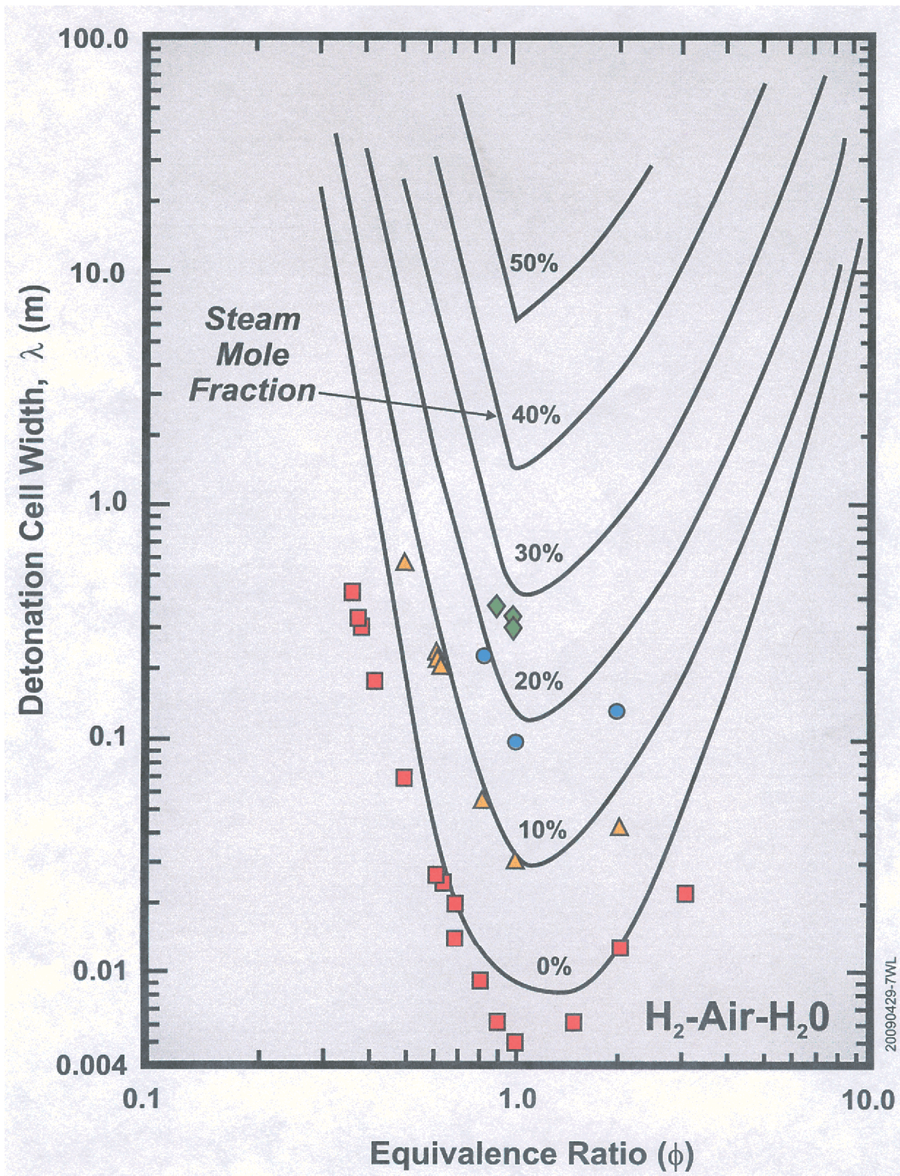


Figure 2-14 Detonation Cell Width Data (Sandia HDT) and Predictions (Shepherd Model) ($H_2$-air-steam, air density = 1.184 kg/m$^3$, T = 100°C for data, T = saturation for prediction). [Reference 57]

