# Estimating Blast Effects from an Accidental Release of High-Pressure Silane

J. Chao, C.R. Bauwens, S.B. Dorofeev
FM Global, Research Division
Norwood, MA, USA

## 1 Introduction

Silane is a pyrophoric gas that can autoignite when exposed to air under normal atmospheric conditions. Because of safety concerns through its widespread usage in the manufacturing of semiconductors, thin-film transistors, LCDs, and photovoltaic cells, numerous studies have been conducted in order to understand the ignition behaviour of silane in air [1-5]. It has been found that a minimum jet velocity (ranging from 4 to 210 m/s) of the released silane is required for spontaneous ignition to occur. For velocities above the critical value, silane can become entrained and mixed into the ambient air and then undergo autoignition following a certain time delay that varies with the concentration of the vapour cloud.

The critical conditions required for autoignition, as well as an understanding of the mechanism that controls ignition delay, are yet to be determined conclusively. It is clear, however, that ignition of silane-air can lead to bulk autoignition or can trigger coherent-autoignition centres (depending on the concentration distribution in the vapour cloud) similar to the SWACER mechanism [6] for deflagration to detonation transition. Therefore, the resulting vapour-cloud explosion (VCE) is generally characterized by very high flame speeds that can result in serious blast damage, even for relatively small releases of silane.

In the present investigation, blast effects (i.e., overpressure and positive impulse) resulting from a silane-air VCE are studied. Although the composition and size of a vapour cloud resulting from an accidental-silane release cannot be determined a priori, an attempt is made to formulate an example of practical estimates of credible worst-case releases and corresponding blast effects, which can be useful in specifying separation distances for various practical silane installations. In addition to blast effects, thermal and projectile hazards due to accidental silane releases should be considered for specification of separation distances, which can be related to various targets and damage criteria. In this study, however, only blast effects are considered; structural damage of buildings is used as an example.

## 2 Methodology

The strength of the blast wave generated by a silane-air explosion will depend on the total amount of chemical energy contained in the vapour cloud and the rate at which it is released. It is, therefore, of interest to estimate how much silane is dispersed into air upon an accidental release and then to approximate how the silane concentration becomes distributed throughout the vapour cloud.

Correspondence to: jenny.chao@fmglobal.com 

Maximum-Flammable Mass

The total mass of silane that is released depends on the ignition delay, which is unknown and, hence, difficult to estimate. Nevertheless, for free-jet releases that are typical of accidental situations, a certain concentration distribution is formed during the release. The resulting silane concentration will range from 100% near the release orifice down to 0% at infinity. The vapour cloud grows with time and approaches a quasi-steady concentration distribution. The mass of flammable gas between the lower and upper flammability limits in this quasi-steady distribution is thus the maximum-flammable mass in the cloud and can be used as a conservative estimate when the ignition delay is unknown (see sketch in Fig. 1a).

The maximum-flammable mass in a silane-air vapour cloud is evaluated in the present study using a similar approach to that developed in [7] for accidental high-pressure releases of hydrogen through small orifices. In general, silane is stored and piped to process equipment at pressures greater than the critical pressure ratio ($p/p_{\mathrm{ambient}}$ = 1.80) such that an accidental release will result in choked flow at the exit orifice with a diameter of $d_0$. The mass flow rate through the exit orifice can be calculated assuming isentropic flow and an infinitely-large reservoir where stagnation conditions do not vary with time:

$$\dot{m} = \frac{\pi d_0^2}{4}\sqrt{\gamma \rho_0 p_0}\left(\frac{\gamma+1}{2}\right)^{\frac{\gamma+1}{2(1-\gamma)}}.$$

The subscript "0" denotes stagnation conditions, and $\gamma = 1.24$ for silane. Compressibility effects should also be included in the density term; i.e., $\rho_0 = p_0/(ZR_sT_0)$ where $R_s$ = 259 J/kg K for silane and $Z$ is the compressibility factor determined from standard charts.

Downstream of the choked orifice, an underexpanded jet is formed as the silane is rapidly expanded to ambient pressure via a series of oblique-shock waves. Concentration gradients in both the axial and radial directions are generated within the jet as entrainment and turbulent mixing occurs with ambient air. In order to bypass the complex region of wave interactions, an equivalent isentropic expansion through a "notional" nozzle with an "effective" diameter of $d_{\mathrm{eff}}$ can be applied, following the work of [8] (see sketch in Fig. 1b). In this manner, the classical relations for concentration decay in a turbulent jet can be used for a supercritical-underexpanded jet and the flammable mass of silane can be calculated once the concentration distribution (in both the axial and radial directions) is known (see [7] for calculation details).

