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BURNING PROPERTIES OF H-764 AND PETN. Closed Vessel Testing.

NEVSTAD Gunnar Ove

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Director of Research

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8) ABSTRACT

Two explosives used in MP (Multipurpose) projectiles have been study in closed vessel for characterisation of burning properties. The two explosives are H-764, a HMX based explosive composition for press filling, and PETN. Both explosives are filled into the projectile by press loading. The obtained press density of the loading can vary and will have effect on the reaction rate of the filling. Loosely packed powder ignition will spread very rapidly to all grains or crystals. Solid pellets may burn only on the surface.

To be able to observe the effect on the burning properties of differences in density of explosive fillings have we prepared cylindrical pellets of different densities and tested these in closed vessel at different loading density. For H-764 in addition to powder, pellets of three different densities have been tested. For PETN powder and one pellet density have been tested.

PETN pellets pressed to a density of 1.63 g/cm^3 burns only on the pellet surface. For the highest pellet density of H-764 the burning start on the pellet surface, but spreads to all single crystals when the pressure increases.

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CONTENTS

BURNING PROPERTIES OF H-764 AND PETN. Closed Vessel Testing.

1 INTRODUCTION

Two explosives used in Multipurpose (MP) ammunition projectiles have been study in closed vessel for determination of the burning properties as function of press density. Both loosely packed powder and pressed pellets have been tested. To be able to experimentally determining the co-volume and impetus have firings with different loading densities been carried out for both powder and pressed pellets.

For H-764, a HMX based explosive has pellets of three different densities been produced and tested. For PETN has only pellets of high density been tested. We did test only one pellet density of PETN because it is an explosive that will have reduced applicability in the future. The burning rate or rate of pressure increase due to the reaction of the explosive has influence on the fragmentation of the shell body. To obtain an optimal fragmentation pattern of a MP-projectile, one of the parameters than can be changed is the pressure used for the press loading of the explosive.

In addition to experimentally testing of the two explosives have theoretical calculations by use of the Cheetah 2.0 (1) code been carried out. And a comparison of some experimentally determined and calculated properties have been performed.

2 EXPERIMENTALLY

2.1 Explosives

The H-764 lot we have used in our experiments was produced and delivered by Dyno Nobel ASA. H-764 is a HMX based explosive containing minimum 98 wt.% HMX. The two other components are Calcium Resinate and graphite in equal amount. The control report for the used lot is given in Appendix A.

The PETN we have used was received from Nammo Raufoss.

2.2 Pressing of pellets

Pellets of different densities have been pressed by use of two different presses and press tools. In figure 2.1 is given a picture of the press and tool for pressing of pellets with low or moderate density. Figure 2.2 gives a better picture of the tool. We have for H-764 with the press and tool given in figure 2.1, pressed cylindrical pellets with density of 1.656 g/cm^3 and 1.749 g/cm^3.

Figure 2.1 Picture of press used to press pellets of moderate density.

Figure 2.3 gives a picture of the press and tool used to press high-density pellets for both H-764 and PETN. Figure 2.4 shows picture of pressed pellets of H-764, density 1.785 g/cm^3.

Figure 2.2 Picture of the press tool used to produce pellets of moderate density.

Figure 2.3 Picture of press and press tool used for production of high-density pellets.

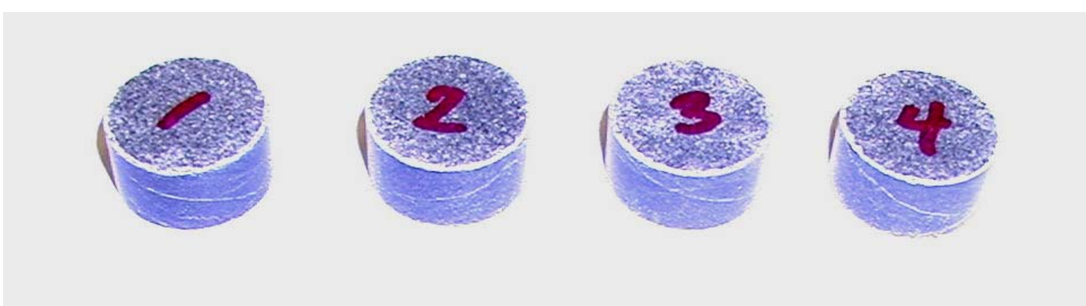

Figure 2.4 Picture of high densities pellets of H-764.

2.3 Closed Vessel

To test the two explosives H-764 and PETN have a 150 ml Closed Vessel been used. Figure 2.5 gives a picture of the CV. Ignition has for all experiments been with 1 g Black Powder and a brown/blue squib. The BP has been placed in a plastic bag around the squib, figure 3.1. For firings with powder explosives the ignition unit was placed in the centre of powder, figure 3.1.