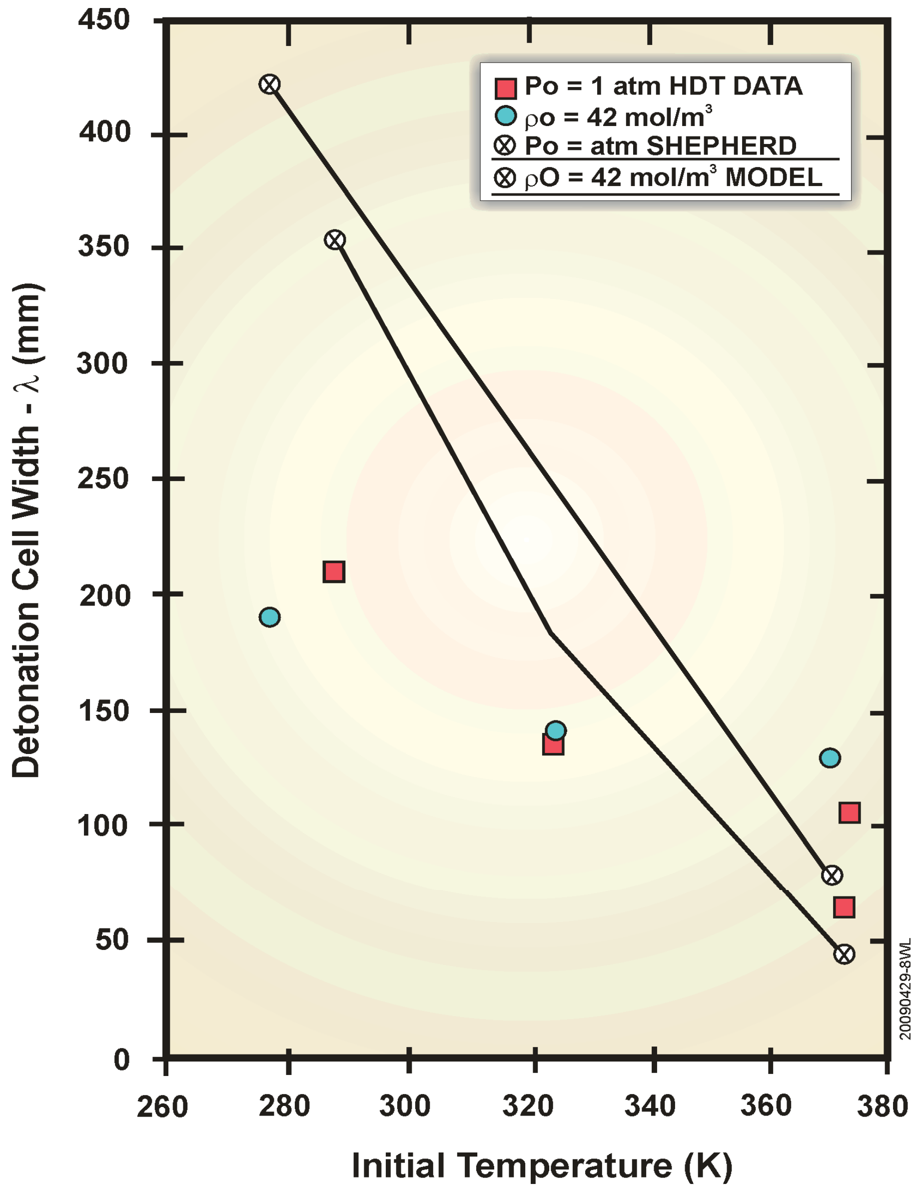


**Figure 2-15 Detonation cell width as a function of temperature [Reference 65]**

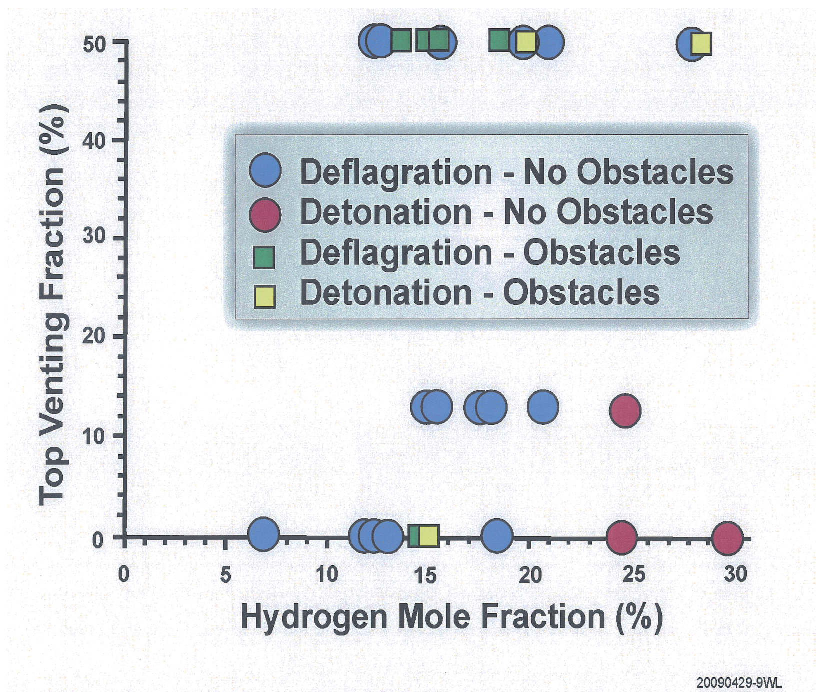


**Figure 2-16 Deflagration-to-detonation transition (DDT) results from the FLAME facility at Sandia [Reference 53]**

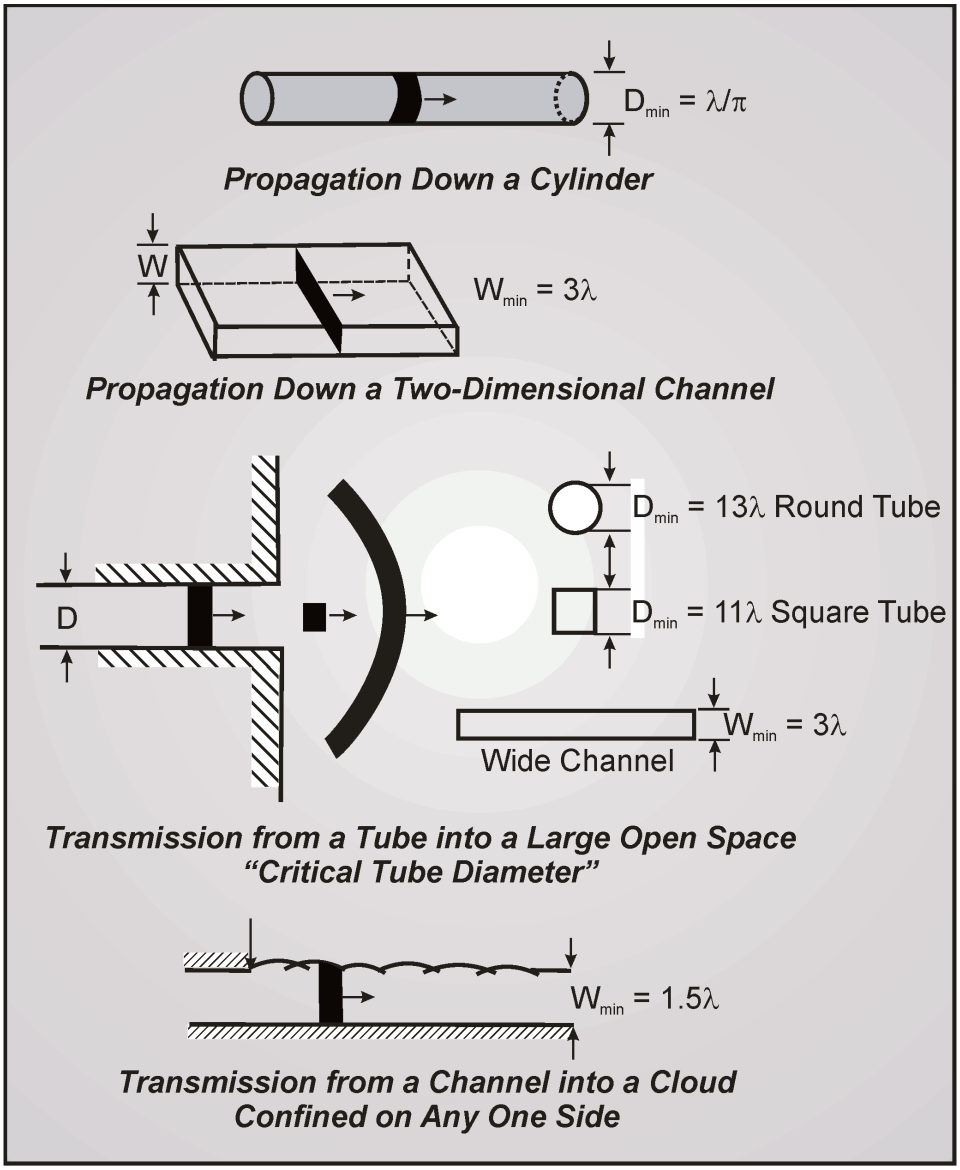


**Figure 2-17 Detonation Propagation and Transmission Correlations for Simple Geometries [Reference 65]**

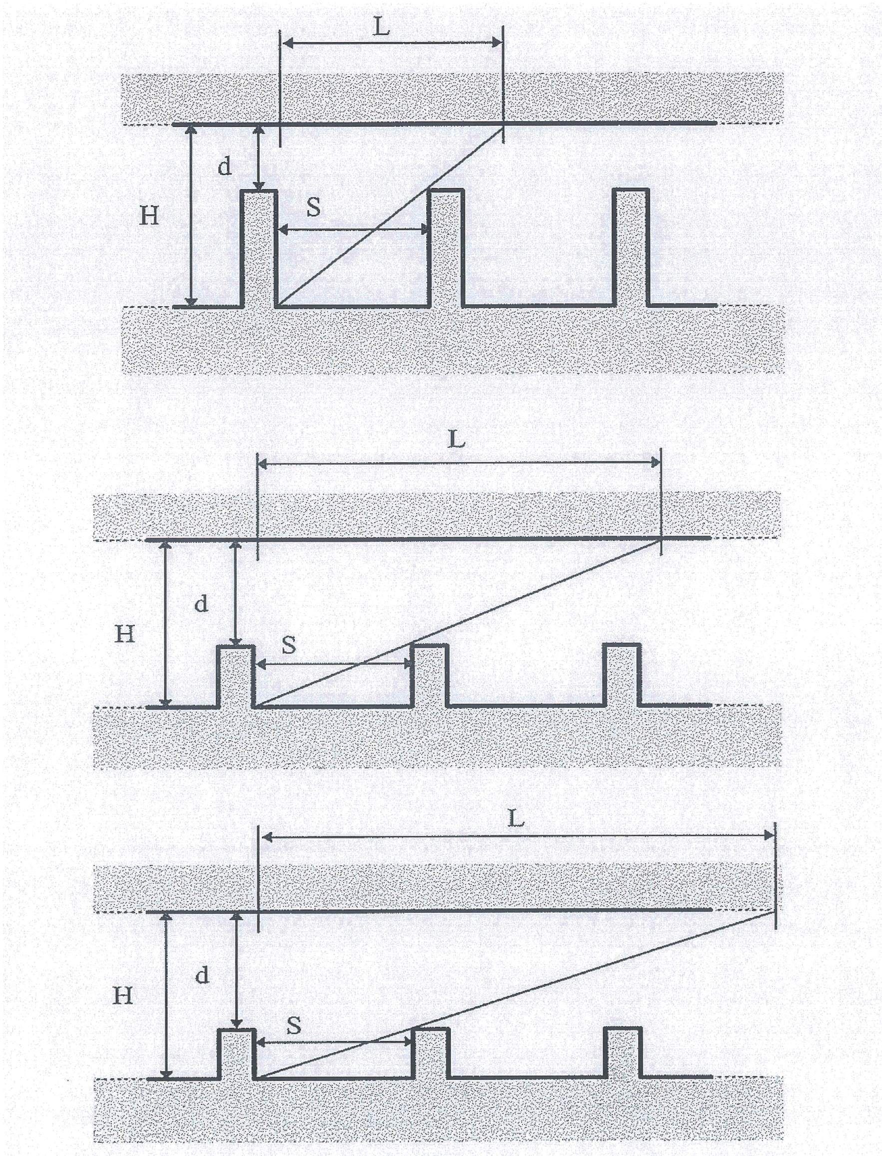


**Figure 2-18 Illustration of Characteristic Size L for Channels with Obstacles and Varying Blockage Ratio [Reference 6]**

## 2.8 Experimental Database for Flame Acceleration Criterion and Onset of Detonation Criterion

As part of the OECD expert group, Dorofeev analyzed a large amount of experimental data on turbulent flame acceleration at conditions applicable to reactor accidents and came up with the idea of critical expansion ratio required for flame acceleration. The following list of experiments in Table 2-1 shows the most extensive database ever assembled together by the expert group [Reference 6]:

(1) High-Temperature Combustion Facility (HTCF) at the Brookhaven National Laboratory (BNL) to study flame acceleration and DDT in hydrogen-air and hydrogen-air-steam mixtures with different hydrogen and steam concentrations. The experiments were performed without venting and with 5.1% venting at initial mixture temperatures