It is also possible that the release can become obstructed or partially confined. In this case, it is well known that the flammable mass in the quasi-steady cloud may be significantly larger than for a free jet, although the effect of the obstruction will depend on geometrical details and the release parameters. In [9], parametric calculations were performed to show that a jet impinging on a flat plate can result in an increase in the flammable volume by up to a factor of 7. Therefore, as a simple-conservative assumption, the same factor is applied to the flammable mass of silane calculated in the present study for obstructed cases.

As an example, the maximum-flammable mass of silane for two different storage conditions (204 bar @ 328 K and 69 bar @ 294 K) is shown as a function of orifice diameter in Fig. 3. Using the present methodology, it can be seen that the flammable mass is described by a power law of the form $m = c_1 d_0^3$ where $m$ is the flammable mass in kg, $d_0$ is the orifice diameter in mm, and $c_1$ is a constant that must be determined specifically for the stagnation conditions of the storage vessel in question. For an obstructed release, the maximum-flammable mass can be approximated as $m_{\mathrm{obs}} = 7c_1d_0^3$.

Blast Effects

Once the total amount of silane released into air is estimated, the distribution of the silane concentration throughout the vapour cloud can be approximated using the simple model developed in [10] for unconfined gaseous explosions. Because the form of the cloud with jet release impinging into a general obstacle array is difficult to characterize, one can assume that the released silane forms a hemispherical-vapour cloud in air with a nonuniform-concentration distribution. The maximum concentration of silane is found in the centre of the vapour cloud, which decreases linearly with the radius of the hemisphere. Only the chemical energy from the portion of the cloud between the upper and lower explosibility limits is considered (see Fig. 2).

Under these assumptions, the maximum concentration and the total mass of silane in the cloud are required to fully define the averaged properties of the vapour cloud. The model in [10,11] can be used for various densities of obstructions that significantly affect the maximum-flame speed. In the case of silane-air, the details of obstructions are not important for the flame speed, which may be very high even without obstacles. Instead, one can choose a sufficiently high visible-flame speed of the order of 500 m/s, which is typical for bulk autoignition or even a detonation. It should be noted that there is very little difference in the resulting blast effect when flame-speed values greater than 500 m/s are chosen. From the flame speed and average-expansion ratio, the blast overpressure and impulse as functions of distance from the explosion centre can be determined (see [12] for details). As an example, the calculated overpressure and impulse using the present approach are shown in Figs. 4a and b for two different vapour-cloud sizes (5.8 and 10 kg of silane).

Damage Levels

For safety practices, it is often of interest to understand the damage associated with the blast effects of a vapour-cloud explosion by defining a safe-separation distance, which is the minimum distance from the explosion centre beyond which the specific level of damage associated with the explosion is considered to be acceptable. For example, the distance to an overpressure of 0.07 bar is generally considered to be a safe-separation distance for moderate structural damage to buildings. The distance to the 0.07-bar overpressure ring is shown in Fig. 5 as a function of the flammable mass of silane. In this example, the separation distance can described by a power law of the form $D = 27m^{1/3}$ where $D$ is the distance in m to the 0.07-bar overpressure ring and $m$ is the flammable mass of silane in kg.

Defining a separation distance based on overpressure, however, does not take the effect of impulse from the blast wave into consideration and does not discern any difference in the hazard resulting from a vapour-cloud explosion with different magnitudes of energy release. A more realistic approach is to define damage criteria based on both pressure and impulse; for e.g., see Table 1 for the damage criteria of buildings [13]. Distances to the various damage levels defined in Table 1 are shown in Fig. 6 as a function of the maximum-flammable mass of silane. For a large vapour cloud (e.g., 100 kg of silane), it can be seen that the onset of total building destruction is estimated to occur in the near field at around 15 m from the explosion centre. The threshold for minor-structural damage is found to be about 128 m from the explosion centre. It is interesting to note that the safe-separation distance for moderate building damage based on overpressure alone (i.e., the 0.07-bar criterion shown in Fig. 5) is comparable at 126 m. For smaller vapour clouds (for e.g., 1 kg of silane), the onset of minor-structural damage occurs in the near field at about 6 m, which is significantly less than the recommended distance of 27 m for an overpressure criterion of 0.07 bar (shown in Fig. 5).

