APPENDIX D: DETONATION CELL SIZE DATA*

D.1 Experimental Data

Hydrogen-air-steam mixtures at elevated initial temperatures and pressures are typical compositions for severe accident conditions in a nuclear containment building. Most of the detonation cell size data for these mixtures are given in References [D.1 to D.7], and are collected in detonation database [D.8], which is also available on the Web at the URL **http://www.galcit.caltech.edu/~jeshep/detn_db/html**. For the system under consideration, the detonation cell size is a function of four main variables: hydrogen concentration, steam concentration, initial temperature, and pressure. Experimental data for detonation cell size for hydrogen-air-steam mixtures at normal initial pressure are presented in Tables D.1-1 and D.1-2. Some data are given in Figures D.1-1 to D.1-4. Considerable data spread for the same initial conditions can be found in these tables and figures; it reflects the accuracy of the cell size measurements. Some values for the same initial conditions differ by a factor of 3, but this is an extreme deviation. The general impression is that the accuracy of the data is within a factor of 2 or so.

Experimental data on the cell size are available only for some particular compositions and initial conditions. These measurements do not permit direct estimation of the cell size for arbitrary compositions and initial conditions typical of severe accidents. Analytical or numerical tools are necessary that can give reliable values of detonation cell sizes for accident analyses. Different approaches have been used to develop the methods for estimation of the cell size data.

One of the approaches was based on fitting of experimental data by an analytical function [D.9]. If the accuracy of such an approximation falls within the range of experimental data, a corresponding analytical function can be used for interpolation of the detonation cell size data. It is clear that such a fit can be used only within the range of experimental data. Extrapolation of the fitted function beyond the range of measurements cannot give reliable values. One of the analytical functions giving the least deviation among other simple expressions is given in Section D.2.

Another approach was based on analysis of a correlation of reaction zone widths calculated from chemical kinetic models with experimental detonation cell sizes [D.10]. This approach allows estimations of detonation cell sizes for mixture compositions that differ from hydrogen-air-steam mixtures. Examples are mixtures with reduced oxygen content (compared with that in air), and multi-component mixtures such as H_2-O_2-N_2-H_2O-CO_2. Both of the above examples can be important for safety analyses, but no experimental data are available, and simple interpolation methods cannot be used. A short description of this approach and its limitations are given in Section D.3.

* Dr. Sergei B. Dorofeev is the lead author for Appendix D.

Table D.1-1 Detonation cell size data for hydrogen-air-steam mixtures at normal initial pressure. Data for spin detonations are also given, assuming $\lambda = \pi d$.

H_2 (dry) (vol %)	T (K)	H_20, (vol %)	λ (cm)	Ref.		H_2 (dry) (vol %)	T (K)	H_20 (vol %)	λ (cm)	Ref.
Data for T ≈ 300 K						**Data for elevated temperatures**				
11.65	296	0.00	135.2	D.2		9.42	375	0.00	135.0	D.2
12.00	300	0.00	135.2	D.2		10.40	375	0.00	135.2	D.2
12.34	300	0.00	135.2	D.2		11.30	375	0.00	135.2	D.2
13.48	300	0.00	42.4	D.4		12.48	376	0.00	30.5	D.2
13.58	300	0.00	121.5	D.1		13.14	373	0.00	44.4	D.2
13.78	300	0.00	119.6	D.1		14.88	370	0.00	15.0	D.2
13.78	300	0.00	61.9	D.1		17.87	375	0.00	3.8	D.2
13.83	300	0.00	42.4	D.4		20.00	370	0.00	2.4	D.2
13.98	300	0.00	63.6	D.1		29.64	375	0.00	0.7	D.2
13.98	300	0.00	56.3	D.1		29.75	371	0.00	2.0	D.2
14.21	300	0.00	46.6	D.1		45.91	374	0.00	1.4	D.2
14.31	300	0.00	42.4	D.4		56.10	374	0.00	3.7	D.2
14.54	300	0.00	33.6	D.1		76.00	375	0.00	135.2	D.2
14.57	300	0.00	41.5	D.1		76.98	375	0.00	135.2	D.2
14.89	300	0.00	24.8	D.4		29.78	375	5.00	2.0	D.2
14.93	300	0.00	18.7	D.4		20.12	375	9.10	18.4	D.2
14.99	300	0.00	33.8	D.1		63.97	375	9.80	61.0	D.2
15.00	300	0.00	25.0	D.4		17.23	376	9.90	47.0	D.2
15.08	300	0.00	30.4	D.1		45.74	375	10.50	4.2	D.2
15.30	300	0.00	29.9	D.1		29.75	375	11.50	2.8	D.2
15.36	300	0.00	30.6	D.1		30.67	375	14.90	4.5	D.2
15.36	300	0.00	26.2	D.1		30.60	374	15.00	5.0	D.2
15.50	300	0.00	26.0	D.4		45.67	376	19.80	29.0	D.2
15.55	300	0.00	35.6	D.1		26.07	375	20.10	25.0	D.2
16.00	300	0.00	24.5	D.5		30.16	376	20.10	16.5	D.2
16.20	300	0.00	23.0	D.4		21.91	375	20.30	100.0	D.2
16.50	300	0.00	18.3	D.5		28.10	375	29.90	127.0	D.2
17.00	300	0.00	13.0	D.4		30.01	375	29.90	65.0	D.2
17.00	300	0.00	16.2	D.5		38.96	375	29.90	50.0	D.2
17.22	300	0.00	9.5	D.4		29.67	375	35.40	135.2	D.2
17.24	297	0.00	7.6	D.2		29.57	375	37.00	135.2	D.2
17.29	300	0.00	9.3	D.4		29.75	375	38.80	135.2	D.2
17.36	300	0.00	14.0	D.5		17.81	400	10.00	30.5	D.4
17.50	300	0.00	12.4	D.5		30.00	400	10.00	1.7	D.4
17.50	300	0.00	8.9	D.4		30.00	400	10.00	1.5	D.4
18.00	300	0.00	11.1	D.5		18.21	400	20.00	84.8	D.4
18.60	300	0.00	8.9	D.5		30.00	400	20.00	17.0	D.4
19.00	300	0.00	8.0	D.5		29.88	400	25.00	16.2	D.4
19.20	300	0.00	7.6	D.5		30.23	400	25.00	21.4	D.4
19.91	300	0.00	2.7	D.4		9.90	500	0.00	42.4	D.4