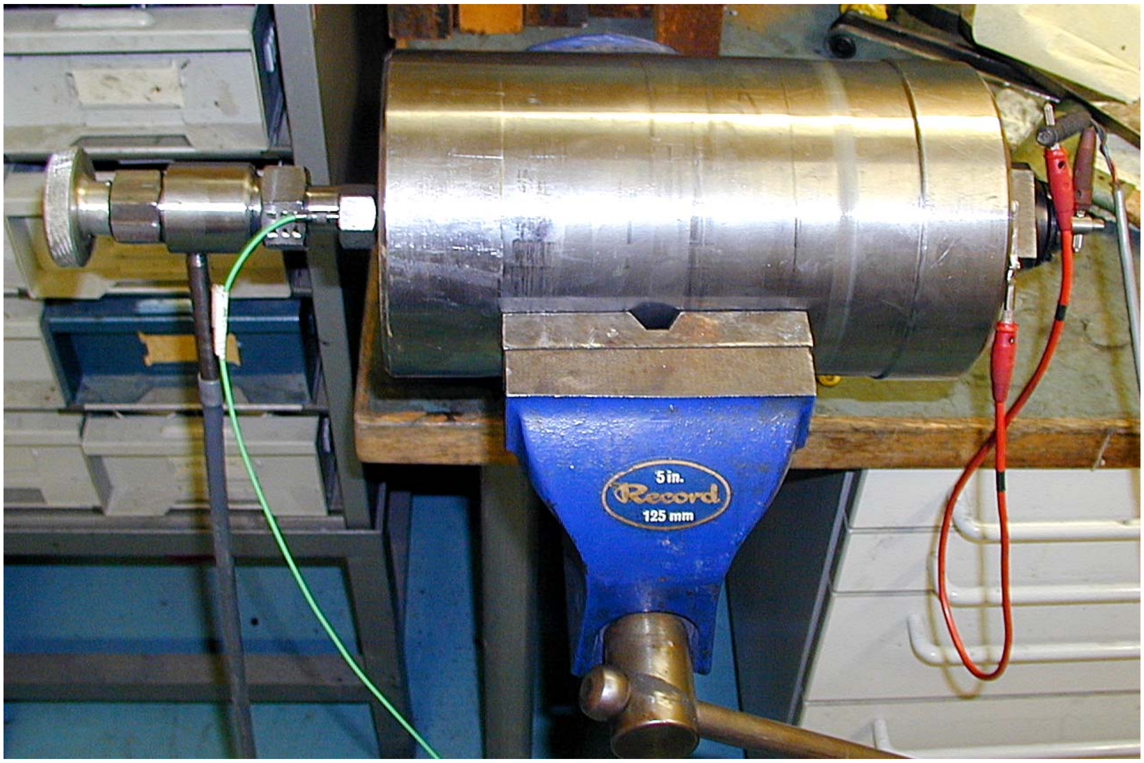

Figure 2.5 Picture of the 150 cm^3 Closed Vessel used to test the explosives H-764 and PETN.

For firings containing pellets the ignition unit was taped to the surface of the stocks of pellets, figure 3.45 shows examples of the configuration.

CV Firing No.	Material	Form	Date of Firing	Sampling time (μs)	Sample size (g)	P_{max} (Bars)	Density (g/cm^3)
410	PETN	Powder	6/5-02	1	20.02	1749	
411	PETN	Powder	6/5-02	1	30.00	2813	
412	PETN	Powder	6/5-02	1	25.00	2250.5	
413	PETN	Powder	6/5-02	1	15.00	1239	
416	PETN	Powder	6/5-02	1	20.00	1700	
417	PETN	Powder	6/5-02	1	25.00	2233.5/2275	
424	PETN	Powder	8/5-02	1	29.90	2797.5	
425	PETN	Powder	8/5-02	1	35.00	3361.5/3437.5	
434	PETN	Pellets	21/8-02	1	18.69	---	
435	PETN	Pellets	21/8-02	4	22.42	1824.5	1.633
436	PETN	Pellets	21/8-02	8	14.94	1135	
441	PETN	Pellets	29/8-02	4	18.68	1485.5	

Table 2.1 Overview of the firings with PETN in 150 ml Closed Vessel.

To measure the pressure a Kistler 6211, SN 87663 pressure gauge was used. Sampling time for most firings was 1 μs. However, for some of the firings with pellets of high density we needed to use longer sampling time. Table 2.1 and 2.2 gives used sampling times for all firings. Independent of the sampling time the number of sample point has been slightly higher than 65000.

CV Firing No.	Material	Form	Date of Firing	Sampling Time (μs)	Sample size (g)	P_{max} (Bars)	Density (g/cm³)
378	H-764	Powder	23/4-02	1	20.00	1923.5	
379	H-764	Powder	23/4-02	1	15.00	1354.5	
380	H-764	Powder	23/4-02	1	25.00	2502	
381**	H-764	Powder	23/4-02	1	30.00	3082.5	
386	H-764	Powder	25/4-02	1	30.00	3037	
387	H-764	Pellets	25/4-02	1	24.92	2375	
388	H-764	Pellets	25/4-02	1	19.93	1892	
389	H-764	Pellets	25/4-02	1	14.86	1330.5	1.6558
390	H-764	Pellets	25/4-02	1	29.82	3205.5	
429	H-764	Pellets	1/6-02	1	24.80	2371	
391	H-764	Powder	26/4-02	1	20.00	1870	
392	H-764	Powder	26/4-02	1	25.00	2396	
393	H-764	Powder	30/4-02	1	20.00	1848	
394	H-764	Powder	30/4-02	1	25.00	2060.5	
395	H-764	Powder	30/4-02	1	25.00	2063.5	
396**	H-764	Powder	2/5-02	1	25.00	2521.5	
397	H-764	Powder	2/5-02	1	20.00	1899	
404	H-764	Powder	3/5-02	1	20.00	1930.5	
405	H-764	Pellets	3/5-02	1	19.90	1853	
406	H-764	Pellets	3/5-02	1	24.91	2392.5	1.7489
407	H-764	Pellets	3/5-02	1	14.97	1325.5	
408	H-764	Pellets	3/5-02	1	29.90	3034.5	
409	H-764	Pellets	3/5-02	1	19.91	1704	
423	H-764	Pellets	7/5-02	2	14.70	1237.5	
427	H-764	Pellets	1/6-02	1	18.89	1688.5	1.7853
428	H-764	Pellets	1/6-02	1	22.06	2114	
432	H-764	Powder	1/6-02	1	20.00	1730.5	
442	H-764	Powder	29/8-02	1	20.04	1938	
443	H-764	Powder	14/9-02	1	25.01	2509.5	

**Leakage

Table 2.2 Properties and conditions for performed firings with H-764 in 150 cm³ Closed Vessel.

3 RESULTS

3.1 H-764

The explosive H-764 has been tested in closed vessel as powder as received from the producer and in form of pressed pellets. The pellets have been pressed to different densities to study possible effect on the burning as function of the density of the pellets. Table 2.2 gives a summary of all firings with H-764.

