

## ESTIMATION OF DETONATION CHARACTERISTICS OF SILANE-AIR MIXTURES

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**Introduction.** Detonation cell size is one of the most important parameters for estimating the detonation hazard of gaseous mixtures [1]. For example, the critical energy of direct initiation of a detonation wave (DW), process of intensification of deflagration-to-detonation process by system of obstacles and geometrical limits of DW propagation depend on detonation cell size. Unfortunately, the detonation cell size in silane-air mixtures was not measured experimentally yet. The detonation cell size in stoichiometric silane-air mixture was firstly estimated in [2]. In the present work more exact estimation, valid for a wide range of silane concentrations will be presented.

One of the major engineering problems of explosion safety is the estimation of the pressure resulting from explosion of the gas mixture cloud formed when a combustible gas flows out of a pressurized vessel and mixes with ambient air. These studies have been carried out for a wide range of hydrogen-oxygen and hydrocarbon-oxygen mixtures. Formulas have been obtained to calculate the spatial pressure profile as a function of the type and weight of the fuel [3]. As shown by recent studies, these formulas do not always apply to silane-air mixtures [4]. In our opinion, a possible reason for this is that one of the main products of explosion of a silane-air mixture are SiO<sub>2</sub> molecules, which are condensed during expansion of the explosion products. This results in changes in the adiabatic index of the mixture and the molar mass of the gas and leads to additional heat release due to the phase transition. Another possible reason may be due to the fact that the range between the upper and lower flammability limits of silane is much wider than that for typical hydrocarbons. As a result, the percentage of silane involved in explosive conversion is significantly higher than the corresponding value in the case of typical hydrocarbons.

As a first step to determine the cause of this discrepancy, we initiated a series of numerical calculations of the silane concentration profile in the cloud formed during its expansion in a free space.

**Estimation of detonation cell size in silane-air mixture.** In our previous publication [5] the modified Arrhenius formula for calculation induction period of chemical reaction  $\tau$  in silane-air mixtures at elevated pressures and temperatures has been proposed:

$$\tau = 1.37 \cdot 10^{-10} \left(\frac{P}{P_0}\right)^{-0.47} \xi_{SiH_4}^{-0.84} \xi_{O_2}^{-0.07} e^{9695/T},$$

where  $\xi_{SiH_4}$  and  $\xi_{O_2}$  are the molar fractions of silane and oxygen. For this purpose the detail chemical kinetic mechanism of silane combustion is used and the process of silane ignition is calculated. This formula and the model [1] of a detonation cell are used to estimate the longitudinal and transverse detonation cell size:

$$b = 4 \frac{E_a}{RT_{SW}} u_D \tau_{SW}, \quad a = 0.6b.$$

Here  $b$  and  $a$  are longitudinal and transverse cell sizes, and  $E_a$  is the energy of activation. Results of calculations are presented in Fig. 1. As can be seen, the cell sizes in silane-air mixture are even a few (3-4) times smaller than in corresponding hydrogen-air and acetylene-air mixtures [6]. Such small values of the cell sizes indicate that the detonation hazard of the mixture is very high.

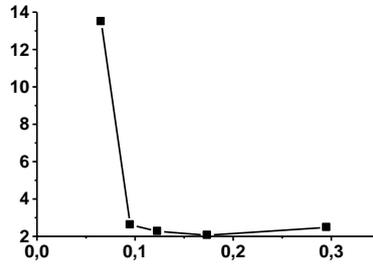


Figure 1. Detonation cell size in silane-air mixture.  $T_0 = 293$  K,  $P_0 = 1$  atm.

The characteristic energy of direct initiation of a spherical detonation wave in gaseous mixtures can be easily estimated via explicit algebraic formulas if the detonation cell size is known (see, for example, [7]):

$$E_{direct} = A\rho_0 D_0^2 b^3.$$

Taking into account, that detonation velocity and cell size in silane-, hydrogen- and acetylene-air mixtures are comparable, the value  $E_{direct}$  in these mixtures are comparable too (for example such energy for these stoichiometric mixtures equals to the energy of explosion of a few grams of TNT [6]).