up to 650K [Reference 11]. The HTCF is 21.3 m long and has an internal diameter of 27.3 cm. Periodic orifice plates were installed down the length of the entire detonation tube. The orifice plates have an outer diameter of 27.3 cm, an inner diameter of 20.6 cm, and a spacing of 1 tube diameter.

(2) Heated Detonation Tube (HDT) Experiments conducted at the Sandia National Laboratories (SNL) with hydrogen-air-steam and hydrogen-air mixtures to determine the region of benign combustion (between the flammability limits and the DDT limits) [Reference 51]. The HDT is 12 m long and has internal diameter of 43 cm. Obstacles were used with 30% blockage ratio annular rings, and alternate rings and disks of 60% blockage ratio. The initial conditions were 383 K and 1 or 3 atm pressure.

(3) RUT facility tests at Russian Research Centre “Kurchatov Institute” with hydrogen-air mixtures with and without steam dilution in a complex geometry [Reference 12, 13]. The first part of the facility was a channel of 2.5 x 2.3-m cross-section and 34.6 m long; the second part was a canyon of 6 x 2.5-m cross-section and 10.5 m long, and the third one was a channel of 2.5 x 2.3-m cross-section and 20 m long. Twelve concrete obstacles were placed along the first channel with a spacing of 2.5 m (blockage ratios were 0.3 and 0.6). Initial temperature in tests with steam was close to 375 K. Initial pressure in all the tests was 1 atm.