3.1.1 H-764 powder

Several firings with H-764 powder at different loading densities have been performed in a 150 cm^3 Closed Vessel (figure 2.5). Table 3.1 gives an overview of all 16 firings we have performed with loosely packed powder. Figure 3.1 gives pictures of how we packed the powder to be tested. In figure 3.2 and 3.3 are given SEM (Scanning Electron Microscope) pictures of the H-764 powder.

Figure 3.1 Picture of from left, the plastic bag containing the explosive, the ignition unit containing a squib and 1 g Black Powder, and a complete shot to the right.

In figures 3.4 – 3.10 are given representative pressure- time curves. Figure 3.11 gives pressure-time curves for all firings with loosely packed powder of H-764.We have performed more firings with powder than necessary to obtain impetus, co-volume and burn rate for H-764. The reason for this is that we have used the powder to check that the test system function as it was expected. For some of the firings we have obtained too low pressures. For two firings we did get leakage.

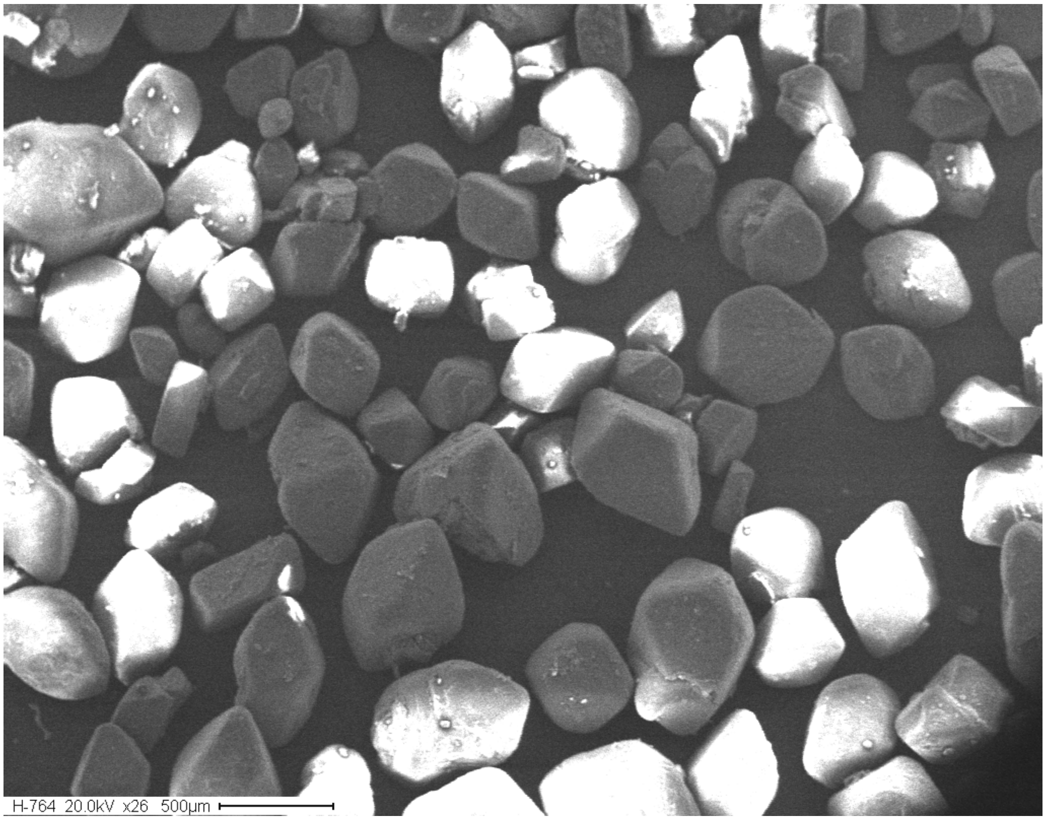

Figure 3.2 Picture of H-764 crystals, magnification 26x.

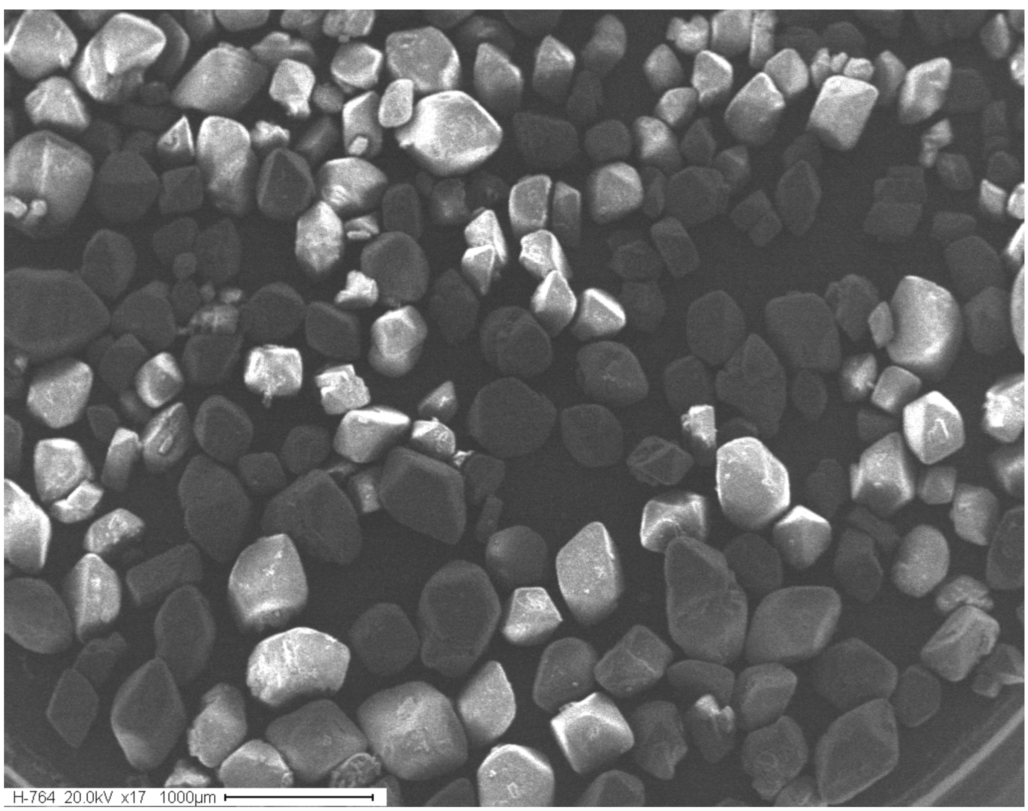

Figure 3.3 Picture of H-764 crystals, magnification 17x.