# 3 Summary

In summary, a methodology to estimate credible worst-case blast effect of silane release has been presented that can be useful to specify separation distances for practical silane installations. This methodology relates only to the blast damage. It should be noted that the values presented for the flammable mass and separation distances are only examples that serve to illustrate the methodology. Actual values for flammable mass and separation distances depend on the release scenario, silane-storage parameters, and the damage criteria chosen to evaluate separation distances.

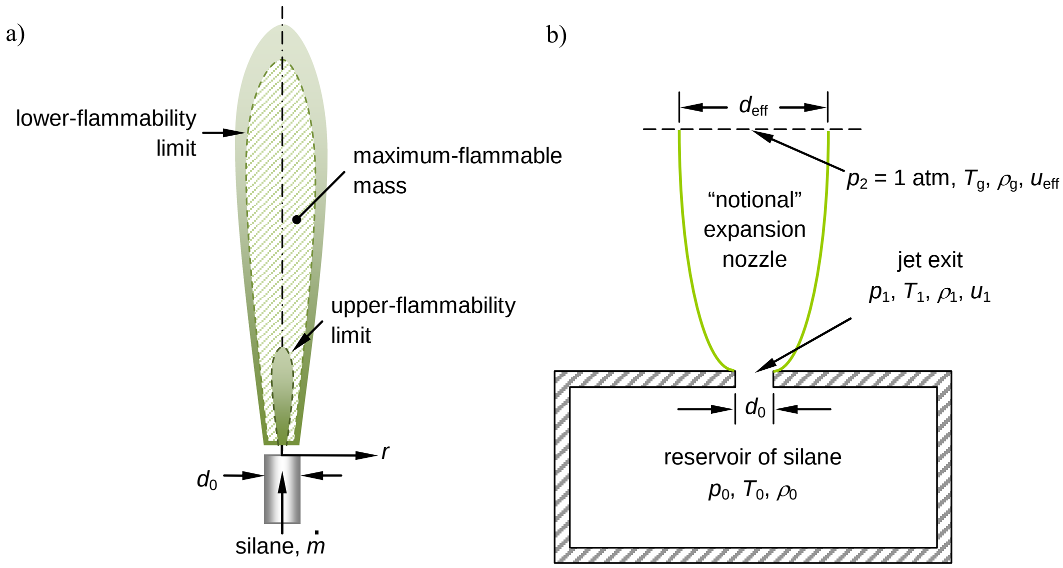


Fig. 1: Sketch of a) lower and upper flammability limits in a silane jet from a choked orifice and b) notional expansion of a supercritical-silane release.

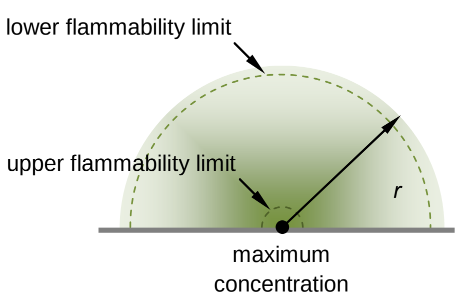


Fig. 2: Distribution of silane concentration in assumed-hemispherical vapour cloud.

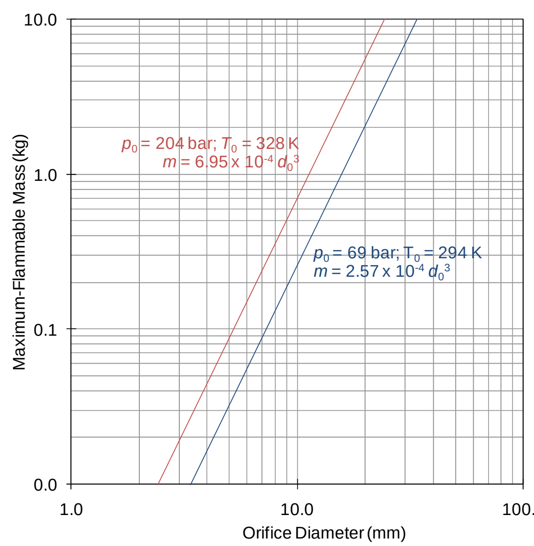


Fig. 3: Maximum-flammable mass from a jet release of silane.