(4) FLAME facility tests at the Sandia National Laboratories in a study of FA and DDT of hydrogen-air mixtures [Reference 53]. FLAME is a large (30.5 m long) rectangular channel that has an interior width of 1.83 m and a height of 2.44 m. The blockage ratio was 0.0 (no obstacles) or 0.33 in the tests. Initial conditions were normal in these tests.

(5) FZK experiments [Reference 26] were performed in a 35-cm-diameter, 12-m-long length with equidistant rings as obstacles (blockage ratio was 0.6, spacing was 35cm). Flame acceleration was studied in hydrogen air mixtures and in hydrogen-oxygen (2:1) mixture, diluted with nitrogen, argon, helium and CO2. Experiments were conducted under normal initial conditions.

(6) CHANNEL, DRIVER, and TORPEDO experiments provided data on turbulent flame propagation regimes in obstructed areas at different scales [Reference 14, 15]. Blockage ratios ranged from 0.1 to 0.9. Distances between obstacles were equal to the transverse size of each tube for all these facilities. Mixture compositions were varied in the tests. Experiments were conducted under normal conditions.

(7) The CHANNEL facility is a tube with a square cross-section of 80 mm x 80 mm and 5.28-m length. Rectangular obstacles were mounted along upper and bottom plates. Different hydrogen-air mixtures and stoichiometric hydrogen-oxygen, diluted by argon or helium were used in these tests.