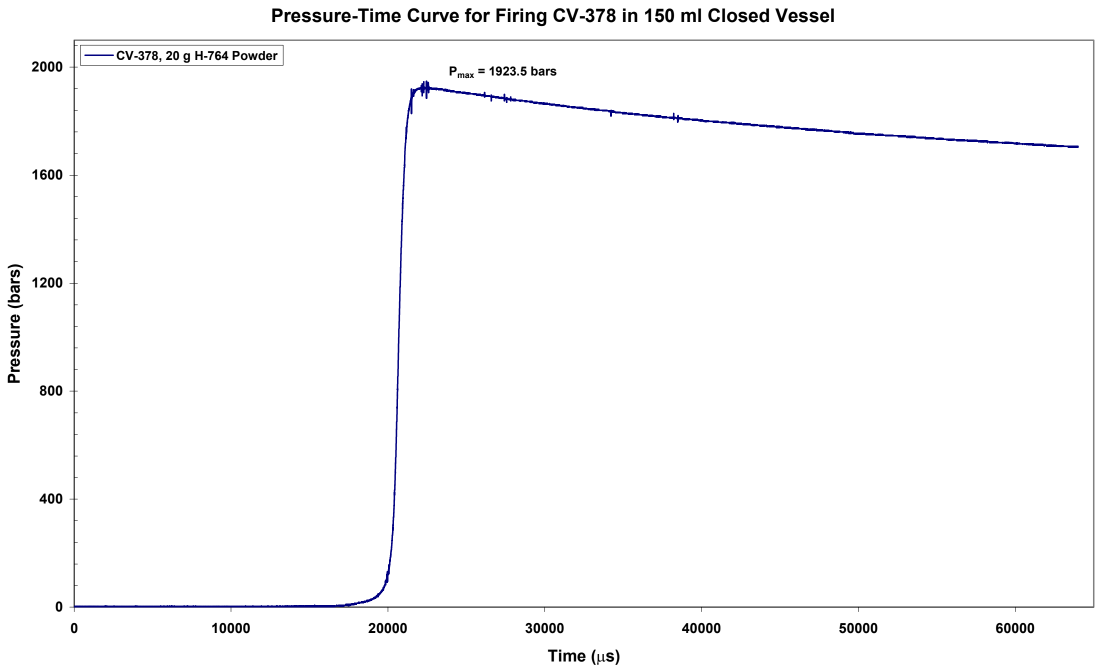

Figure 3.4 Pressure-time curve for firing CV-378 with H-764 powder.

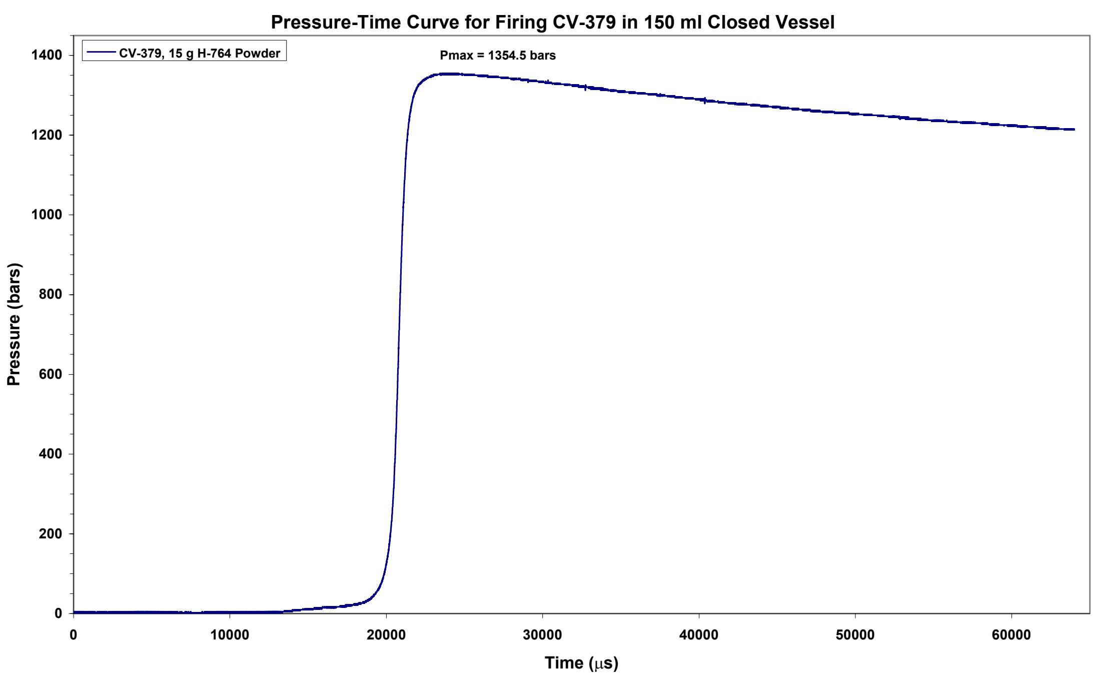

Figure 3.5 Pressure-time curve for firing CV-379 with H-764 powder.