Typically, in the case of silane leak from a gas cylinder, only the deflagration (not detonation) mode of explosion was registered [4]. But it is known that a system of obstacles can essentially accelerate transition of deflagration into multi-front detonation if characteristic scales of obstacles and distances between them are comparable with the detonation cell size (see, for example, [1]). Therefore in the case of silane leak into an area with some system of obstacles, detonation of silane-air cloud is possible, if the characteristic scales of the obstacles and the gaps between them are comparable with the detonation cell size of the stoichiometric silane-air mixture ( $a_p = 3$  mm, see above). Such possibility should be taken into account in the corresponding estimations of detonation hazard. In order to prevent detonation mode of explosion caused by silane leaks into air, it is necessary to avoid blocking up of a space (in which leakage of silane is possible) by small (a few centimeters in size) obstacles. However, if it is necessary to create a detonation wave in silane-air mixtures for investigations, a system of obstacles with the proper characteristic scales for acceleration deflagration-to-detonation transition should be used. Direct initiation of detonation wave in silane-air mixtures via explosion of a few grams of TNT can be used too.

It is known that the regular cellular structure of a detonation wave, which is characterized by the presence of symmetric transverse waves and a small variation in the cell size, corresponds to the activation energy in the formula for calculating the induction period. Among the mixtures with a regular cellular structure are, for example, hydrogen-oxygen mixtures. In contrast, irregular structures of the detonation wave correspond to high activation energies. Irregular structures of a detonation wave are characterized by the presence of asymmetric main transverse waves, a hierarchy of secondary transverse waves, and a large variation in the detonation cell size. Such mixtures include, for example, methane-oxygen mixtures. As seen from the above formula for calculating the induction period in silane-air mixtures, the activation energy is comparable with the corresponding value for oxygen-air mixtures. Therefore, it should be expected that the cellular structure of the detonation wave in silane-air mixture will be regular.

**Calculation of a leak of silane; silane distribution in a cloud.** Numerical simulation of the discharge of a laminar subsonic jet of silane into a submerged space was conducted by solving unsteady Reynolds-averaged Navier-Stokes equations using the ANSYS Fluent 14.5 soft-

ware. Diameter of an orifice and velocity of silane discharge are  $d = 3.86$  mm  $u = 2$  m/s respectively. Results of calculation are shown in Fig's 2, 3. Chemical composition of the mixture inside the cloud:  $\alpha\text{SiH}_4 + (1 - \alpha)\text{Air}$ ,  $\alpha$  depends on spatial coordinates and time. Similar calculations have been performed for methane and propane mixtures. It can be seen that the percentage of mass of silane between the flammable limits is much more than corresponding value for methane and propane. As a result, the percentage of silane involved in explosive conversion is significantly higher than the corresponding value in the case of typical hydrocarbons.

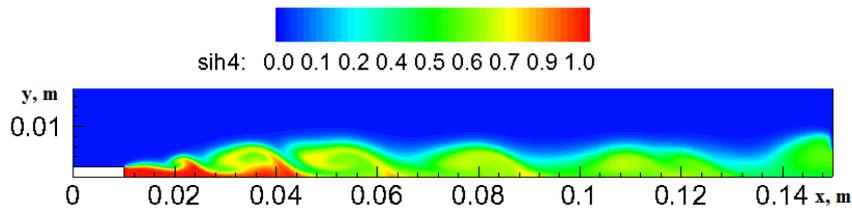


Figure 2. Mass fraction of silane in the cloud.

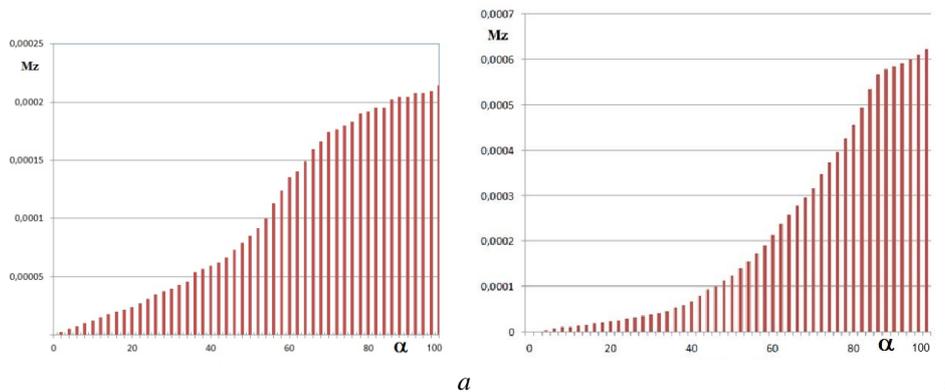


Figure 3. Total mass of silane  $M_z$  in the areas of the cloud, in which molar fraction of silane is less than  $\alpha$  for different moments in time.  $a$ :  $t = 0.1$  s;  $b$ :  $t = 0.3$  s.

#### LIST OF LITERATURE

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