(8) The DRIVER facility is a detonation tube of 174 mm id and approximately 12-m length. Hydrogen-air mixtures and stoichiometric hydrogen-oxygen mixtures diluted with nitrogen, argon, or helium were used in this facility.

(9) The TORPEDO facility is a 520-mm tube of 30.3-m length. Hydrogen-air mixtures and stoichiometric hydrogen-oxygen, diluted by helium were used in these tests.

This was an extensive undertaking that provided better insight into the combustion regime of slow and fast deflagrations. It also made possible a quantitative prediction of flame acceleration in code calculations. Figure 2-20 shows for hydrogen-lean mixtures the correlation between the expansion ratio, the Zeldovich number and the resulting combustion regime. Here, the Zeldovich number is defined as $\beta = Ea(T_b - T_u)/(RT_b^2)$ where *Ea* is the effective activation energy, $T_u$ is the initial, and $T_b$ is the maximum flame temperature. There is clearly a boundary between fast combustion and slow combustion. This boundary line defines the critical expansion ratios for a wide range of initial temperatures. Similarly, for hydrogen-rich (including stoichimetric) mixtures, the boundary line between fast and slow combustions shown in Figure 2-21 is a horizontal line with expansion ratio between 3.5 to 4.0. Based on these results, Dorofeev established the so-called "σ criterion" which states that for flame acceleration to occur, the expansion ratio of the mixture must be equal or greater than the critical expansion ratio. Figure 2-22 shows the relation between the acceleration limits and expansion ratios for hydrogen-air-steam mixtures at 373 K.

Dorofeev also correlated the onset conditions for DDT based on the above large amount of experimental data and some additional experiments that are listed below:

(1) McGill University small-scale tests on DDT [Reference 63, 27],

(2) Whiteshell Laboratories (AECL) data [Reference 8].

(3) Large-scale DDT experiments with hydrogen-air, hydrogen-air-steam, and hydrogen-air-CO2 mixtures at Russian Research Centre 'Kurchatov Institute' RUT facility [Reference 12, 13, 14, 33,54, 55, 56]

(4) Small scale experiments in MINIRUT experimental apparatus at scale 1:50 of RUT facility [Reference 33, 14].

(5) Data on DDT conditions obtained in obstructed channels with transverse sizes 80, 174, 350, 520 mm [Reference 33, 26] for a wide range of hydrogen mixtures

A summary of experiments is given in Table 2-2 and experimental results are presented in Figure 2-23. Data are marked with light and dark labels where "light" means no DDT and "dark" means DDT. Figure 2-23 shows combustion modes (DDT or no DDT) as a function of characteristic length *L* of the compartment or the mixture cloud, and detonation cell width λ. A good correlation is observed for $L/\lambda$=7 within the accuracy of the cell size data over a wide range of scales. The minimum ratio of $L/\lambda$= 5.6 for few cases of DDT (i.e. dark data points above L/λ=7 line) can be found among the general borderline of $L/\lambda$=7 in the correlation presented in Figure 2-23. This is just a 20% deviation, which is much smaller than inaccuracy of the cell size data. Based on these results, the so-called "7λ criterion" was recommended for reactor safety applications.

## 2.9 Effects of $H_2$ Stratification on Deflagrations

So far we have only considered combustion in a well-mixed mixture. However, in reality, stratified regions of hydrogen or steam concentrations may exist prior to complete mixing. Whitehouse et al. (1994) found, from a series of experiments in a 10.7 $m^3$ cylinder, that combustion of a stratified mixture could be the same, less, or more severe than a well-mixed mixture for the same amount of hydrogen. For the case of stratified mixtures with average concentrations of hydrogen below the downward flammability limits, the combustion pressures were significantly greater than well-mixed mixtures when ignited at the top of the vessel and about the same when ignited at the bottom. A higher concentration at the top leads to a considerably higher burn completeness in the stratified mixture for top ignition.

For the case with average concentrations above the downward flammability limits, the combustion pressures were nearly the same for top ignition and lower for bottom ignition. The burn completeness was near 100% for top ignition. Much higher flame speeds for top ignition and slower flame speeds for bottom ignition were observed in the stratified mixtures. Since stratification could result in an incomplete burn, one can conservatively neglect the stratification effects on combustion by assuming a complete burn.