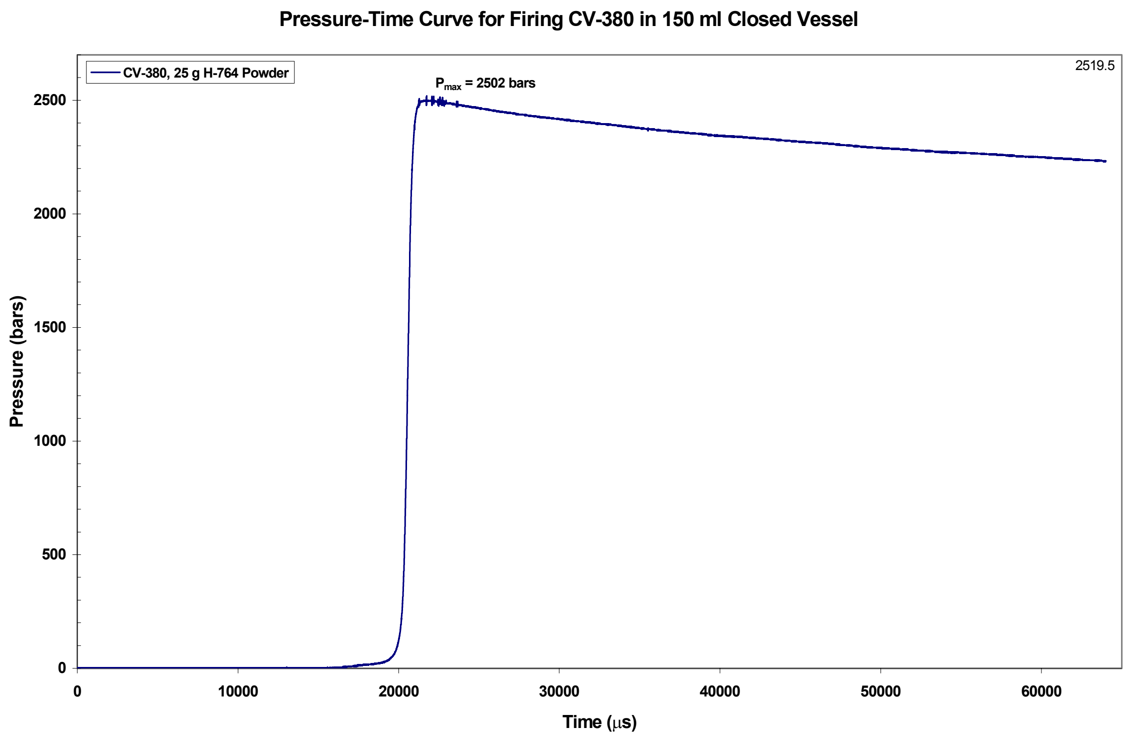

Figure 3.6 Pressure-time curve for firing CV-380 with H-764 powder.

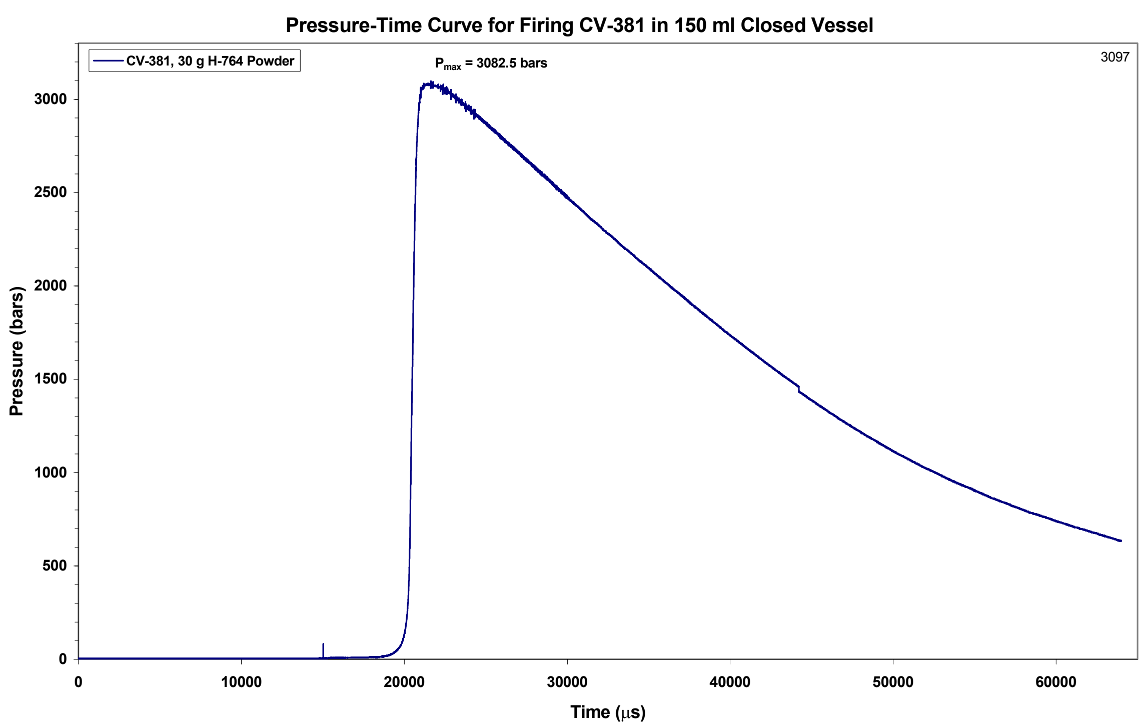

Figure 3.7 Pressure-time curve for firing CV-381 with H-764 powder. The drop in pressure is due to leakage.