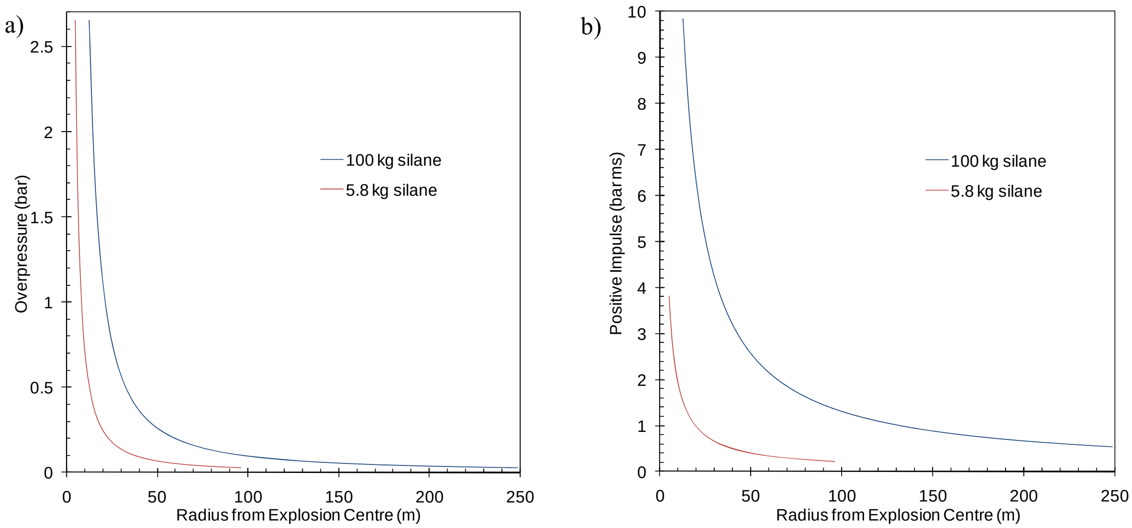


Fig. 4: a) Overpressure and b) positive impulse as functions of radius from the explosion centre.

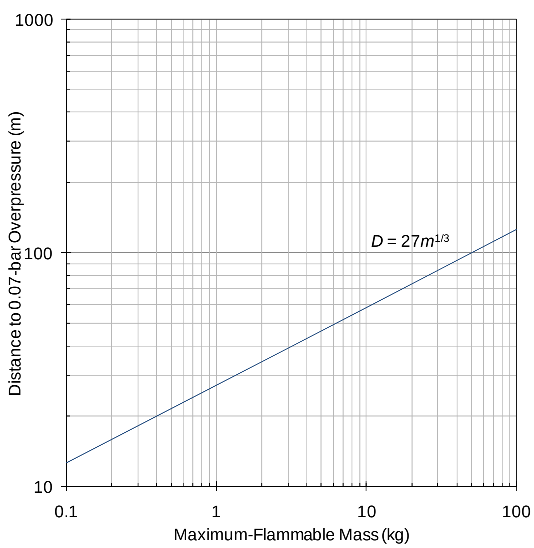


Fig. 5: Distance to 0.07-bar overpressure ring.

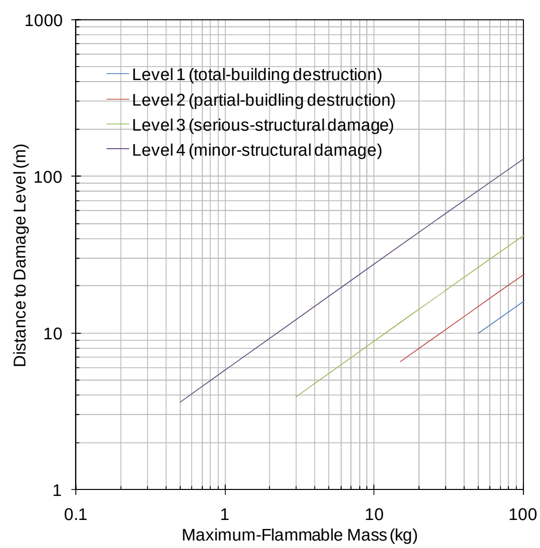


Fig. 6: Distance to damage levels based on a P-I criterion.

Table 1: Criteria for damage levels ($p(R) \geq p_a$ ; $I(R) \geq I_a$ ; $(I(R) - I_a)(p(R)-p_a) \geq k$).

| Building-Damage Level Description | $p_a$ (bar) | $I_a$ (bar ms) | $k$ (bar$^2$ ms) |
|---|---|---|---|
| 1 : total destruction | 0.701 | 7.7 | 0.0866 |
| 2 : threshold for partial destruction; 50–75% of walls destroyed | 0.345 | 5.2 | 0.0541 |
| 3 : threshold for serious structural damage; some load-bearing members fail | 0.146 | 3.0 | 0.0119 |
| 4 : threshold for minor structural damage | 0.036 | 1.0 | 0.00895 |

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