**Table 2-1 Experiments Used in Correlations for Flame Acceleration Criterion**

| Data Source | Label | Blockage Ratio BR | Tube or channel size L,mm | Initial temperature e T,K | Mixture type | Equivalence Ratio $\Phi$ |
|---|---|---|---|---|---|---|
| HfCF-BNL [3.11] | bl | 0.43 | 273 | 300 | H2/air | ‹1 |
| HfCF-BNL [3.11] | b2 | 0.43 | 273 | 500 | H2/air | ‹1 |
| HfCF-BNL [3.11] | b3 | 0.43 | 273 | 650 | H2/air | ‹1 |
| HfCF-BNL [3.11] | b4 | 0.43 | 273 | 400 | H2/air/$H_20$ | ‹1 |
| HfCF-BNL[3.11] | b5 | 0.43 | 273 | 500 | H2/air/$H_20$ | ‹1 |
| HfCF-BNL[3.11] | b6 | 0.43 | 273 | 650 | H2/air/$H_20$ | ‹1 |
| CHANNEL-RRCKI [3.9] | c1 | 0.1 | 80 | 293 | H2/air | ‹ 1; ›1 |
| CHANNEL-RRCKI [3.9] | c2 | 0.3 | 80 | 293 | H2/air | ‹ 1; ›1 |
| CHANNEL-RRCKI [3.9] | c3 | 0.6 | 80 | 293 | H2/air | ‹ 1; ›1 |
| CHANNEL-RRCKI [3.9] | c4 | 0.9 | 80 | 293 | H2/air | ‹ 1; ›1 |
| CHANNEL-RRCKI [3.9] | c5 | 0.6 | 80 | 293 | $H_2/0_2/He$ | 1 |
| CHANNEL-RRCKI [3.9] | c6 | 0.6 | 80 | 293 | $H_2/0_2/Ar$ | 1 |
| DRIVER-RRCKI[3.9] | dl | 0.09 | 174 | 293 | $H_2$/air | ‹ 1; › I |
| DRIVER-RRCKI[3.9] | d2 | 0.3 | 174 | 293 | $H_2$/air | ‹ 1; ›1 |
| DRIVER-RRCKI[3.9] | d3 | 0.6 | 174 | 293 | $H_2$/air | ‹ 1; ›1 |
| DRIVER-RRCKI[3.9] | d4 | 0.9 | 174 | 293 | $H_2$/air | ‹ 1;› I |
| DRIVER-RRCKI[3.9] | d5 | 0.09 | 174 | 293 | $H_2/0_2/N_2$ | 1 |
| DRIVER-RRCKI[3.9] | d6 | 0.3 | 174 | 293 | $H_2/0_2/N_2$ | 1 |
| DRIVER-RRCKI[3.9] | d7 | 0.6 | 174 | 293 | $H_2/0_2/N_2$ | 1 |
| DRIVER-RRCKI[3.9] | d8 | 0.9 | 174 | 293 | $H_2/0_2/N_2$ | 1 |
| DRIVER-RRCKI[3.9] | e1 | 0.09 | 174 | 293 | $H_2/0_2/He$ | 1 |
| DRIVER-RRCKI[3.9] | e2 | 0.3 | 174 | 293 | $H_2/0_2/He$ | 1 |
| DRIVER-RRCKI[3.9] | e3 | 0.6 | 174 | 293 | $H_2/0_2/He$ | 1 |
| DRIVER-RRCKI[3.9] | e5 | 0.09 | 174 | 293 | $H_2/0_2/Ar$ | 1 |
| DRIVER-RRCKI[3.9] | e6 | 0.3 | 174 | 293 | $H_2/0_2/Ar$ | 1 |
| DRIVER-RRCKI[3.9] | e7 | 0.6 | 174 | 293 | $H_2/0_2/Ar$ | 1 |
| FLAME-SNL [3.15] | fl | 0.33 | 1830 | 293 | $H_2$/air | ‹1 |
| FLAME-SNL [3.15] | f2 | 0 | 1830 | 293 | $H_2$/air | ‹1 |
| FZK [3.9] | gl | 0.6 | 350 | 293 | $H_2$/air | ‹ 1; ›1 |
| FZK [3.9] | g2 | 0.6 | 350 | 293 | $H_2/0_2/N_2$ | 1 |
| FZK [3.9] | g3 | 0.6 | 350 | 293 | $H_2/0_2/He$ | 1 |
| FZK [3.9] | g4 | 0.6 | 350 | 293 | $H_2/0_2/Ar$ | 1 |
| FZK [3.9] | g5 | 0.6 | 350 | 293 | $H_2/0_2/C0_2$ | 1 |
| FZK [3.9] | g6 | 0.6 | 350 | 293 | $H_2$/air/$C0_2$ | 0.5 |
| FZK [3.9] | g7 | 0.6 | 350 | 293 | $H_2$/air/$C0_2$ | 1 |
| FZK [3.9] | g8 | 0.6 | 350 | 293 | $H_2$/air/$C0_2$ | 2 |
| FZK [3.9] | g9 | 0.6 | 350 | 293 | $H_2$/air/$C0_2$ | 4 |
| RUT-RRCKI [3.13] | r1 | 0.6 | 2250 | 293 | $H_2$/air | ‹1 |

| | | | | | | |
|---|---|---|---|---|---|---|
| RUT-RRCKI [3.13] | r2 | 0.3 | 2250 | 293 | $H_2$/air | ‹1 |
| RUT-RRCKI [3.13] | r3 | 0 | 2250 | 293 | $H_2$/air | ‹1 |
| RUT-RRCKI [3.13] | r4 | 0.3 | 2250 | 293 | $H_2$/air/ $H_2$0 | ≤1 |
| HDT-SNL [3.12] | s1 | 0.6 | 406 | 383 | $H_2$/air | ›1 |
| HDT-SNL [3.12] | s2 | 0.3 | 406 | 383 | $H_2$/air/ $H_2$0 | ›1 |
| TORPEDO-RRCKI [3.9] | t1 | 0.6 | 520 | 293 | $H_2$/air | ‹1;›1 |
| TORPEDO-RRCKI [3.9] | t2 | 0.6 | 520 | 293 | $H_2/O_2$/He | 1 |
| TORPEDO-RRCKI [3.9] | t3 | 0.3 | 520 | 293 | $H_2$/air | ‹1;›1 |
| TORPEDO-RRCKI [3.9] | t4 | 0.1 | 520 | 293 | $H_2$/air | ‹1;›1 |