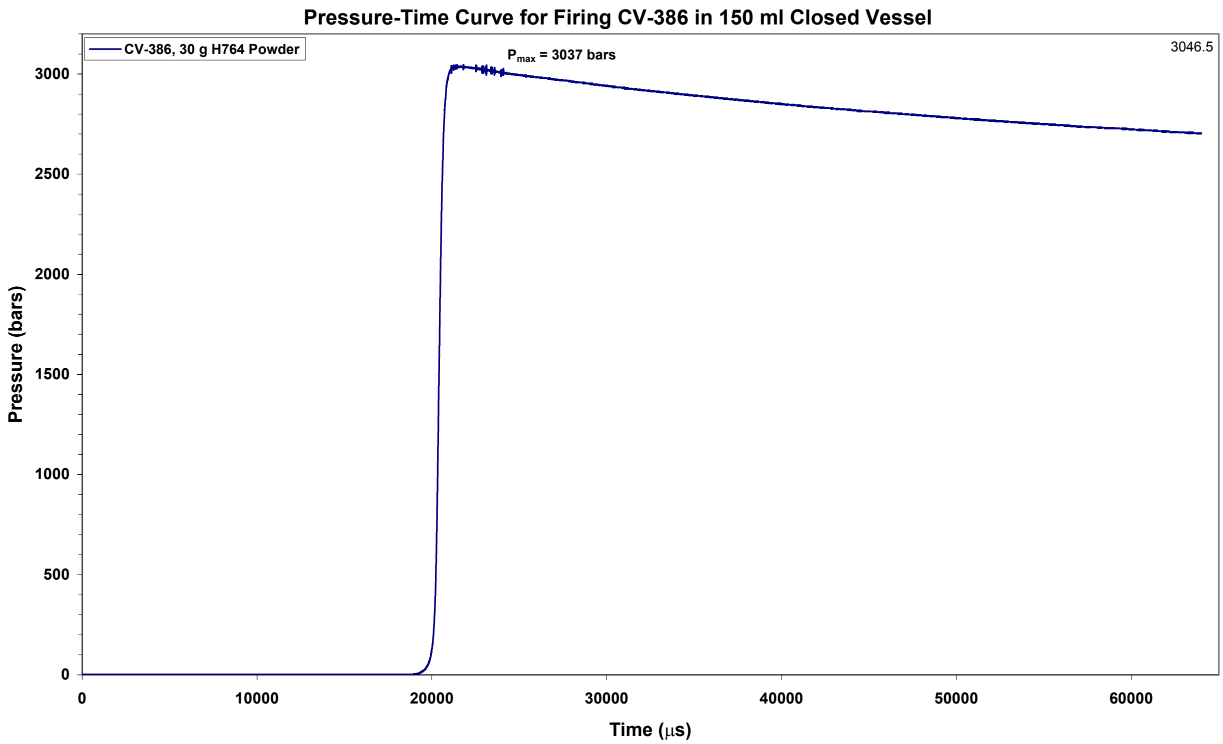

Figure 3.8 Pressure-time curve for firing CV-386 with H-764 powder.

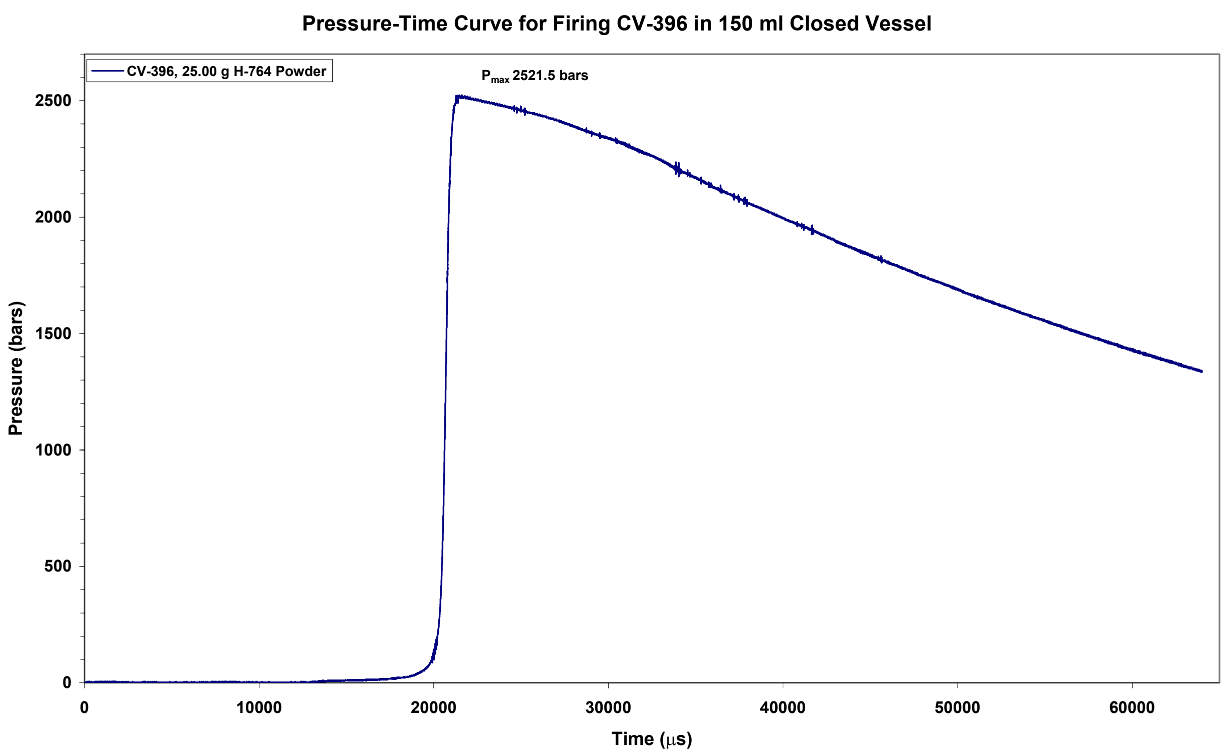

Figure 3.9 Pressure-time curve for firing CV-396 with H-764 powder. The drop in pressure is due to leakage.