Table D.1-1 (continued)

H_2 (dry) (vol %)	T (K)	H_20 (vol %)	λ (cm)	Ref.		H_2 (dry) (vol %)	T (K)	H_20 (vol %)	λ (cm)	Ref.
Data for T ≈ 300 K						**Data for elevated temperatures**				
20.00	300	0.00	5.5	D.5		10.87	500	0.00	42.9	D.4
20.00	300	0.00	4.0	D.4		11.16	500	0.00	19.6	D.4
20.13	300	0.00	5.1	D.5		12.50	500	0.00	9.8	D.4
21.00	300	0.00	4.4	D.5		12.93	500	0.00	12.0	D.4
22.00	300	0.00	3.1	D.5		13.96	500	0.00	8.0	D.4
22.73	300	0.00	2.6	D.5		13.96	500	0.00	6.5	D.4
23.00	300	0.00	2.6	D.5		14.61	500	0.00	5.2	D.4
23.96	300	0.00	2.2	D.5		16.00	500	0.00	2.9	D.4
24.00	300	0.00	2.1	D.5		16.00	500	0.00	2.3	D.4
24.11	300	0.00	1.1	D.4		17.43	500	0.00	2.0	D.4
25.00	300	0.00	1.8	D.5		17.59	500	0.00	1.5	D.4
25.00	300	0.00	1.2	D.4		21.96	500	0.00	0.8	D.4
25.16	300	0.00	1.9	D.5		29.58	500	0.00	0.6	D.4
26.00	300	0.00	1.7	D.5		29.98	500	0.00	0.9	D.4
27.00	300	0.00	1.6	D.5		29.98	500	0.00	0.6	D.4
27.44	300	0.00	1.6	D.5		50.00	500	0.00	1.8	D.4
28.00	300	0.00	1.6	D.5		50.00	500	0.00	1.1	D.4
28.53	300	0.00	1.6	D.5		50.30	500	0.00	1.0	D.4
29.00	300	0.00	1.5	D.5		30.00	500	10.00	1.3	D.4
29.17	282	0.00	1.5	D.2		30.00	500	10.00	1.2	D.4
29.46	302	0.00	1.1	D.2		30.00	500	20.00	5.6	D.4
29.57	300	0.00	1.6	D.5		30.00	500	20.00	5.3	D.4
29.60	300	0.00	1.5	D.5		30.30	500	30.00	28.6	D.4
29.67	300	0.00	0.8	D.4		30.00	601	30.00	17.0	D.4
30.00	300	0.00	1.5	D.5		6.24	650	0.00	84.8	D.4
30.00	300	0.00	0.9	D.4		7.02	650	0.00	42.4	D.4
30.12	300	0.00	0.9	D.4		7.39	650	0.00	84.8	D.4
30.54	300	0.00	1.3	D.4		7.51	650	0.00	23.0	D.4
30.54	300	0.00	2.1	D.4		7.83	650	0.00	21.3	D.4
32.00	300	0.00	1.6	D.5		8.77	650	0.00	9.4	D.4
34.00	300	0.00	1.7	D.5		8.83	650	0.00	7.4	D.4
36.00	300	0.00	1.9	D.5		9.58	650	0.00	4.6	D.4
38.00	300	0.00	2.2	D.5		9.90	650	0.00	8.0	D.4
40.00	300	0.00	2.3	D.5		9.90	650	0.00	8.0	D.4
40.00	300	0.00	0.9	D.4		9.94	650	0.00	4.8	D.4
42.00	300	0.00	2.7	D.5		10.83	650	0.00	4.0	D.4
44.00	300	0.00	3.1	D.5		10.87	650	0.00	3.7	D.4
46.00	300	0.00	3.7	D.5		10.87	650	0.00	3.6	D.4
48.00	300	0.00	4.2	D.5		11.42	650	0.00	3.0	D.4
50.00	300	0.00	5.0	D.5		11.88	650	0.00	3.2	D.4
50.00	300	0.00	2.6	D.4		11.88	650	0.00	3.3	D.4

Table D.1-1 (concluded)