**Table 2-2 Experiments Used in the L/λ Correlation for Onset of Detonations**

| Data Source | Label | Blockage Ratio BR | Tube or channel size D (H),mm | Initial temperature e T,K | Mixture type | Equivalence Ratio $\Phi$ |
|---|---|---|---|---|---|---|
| AECL [3.12] | a1 | 0.31 | 280 | 373 | $H_2$/air/$H_20$ | |
| HTCF-BNL [3.11] | b1 | 0.43 | 273 | 300 | $H_2$/air | ‹1 |
| HTCF-BNL [3.11] | b2 | 0.43 | 273 | 500 | $H_2$/air | ‹1 |
| HTCF-BNL [3.11] | b3 | 0.43 | 273 | 650 | $H_2$/air | ‹1 |
| HTCF-BNL [3.11] | b4 | 0.43 | 273 | 400 | $H_2$/air/$H_20$ | ‹1 |
| HTCF-BNL [3.11] | b5 | 0.43 | 273 | 500 | $H_2$/air/$H_20$ | ‹1 |
| HTCF-BNL [3.11] | b6 | 0.43 | 273 | 650 | $H_2$/air/$H_20$ | ‹1 |
| CHANNEL-RRCKI [3.9] | c1 | 0.1 | 80 | 293 | $H_2$/air | ‹1;›1 |
| CHANNEL-RRCKI [3.9] | c2 | 0.3 | 80 | 293 | $H_2$/air | ‹1;›1 |
| CHANNEL-RRCKI [3.9] | c3 | 0.6 | 80 | 293 | $H_2$/air | ‹1;›1 |
| DRIVER-RRCKI [3 .9] | d1 | 0.09 | 174 | 293 | $H_2$/air | ‹1;›1 |
| DRIVER-RRCKI [3 .9] | d2 | 0.3 | 174 | 293 | $H_2$/air | ‹1;›1 |
| DRIVER-RRCKI [3 .9] | d3 | 0.6 | 174 | 293 | $H_2$/air | ‹1;›1 |
| DRIVER-RRCKI [3 .9] | d4 | 0.9 | 174 | 293 | $H_2$/air | ‹1 |
| FLAME-SNL [3 .15] | f1 | 0.33 | 1830 | 293 | $H_2$/air | ‹1 |
| mini-FLAME-SNL [3.47] | f3 | 0.33 | 150 | 293 | $H_2$/air | ‹1 |
| FZK [3 .9] | g1 | 0.6 | 350 | 293 | $H_2$/air | ‹1;›1 |
| FZK [3 .9] | g2 | 0.6 | 350 | 293 | $H_2/0_2/N_2$ | 1 |
| FZK [3 .9] | g3 | 0.3 | 350 | 293 | $H_2$/air | 1 |
| FZK [3 .9] | g6 | 0.6 | 350 | 293 | $H_2$/air/$C0_2$ | .5 |
| FZK [3 .9] | g7 | 0.6 | 350 | 293 | $H_2$/air/$C0_2$ | 1 |
| FZK [3 .9] | g8 | 0.6 | 350 | 293 | $H_2$/air/$C0_2$ | 2 |
| FZK [3 .9] | g9 | 0.6 | 350 | 293 | $H_2$/air/$C0_2$ | 4 |
| McGill [3.25] | m1 | 0.44 | 16x57x 50 | 293 | $H_2$/air | ‹1 |
| McGill [3.25] | m2 | 0.44 | 16 X 57 X 100 | 293 | $H_2$/air | ‹1 |
| McGill [3.25] | m3 | 0.43 | 50 | 293 | $H_2$, CH-fuels/air | ‹1 |
| McGill [3.25] | m4 | 0.43 | 150 | 293 | $H_2$, CH-fuels/air | ‹1 |
| McGill [3.25] | m5 | 0.43 | 300 | 293 | $H_2$, CH-fuels/air | ‹1 |
| McGill [3.25] | m6 | 0.44 | 65 X 52 X 32 | 293 | $H_2$, CH-fuels/air | ‹1 |
| McGill [3.25] | m7 | 0.44 | 65 X 52 X 64 | 293 | $H_2$, CH-fuels/air | ‹1 |
| McGill [3.25] | m8 | 0.44 | 65 X 52 X 128 | 293 | $H_2$, CH-fuels/air | ‹1 |
| RUT-RRCKI [3.13] | r1 | 0.6 | 2250 | 293 | $H_2$/air | ‹1 |
| RUT-RRCKI [3.13] | r2 | 0.3 | 2250 | 293 | $H_2$/air | ‹1 |
| RUT-RRCKI [3.13] | r3 | room | 10.5 X 6 X 2.3 m | 293 | $H_2$/air | ‹1 |
| RUT-RRCKI [3.13] | r4 | room | 10.5 X 6 X 2.3 m | 375 | $H_2$/air/$H_20$ | ≤1 |
| RUT-RRCKI [3.13] | r5 | 0.3 | 2250 | 375 | $H_2$/air/$H_20$ | ≤1 |