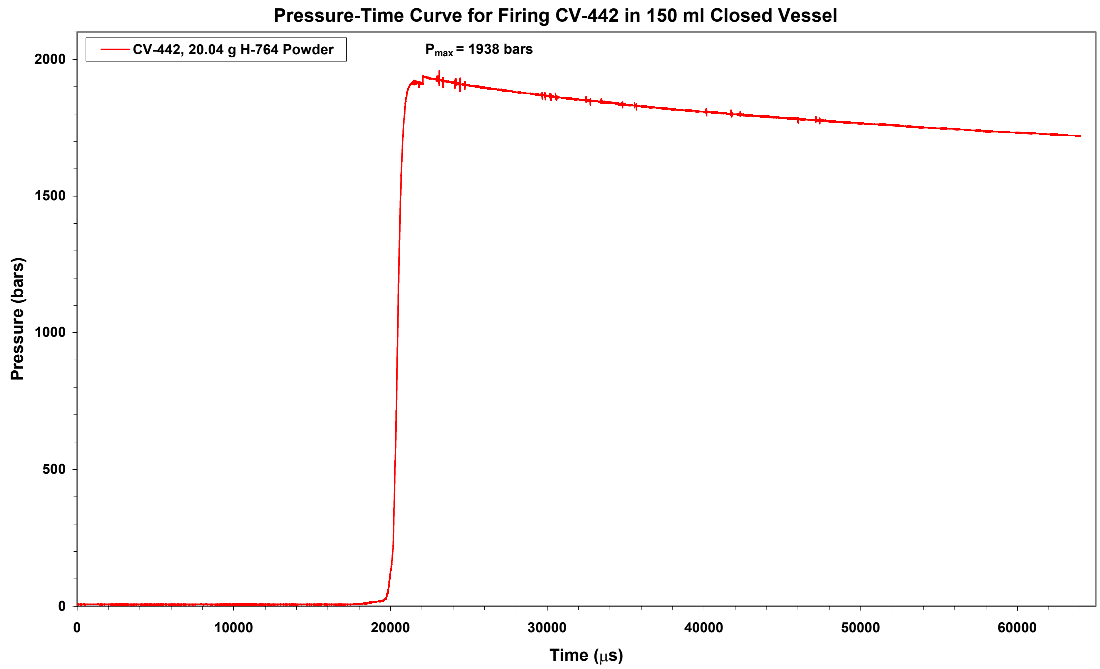

Figure 3.10 Pressure-time curve for firing CV-442 with H-764 powder.

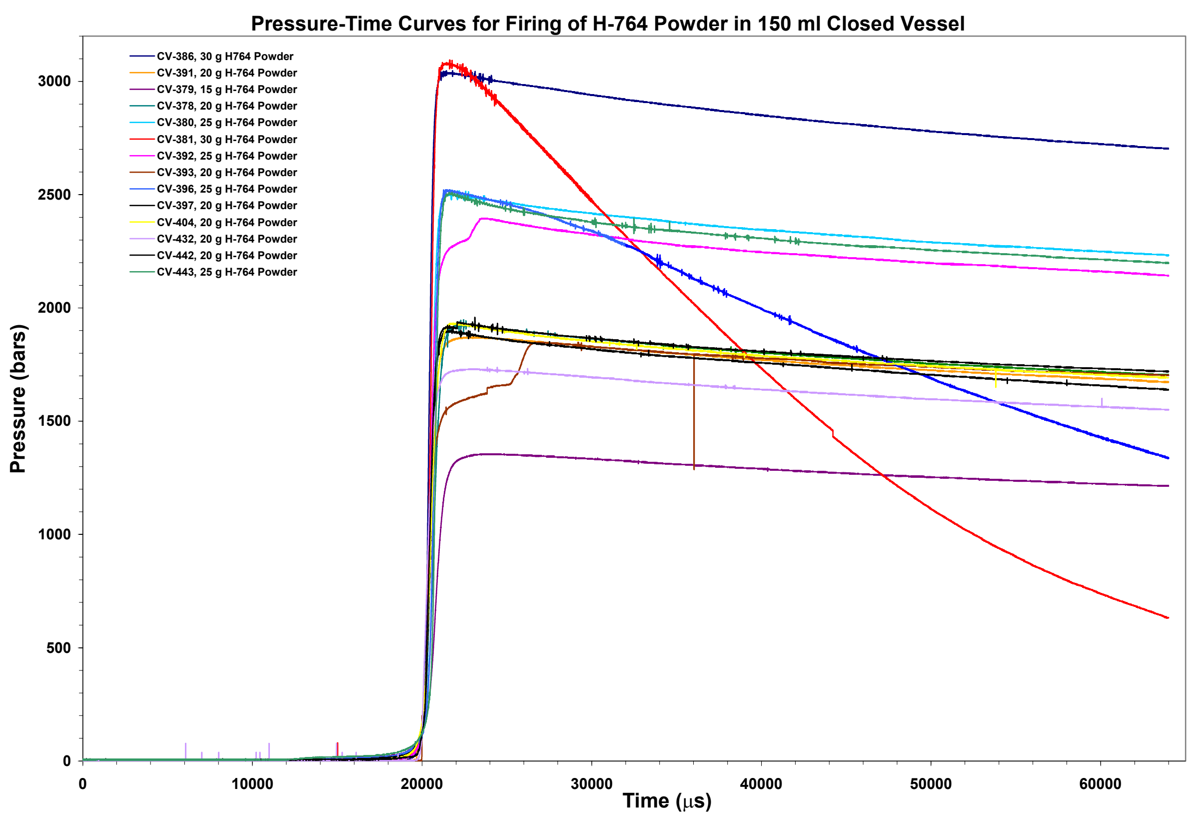

Figure 3.11 Pressure-time curves obtained for firings with H-764 powder.