H_2 (dry) (vol %)	T (K)	H_20 (vol %)	λ (cm)	Ref.		H_2 (dry) (vol %)	T (K)	H_20 (vol %)	λ (cm)	Ref.
Data for T ≈ 300 K						Data for elevated temperatures				
51.36	300	0.00	1.8	D.4		12.00	650	0.00	3.3	D.4
52.00	300	0.00	5.5	D.5		14.28	650	0.00	1.7	D.4
54.00	300	0.00	7.9	D.5		15.00	650	0.00	1.8	D.4
54.50	300	0.00	4.6	D.4		15.03	650	0.00	1.7	D.4
55.00	300	0.00	9.5	D.5		17.48	650	0.00	1.2	D.4
56.00	300	0.00	10.0	D.5		17.50	650	0.00	1.9	D.4
58.00	300	0.00	14.2	D.5		30.00	650	0.00	0.4	D.4
58.00	300	0.00	8.0	D.4		30.29	650	0.00	0.5	D.4
58.00	300	0.00	7.8	D.4		50.00	650	0.00	1.0	D.4
60.00	300	0.00	18.9	D.5		50.00	650	0.00	1.0	D.4
70.46	300	0.00	135.2	D.2		50.00	650	0.00	1.1	D.4
73.08	300	0.00	135.2	D.2		9.85	650	7.50	42.9	D.4
75.00	299	0.00	135.2	D.2		17.55	650	10.00	3.3	D.4
30.54	298	3.10	1.3	D.2		30.00	650	10.00	0.8	D.4
29.53	311	0.00	0.9	D.2		9.86	650	15.00	84.8	D.4
						17.63	650	20.00	9.1	D.4
						30.00	650	20.00	2.3	D.4
						30.00	650	20.00	2.2	D.4
						18.06	650	25.00	27.5	D.4
						30.00	650	25.00	2.6	D.4
						17.26	650	30.00	42.4	D.4
						29.46	650	30.00	7.5	D.4
						30.00	650	30.00	7.3	D.4
						30.00	650	30.00	6.2	D.4
						30.00	650	30.00	6.5	D.4
						30.00	650	30.00	5.7	D.4
						28.64	650	35.00	17.5	D.4
						29.43	650	40.00	50.3	D.4
						29.37	650	50.00	84.8	D.4

Table D.1-2 Detonation cell size data for hydrogen-air-steam mixtures at sub-atmospheric and elevated initial pressures

H_2 (dry) (vol %)	T (K)	P (MPa)	H_20 (vol %)	λ (cm)	Ref.	H_2 (dry) (vol %)	T (K)	P (MPa)	H_20 (vol %)	λ (cm)	Ref.
30.00	300	0.003	0.00	2.3	D.6	15.00	373	0.146	0.00	17.0	D.2
30.00	300	0.007	0.00	13.0	D.6	17.36	373	0.149	0.00	6.3	D.2
30.00	300	0.008	0.00	14.0	D.6	17.36	373	0.164	10.00	53.0	D.2
30.00	300	0.01	0.00	11.0	D.6	20.13	373	0.168	10.00	23.0	D.2
30.00	300	0.0105	0.00	7.8	D.6	20.40	373	0.153	0.00	2.4	D.2
30.00	300	0.0115	0.00	6.4	D.6	20.40	373	0.169	10.00	21.0	D.2
30.00	300	0.012	0.00	6.3	D.6	20.67	373	0.154	0.00	2.3	D.2
30.00	300	0.013	0.00	4.7	D.6	20.67	373	0.169	10.00	20.0	D.2
30.00	300	0.02	0.00	4.1	D.6	21.45	373	0.155	0.00	1.8	D.2
30.00	300	0.023	0.00	3.4	D.6	22.73	373	0.156	0.00	1.3	D.2
30.00	300	0.025	0.00	3.2	D.6	25.16	373	0.159	0.00	0.9	D.2
30.00	300	0.035	0.00	2.1	D.6	25.16	373	0.175	10.00	5.3	D.2
30.00	300	0.05	0.00	2.0	D.6	25.63	373	0.192	20.00	22.0	D.2
30.00	300	0.07	0.00	1.8	D.6	27.44	373	0.162	0.00	0.6	D.2
30.00	300	0.1	0.00	1.6	D.6	27.44	373	0.211	30.00	35.0	D.2
17.29	303	0.010	0.00	25.0	D.2	29.59	373	0.165	0.00	0.5	D.2
14.39	293	0.114	0.00	40.0	D.2	29.59	373	0.180	0.00	0.5	D.2
17.50	293	0.118	0.00	11.0	D.2	29.59	373	0.200	10.00	3.0	D.2
19.05	293	0.119	0.00	3.8	D.2	29.59	373	0.225	20.00	9.5	D.2
24.44	293	0.124	0.00	1.2	D.2	29.59	373	0.255	30.00	28.0	D.2
28.10	293	0.128	0.00	1.0	D.2	29.59	373	0.255	30.00	32.0	D.2
43.06	293	0.143	0.00	1.3	D.2	29.69	373	0.165	0.00	0.5	D.2
29.63	296	0.025	0.00	2.4	D.2	37.04	373	0.174	0.00	0.6	D.2
16.72	296	0.026	0.00	45.0	D.2	45.66	373	0.185	0.00	1.1	D.2
29.19	296	0.051	0.00	1.5	D.2	45.66	373	0.204	10.00	4.0	D.2
17.04	296	0.015	0.00	21.5	D.2	45.66	373	0.223	20.00	13.0	D.2
29.02	297	0.151	0.00	0.8	D.2	55.76	373	0.198	0.00	2.0	D.2
17.01	297	0.051	0.00	15.7	D.2	29.60	375	0.215	29.60	25.0	D.2
17.44	299	0.026	0.00	26.0	D.2	9.30	650	0.240	0.00	8.5	D.4
17.13	301	0.264	0.00	10.0	D.2	17.78	650	0.200	20.00	10.7	D.4
12.50	373	0.143	0.00	42.0	D.2	17.91	650	0.150	20.00	10.3	D.4
13.45	373	0.144	0.00	32.0	D.2	30.13	650	0.150	30.00	4.5	D.4
13.77	373	0.145	0.00	29.0	D.2	30.22	650	0.200	30.00	3.7	D.4