| | | | | | | |
|---|---|---|---|---|---|---|
| RUT-RRCKI [3.13] | r6 | 0.3 | 2250 | 293 | $H_2$/air/$H_2$0 | ‹1 |
| RUT-RRCKI [3.13] | r7 | room | 10.5 X 6 X 2.3 m | 293 | $H_2$/air/$H_2$0 | ‹1 |
| RUT-RRCKI [3.13] | ri | room | 15 X 6 X 2.3 m | 293 | $H_2$-ingection | ≤1 |
| HDT-SNL [3.12] | s1 | 0.6 | 406 | 383 | $H_2$/air | ›1 |
| HDT-SNL [3.12] | s2 | 0.3 | 406 | 383 | $H_2$/air/$H_2$0 | ›1 |
| TORPEDO-RRCKI[3.9] | t1 | 0.6 | 520 | 293 | $H_2$/air | ‹1;›1 |
| TORPEDO-RRCKI[3.9] | t3 | 0.3 | 520 | 293 | $H_2$/air | ‹1;›1 |
| TORPEDO-RRCKI[3.9] | t4 | 0.1 | 520 | 293 | $H_2$/air | ‹1;›1 |
| mini-RUT-RRCKI[3.44] | v1 | 0.3 | 46 | 293 | $H_2$/air | ‹1 |
| mini-RUT-RRCKI[3.44] | v2 | room | 210 X 120 X 50 | 293 | $H_2$/air | ‹1 |

**Table 2-3 References Cited in Tables 2-1 and 2-2**

| Number | References |
|---|---|
| 3.9 | [Kuznetsov et al. 1999] |
| 3.11 | [Ciccarelly et al. 1998] |
| 3.12 | [Sherman et al. 1993] |
| 3.13 | [Dorofeev et al. 1996] |
| 3.14 | [Dorofeev et al. 1997] |
| 3.15. | [Sherman et al. 1989] |
| 3.21 | [Chan et al. 1996] |
| 3.25 | [Teodorczyk et al. 1990] |
| 3.26 | [Lee et al. 1984] |
| 3.27 | [Teodorczyk et al 1988] |
| 3.38 | [Sidorov et al. 1998 (a)] |
| 3.39 | [Sidorov et al. 1998 (b)] |
| 3.40 | [Sidorov et al. 1999] |
| 3.44 | [Dorofeev et al. 1999] |
| 3.45 | [Matsukov et al. 1999] |
| 3.47 | [Sherman et al. 1989] |

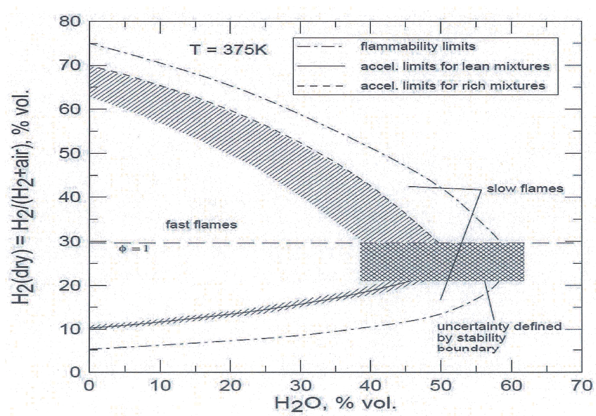


**Figure 2-19 Limits of Flame Acceleration for Hydrogen-Air-Steam Mixtures at 375 K and 1 atm. [Reference 6]**

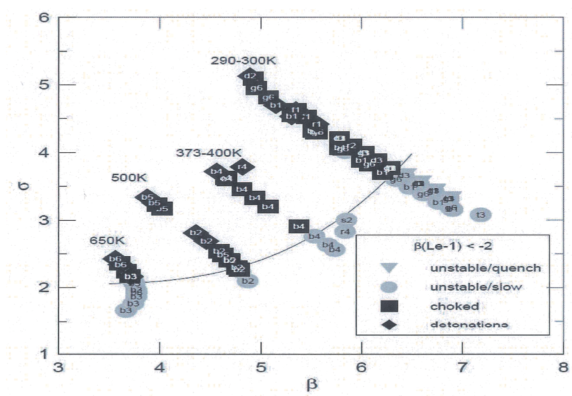


**Figure 2-20 Combustion regime as function of expansion ratio σ and Zeldovich number β for hydrogen-lean mixtures (i.e., β(Le-1)< -2). [Reference 6]**