10^3$  cm/s. Substitute  $\aleph = 0.3$  cm<sup>2</sup>/s

$$l = 3 \cdot 10^{-1} / 10^3 = 3 \cdot 10^{-4} \text{ cm} (\text{H}_2);$$
  $l = 3 \cdot 10^{-1} / 5 = 0,06 \text{ cm} (\text{CH}_4)$ 

In both cases, the width of the heating zone is many times greater than the mean free path of gas molecules, which is natural, because the speed of  $U_n$  is much less than the speed of sound; from kinetic theory it follows

$$\aleph \approx \Lambda c_s \tag{4}$$

( $\Lambda$  - average mean free path,  $c_s$  is the thermal velocity of molecules, which is of the order of sound) and therefore

$$\boldsymbol{l} \sim \frac{\Lambda^{*}\boldsymbol{c}_{s}}{\boldsymbol{U}_{n}} \gg \Lambda \tag{5}$$

The order of magnitude of the residence time of a substance in a flame can be determined by dividing, for example, the heating zone by the flame velocity CH<sub>4</sub>

$$6 \cdot 10^{-2} \text{ cm}/5 = 1, 2 \cdot 10^{-2} \text{ s}; 2\text{H}_2\text{-}\text{O}_2 - 3 \cdot 10^{-7} \text{ s}.$$

It should be emphasized that T and the composition of the mixture in the flame changes not only as a result of a chemical reaction, but also in the heating zone; T changes due to the thermal conductivity of the gas, and the composition due to diffusion. The chemical reaction takes place in a mixture that has already undergone heating and whose composition has already changed.

## Detonation

Detonation is the process of the spread in a gas, liquid or solid of an exothermic chemical transformation in the form of a narrow zone moving relative to the starting material at a speed exceeding the speed of sound. This zone is called the detonation wave.

A quick reaction in the zone is not excited due to heat transfer from the reacted layer of the substance to the unreacted one, but by shock compression and corresponding heating of the initial medium caused by the pressure of the reaction products. Therefore, detonation is possible only in environments where reaction products occupy a larger volume than the starting material.

A strict criterion for the fundamental possibility of detonation in a given medium is the positive sign of the isobaric-isochoric thermal effect of the corresponding  $Q_{pV}$  reaction.

This value is measured by the heat released under constant pressure and specific volume.

In practice, detonation is observed during the decomposition of explosives. Gaseous explosives are more often called combustible mixtures.

The main characteristic of explosives is the so-called detonation adiabat (Fig. 9.2). It is a curve in the p-V plane, described by the equation

$$E_{(p,V)} - E_0 = \frac{p - p_0}{2} (V_0 - V)$$

where values with an index of 0 (zero) refer to the initial explosive, and without an index, to the reaction products; E is the specific internal energy, considered as a function of pressure p and specific volume V.

The velocity of the detonation wave relative to the original substance is called the detonation velocity  $u_D$ :

$$u_D = V_0 \left(\frac{p - p_0}{V_0 - V}\right)^{\frac{1}{2}} = V_0 (tg \alpha)^{\frac{1}{2}},$$

where  $\alpha$  is the angle of inclination of the Michelson straight line. This is the name of the line on the p - V plane, passing through the points that depict the initial and final thermodynamic state of the medium. The smallest possible value of the detonation velocity corresponds to the contact of the Michelson straight line with the detonation adiabat. This point of contact, called the Jouguet point, is remarkable in that, with respect to the reaction products in the corresponding state, the detonation wave moves at a speed equal to the local speed of sound. Such detonation is called normal. It is distributed in the explosive independently, without any outside support. The higher points of the detonation adiabat correspond to the subsonic nature of the motion of the detonation wave relative to the reaction products. Such detonation is called overcompressed. It can propagate only under the action of a piston, which follows the detonation wave and compresses the reaction products. If the piston is stopped, detonation returns to normal. The role of the piston can be played by the products of the normal detonation of another, more powerful explosive. The points located on the detonation adiabat below the Jouguet point correspond to the supersonic nature of the motion of the detonation wave relative to the reaction products. Such a detonation is called underexposed. Uncompressed detonation, like normal, propagates independently. But it is possible only in the exceptional case, when the sign of the isobaric-isochoric thermal effect  $Q_{pV}$  changes from positive to negative (in the case of simultaneous occurrence of exothermic and endothermic reactions, of which the first ends earlier).

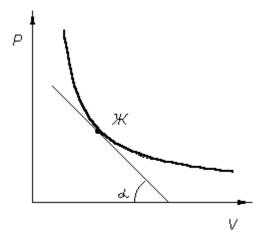


Fig. 9.2. Adiabat:  $\mathcal{K}$  - Jouguet point,  $\alpha$  - tilt angle on the Michelson line

The rate of normal detonation  $u_n$  is determined only by the thermodynamic properties of the starting material and reaction products and does not depend on the kinetics of the decomposition of explosives in the detonation wave.

In the general case, the relation

$$u_{\mu}^{2} = V_{0}(n+1)(p_{\mu}-p_{0}),$$

where  $p_{\pi}$  is the pressure at the Jouguet point; n is the polytropic index taken for a given point (if it is constant). This indicator is determined by the expression  $n = \frac{V}{p} : \left(\frac{dp}{dV}\right)_S$ , where S is the specific entropy. For dense detonation products of condensed explosives,  $n \approx 3$ . For ideal gases, it coincides with the Poisson exponent  $\gamma = \frac{C_p}{C_V}$ . In the particular case of detonation of an ideal gas, in which the reaction products have the same Poisson's ratio, the formula follows from the previous relation

$$u_{\scriptscriptstyle H}^2=2(\gamma^2-1)Q,$$

where Q can be understood as isobaric-isochoric  $Q_{pV}$  and isobaric-isothermal thermal effects of the reaction commonly used in chemistry (in the present case,  $Q_{pV} = Q_{pT}$ ).

## Literature

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