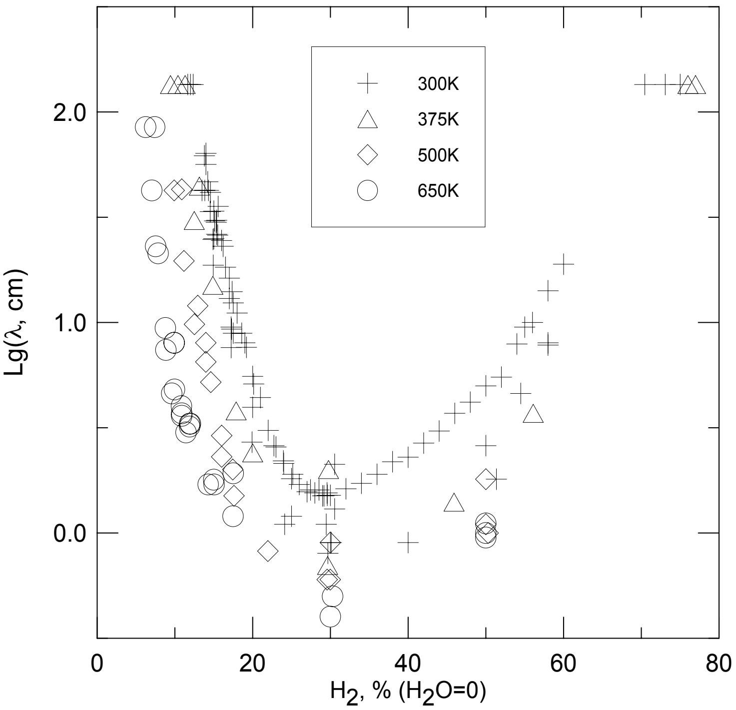

Figure D.1-1 Experimental data on detonation cell width versus hydrogen concentration at different initial temperatures for mixtures without steam

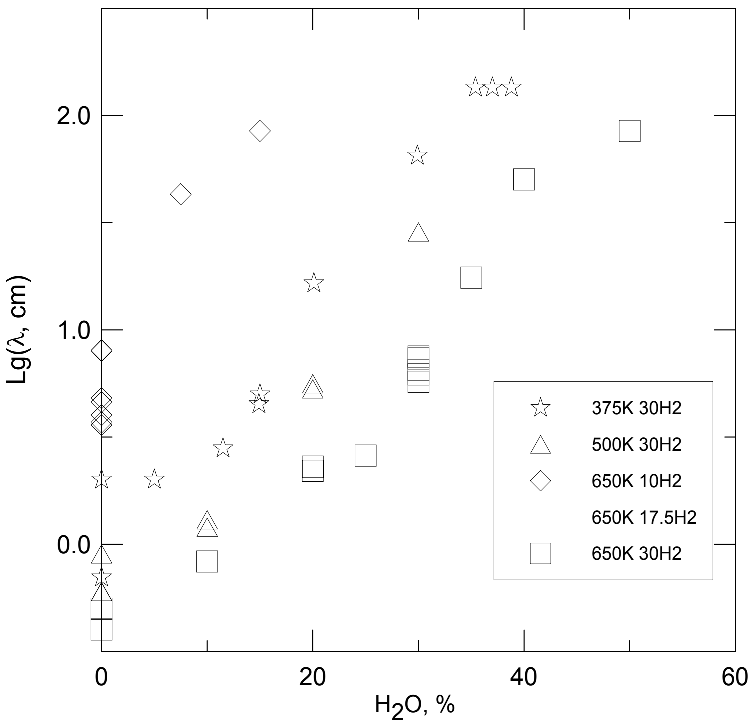

Figure D.1-2 Experimental data on detonation cell width versus steam concentration at different initial temperatures and dry hydrogen concentrations

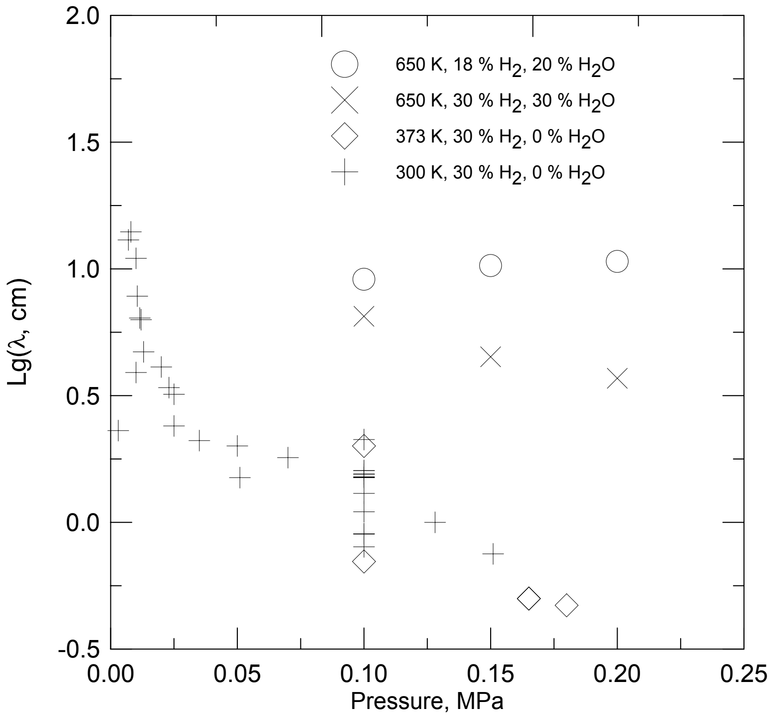

Figure D.1-3 Experimental data on detonation cell width versus initial pressure at different initial temperatures, dry hydrogen, and steam concentrations

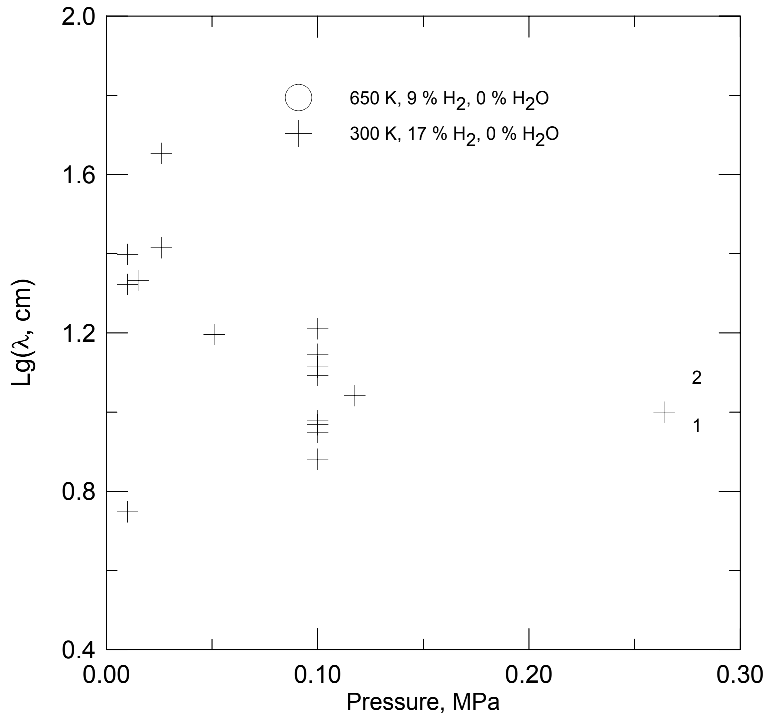

Figure D.1-4 Experimental data on detonation cell width versus initial pressure at different initial temperatures and dry hydrogen concentrations without steam

D.2 Data Interpolation with Analytical Functions

Different analytical functions $\lambda([H_2], [H_2O], T, p)$ were applied to fit experimental data [D.9]. One of the functions giving the least deviation among other simple expressions is given here.

Function B67p. Variables: A - dry hydrogen concentration $[H_2]_{dry} = H_2/(H_2+air)$, vol %; B - initial temperature T, K; C - steam concentration, vol %; D - initial pressure, MPa. Cell size λ is in cm.

$$\lg(\lambda) = (a-m+(b/(A-k/B)^{f} + h\cdot(A-g\cdot B)^2+i\cdot(A-g\cdot B))\cdot(1+d\cdot C+e\cdot B\cdot C^2)\cdot j/B)\cdot$$

$$\cdot(D-c)\cdot(1/(0.1-c)+n\cdot(D-0.1))+m$$

Parameters:
a = -1.13331E+00
b = 4.59807E+01
c = -1.57650E-01
d = 4.65429E-02
e = 3.59620E-07
f = 9.97468E-01
g = -2.66646E-02
h = 8.74995E-04
i = -4.07641E-02
j = 3.31162E+02
k = -4.18215E+02
m = 2.38970E+00
n = -8.42378E+00

The regression mean-square deviation is σ = 1.72128E-01.

Deviation of experimental data from the fitted function can be calculated as $\lambda_{fit}/\lambda_{exp} = 10\sigma$. The mean standard deviation is about 1.5. The maximum deviation is about 2.6.

Examples of comparison of experimental data with function B67p are given in Figures D.2-1 and D.2-2. A "map" of the cell widths plotted in $[H_2]_{dry}$ - $[H_2O]$ plane for T = 375 K, p = 1 bar* using function B67p, is shown as an example in Figure D.2-3 ($[H_2]_{dry} = [H_2]/([H_2]+[air])$).

*1 bar = 100 kPa.

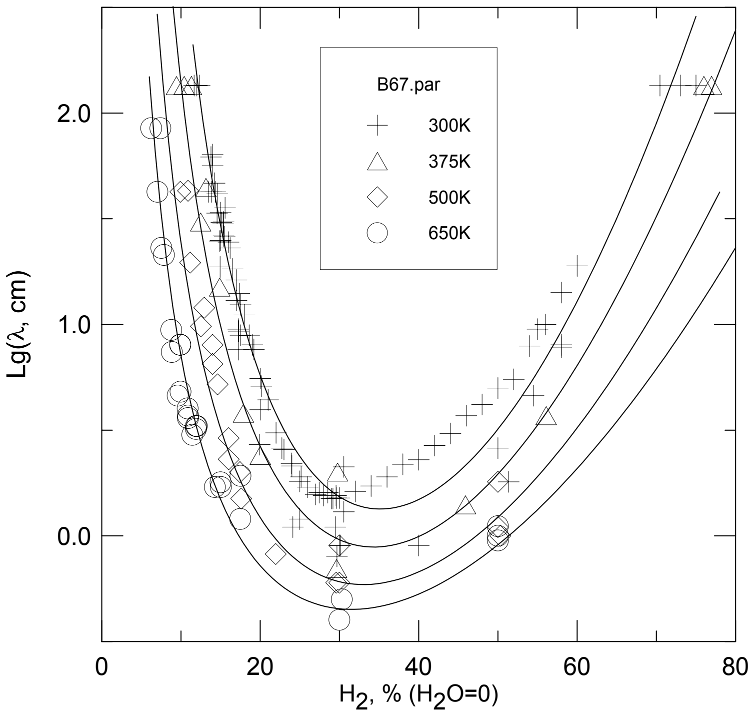

Figure D.2-1 Experimental data and fitting function B67. Cell width versus hydrogen concentration at different initial temperatures for mixtures without steam

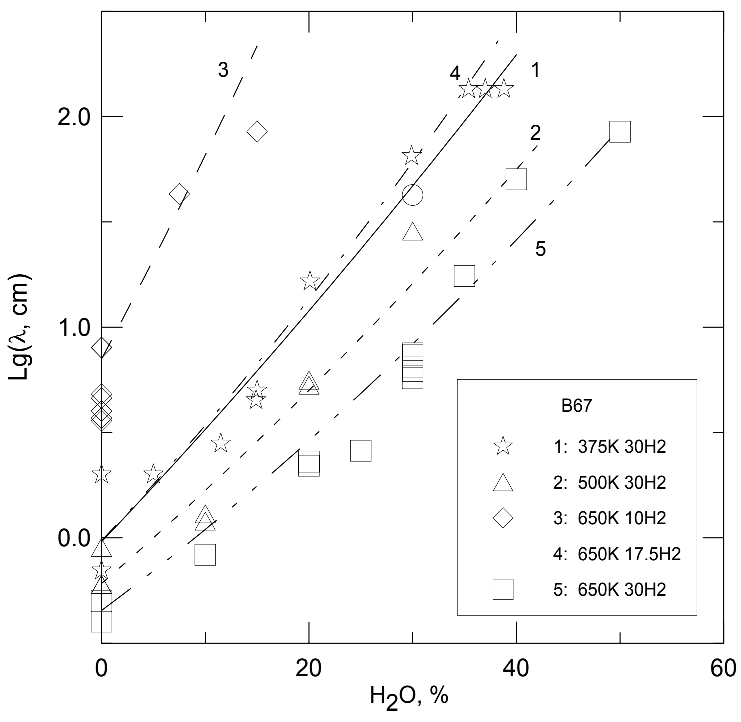

Figure D.2-2 Experimental data and fitting of function B67. Cell width versus steam concentration at different initial temperatures and dry hydrogen concentration

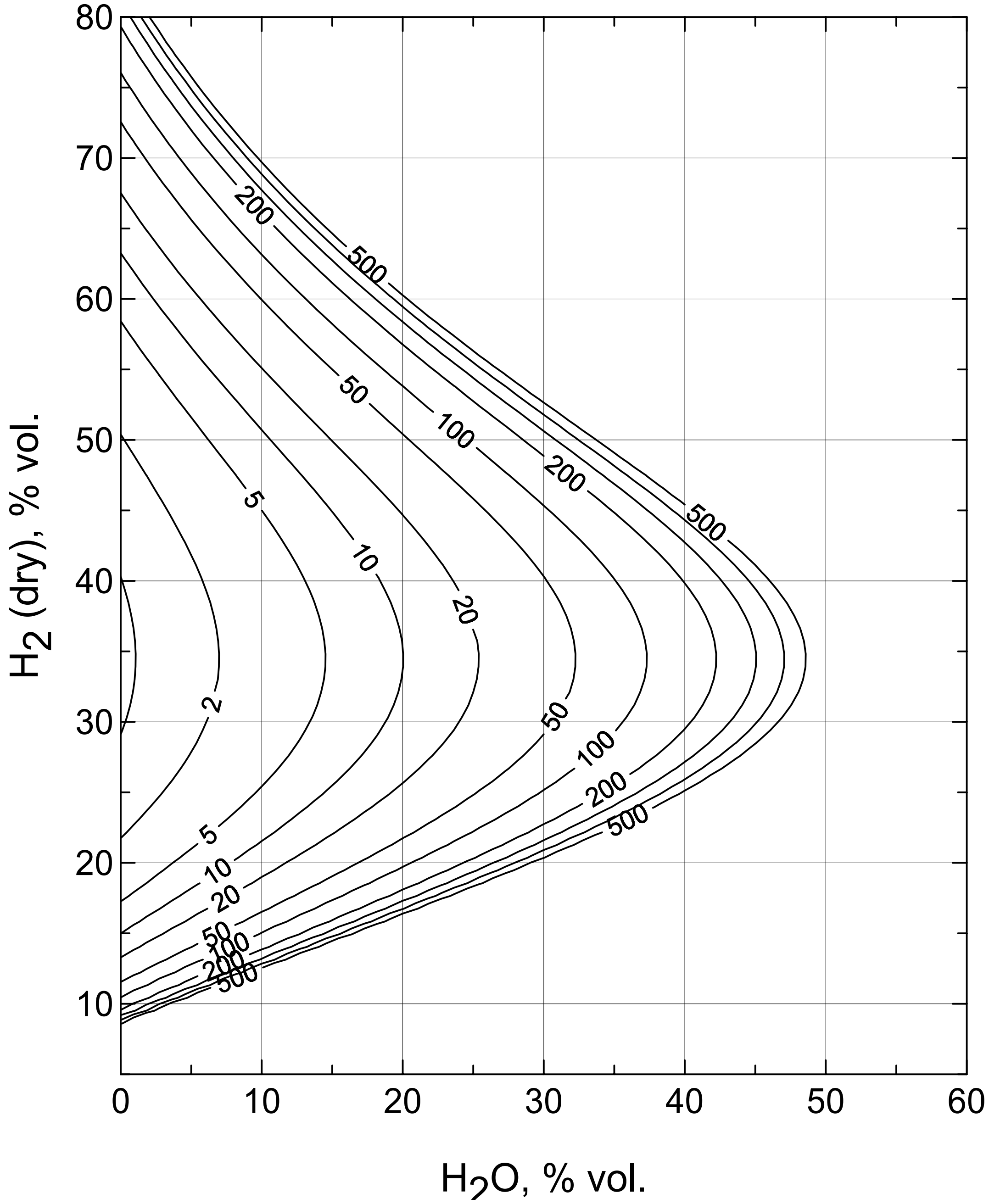

Figure D.2-3 Cell widths (cm) in $[H_2]_{dry}$ - $[H_2O]$ plane. Function B67, T = 375 K, p = 1 bar, ($[H_2]_{dry} = [H_2]/([H_2]+[air])$)

D.3 Generalization of the Zeldovich-von Neumann-Döring (ZND) Correlation

A simple model was proposed in Reference [D.10] to generalize the correlation between characteristic reaction zone widths δ and the cell sizes λ. As typical of ZND correlations, it was assumed that characteristic reaction zone width, δ, can be estimated from a detailed chemical reaction model. It was suggested that parameters influencing the wave stability and regularity of the cellular structure should play a role in a correlation between the detonation cell sizes and reaction zone widths. Two parameters were considered to be of the main importance. The first one – dimensionless activation energy Ea/RT_{ps} – gives a measure of the reaction time sensitivity to changes of the initial reaction conditions (shock strength). The second parameter, T_{vn}/T_0, gives a measure of the chemical energy release compared with the initial thermal energy. Here Ea is effective activation energy, R is gas constant, T_{ps} is representative post-shock temperature, and T_{vn} and T_0 are von Neumann and initial temperatures respectively.

An attempt was made to take into account the multi-dimensional structure of real detonations in this model by choosing representative reaction conditions (or characteristic post-shock temperature T_{ps}) that allow one to correlate reaction zone width $\delta(T_{ps})$ and detonation cell size λ. The CHEMKIN-II code was used for kinetic calculations. An analytical expression was suggested to describe the function of $\lambda/\delta(Ea/RT_{ps}, T_{vn}/T_0)$ in the range of $Ea/RT_{ps} = 3 \div 16$, and $Tvn/T_0 = 1.5 \div 8$. The mean deviation of the calculated values from experimental data was about 50%.

A numerical model was developed [D.10], which permits one to calculate detonation cell sizes from mixture composition and initial temperature and pressure. The corresponding computer code is available on the Web at URL **http://www.iacph.kiae.ru/lichr**.

Compared with the standard ZND models, which are able to give only general trends in the cell size behaviour, the numerical model [D.10] gives more reliable estimates for the cell sizes. In most cases, the deviation is within the scatter of the experimental data. The estimates of λ values, however, should be treated carefully if the stability parameters appear outside the range of variables, where the λ/δ-function was defined. The limitations of kinetic calculations with the CHEMKIN-II code should be also taken into consideration.

Examples of comparison of experimental data with calculations are given in Figures D.3-1 and D.3-2. A "map" of the cell widths plotted in $[H_2]_{dry}$ - $[H_2O]$ plane for T = 375 K, p = 1 bar using this model, is shown as an example in Figure D.3-3 ($[H_2]_{dry} = [H_2]/([H_2]+[air])$).

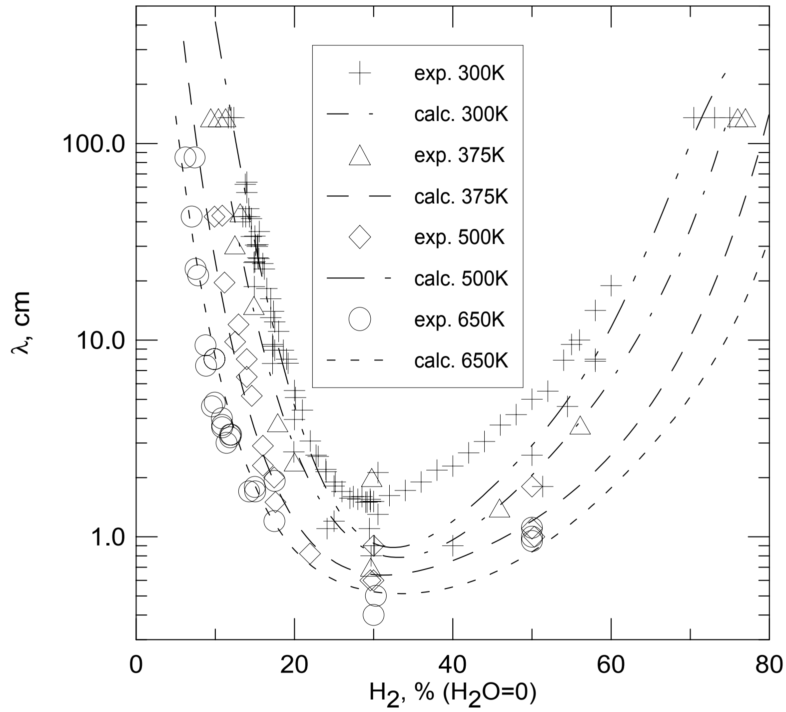

Figure D.3-1 Cell width versus hydrogen concentration at different initial temperatures for hydrogen-air mixtures without steam. Experimental data and calculations.

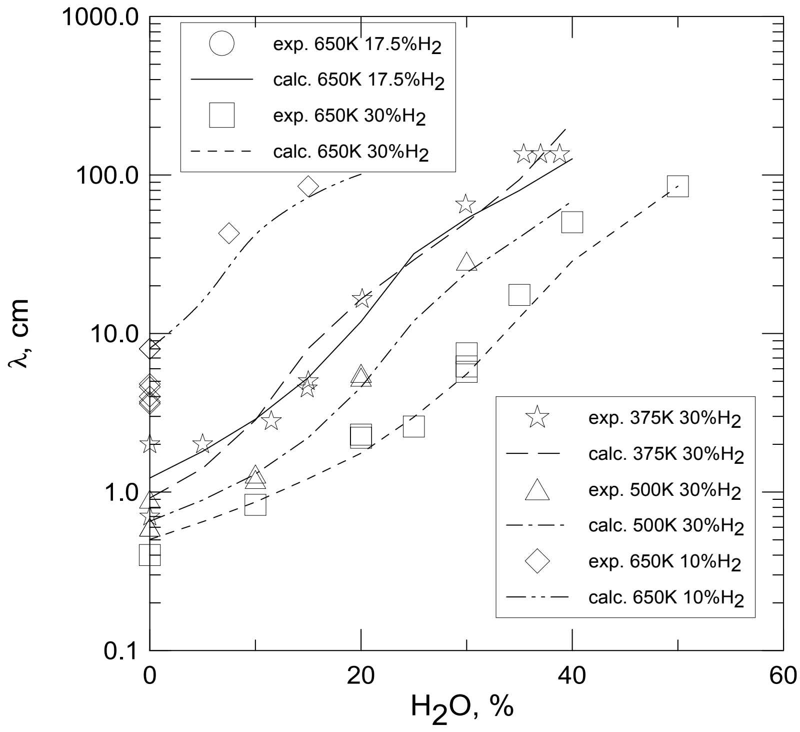

Figure D.3-2 Cell width for hydrogen-air-steam mixtures versus steam concentration at different initial temperatures and dry hydrogen concentrations. Experimental data and calculations.

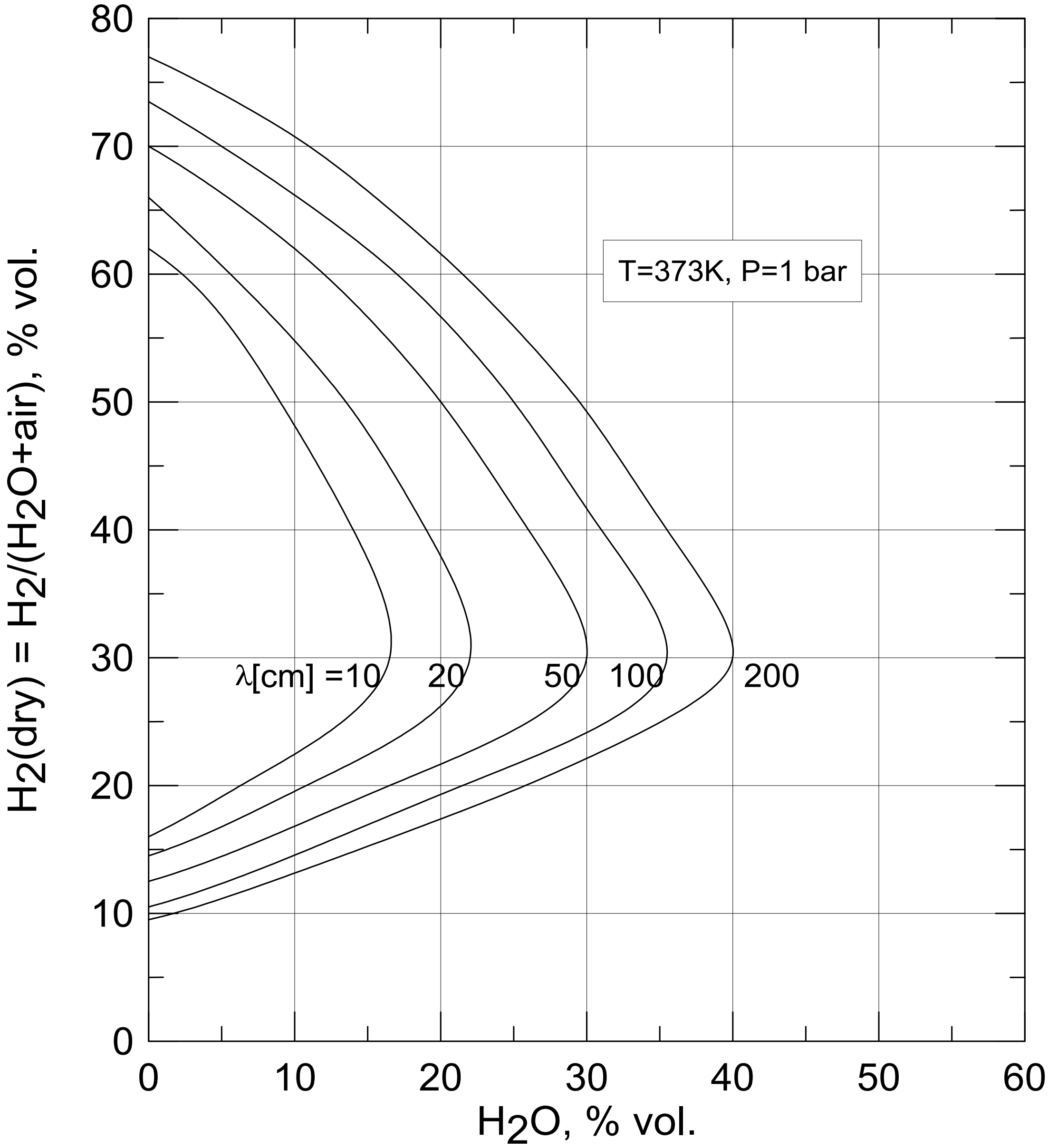

Figure D.3-3 Cell widths (cm) in $[H_2]_{dry}$ - $[H_2O]$ plane. Calculations with model [D.10], T = 373 K, p = 1 bar, ($[H_2]_{dry} = [H_2]/([H_2]+[air])$)

D.4 References

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