Firing No.	Weight (g)	Loading Density (g/cm^3)	Maximum Pressure (MPa)	P_{max}/LD (MPa/g/cm^3)
CV-378	20	0.1333	192.35	1442.63
CV-379	15	0.1000	135.45	1354.50
CV-380	25	0.1667	250.20	1501.20
CV-381	30	0.2000	308.25	1541.25
CV-386	30	0.2000	303.70	1518.50
CV-391	20	0.1333	187.00	1402.50
CV-392	25	0.1667	239.60	1437.60
CV-393	20	0.1333	184.80	1386.00
CV-394	25	0.1667	206.05	1236.30
CV-395	25	0.1667	206.35	1238.10
CV-396	25	0.1667	252.15	1512.90
CV-397	20	0.1333	189.90	1424.25
CV-404	20	0.1333	193.05	1451.25
CV-432	20	0.1333	173.05	1297.88
CV-442	20.04	0.1336	193.80	1450.60
CV-443	25.01	0.1667	250.95	1503.30

Table 3.1 Properties of firings with H-764 powder.

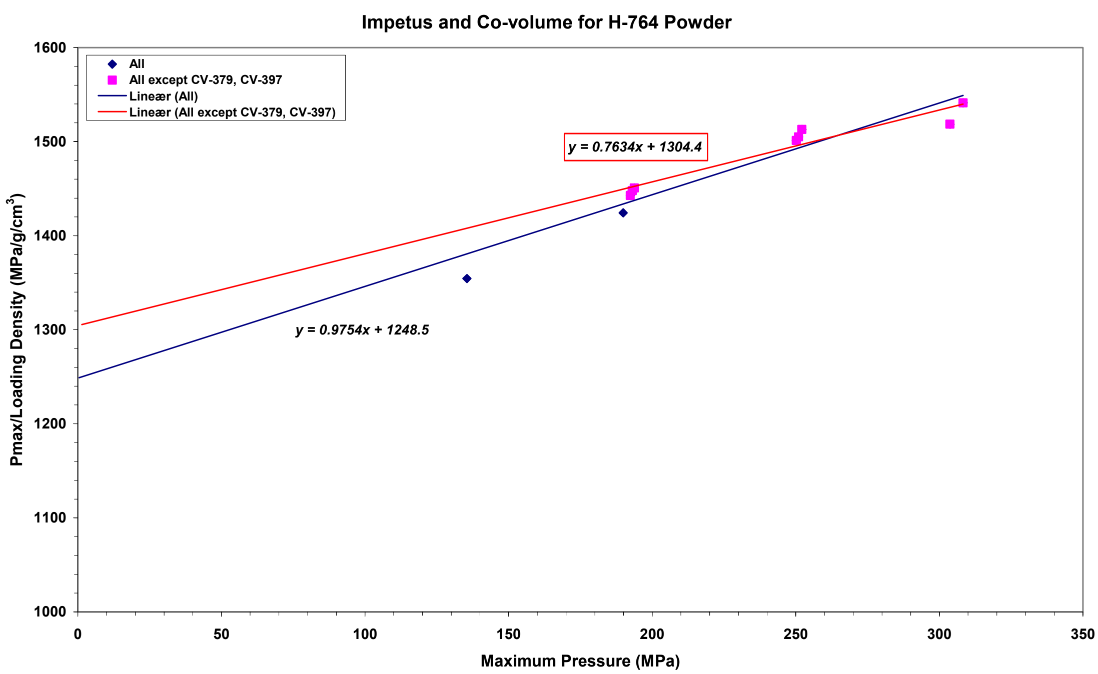

Figure 3.12 Impetus and Co-volume of H-764 powder.

In figure 3.12 has impetus and co-volume been determined by use of 11 and 9 of the firings with H-764 powder. The firings CV-392, 393, 394, 395 and 432 have not been used because we think they in one or other way are wrong. From figure 3.11 one can see that for these firings there are either some jumps in the pressure-time curves, or the obtained maximum pressure is too low. The main explanation to these unexpected curve forms may be found in the properties of the grease we have use in channel leading to the pressure gauge. We did for some of the experiments use some grease that after some firings cured or get harder. This may have an influence on the measurement of the pressure.

3.1.2 H-764 pellets pressed with 1900 kg pressure

Twenty-three pellets were pressed with a pressure of 1900 kg. The measured weight and dimensions for each pellet is given in table 3.2. The table also contains calculated volume and density of each pellet. The pellets in table 3.2 were used to perform 5 firings in the CV at four different loading densities.

Pellet No.	Weight (g)	Height (mm)	Volume (cm^3)	Density (g/cm^3)	Firing No. Weight
1	4.95	10.97	2.9888	1.6562	CV-429. 24.80 g
2	5.00	11.02	3.0025	1.6653	
3	4.97	11.02	3.0025	1.6553	
4	4.99	11.03	3.0052	1.6605	
5	4.98	11.02	3.0025	1.6586	
6	4.99	11.03	3.0052	1.6605	CV-390, 29.82 g
7	4.95	10.99	2.9943	1.6531	
8	4.97	11.05	3.0106	1.6508	
9	4.98	11.03	3.0052	1.6571	
10	4.99	11.03	3.0052	1.6605	
11	4.97	11.07	3.0161	1.6478	
12	4.96	11.01	2.9997	1.6535	CV-389, 14.86 g
13	4.97	11.02	3.0025	1.6553	
14	4.94	10.95	2.9834	1.6558	
15	5.00	11.12	3.0297	1.6503	CV-388, 19.93 g
16	5.01	11.09	3.0215	1.6581	
17	4.97	11.08	3.0188	1.6463	
18	4.98	11.05	3.0106	1.6541	
19	5.01	11.1	3.0243	1.6567	CV-387, 24.92 g
20	4.96	10.98	2.9916	1.6580	
21	4.95	10.96	2.9861	1.6577	
22	4.99	11.06	3.0134	1.6560	
23	4.97	11.01	2.9997	1.6568	
*Diameter 18.63 mm		**Average density**		**1.6558**	

Table 3.2 Properties of H-764 pellets pressed with 1900 kg pressure.

In figure 3.13 –3.18 are the obtained pressure-time curves given. Figure 3.18 gives all curves and shows that the form of all curves is similar except for CV-390, which has some ringing. However, after the maximum pressure has been reached the pressure seems to be correct, and the drop in pressure due to heat loss to the bomb seems to be of same magnitude as for the other firings.

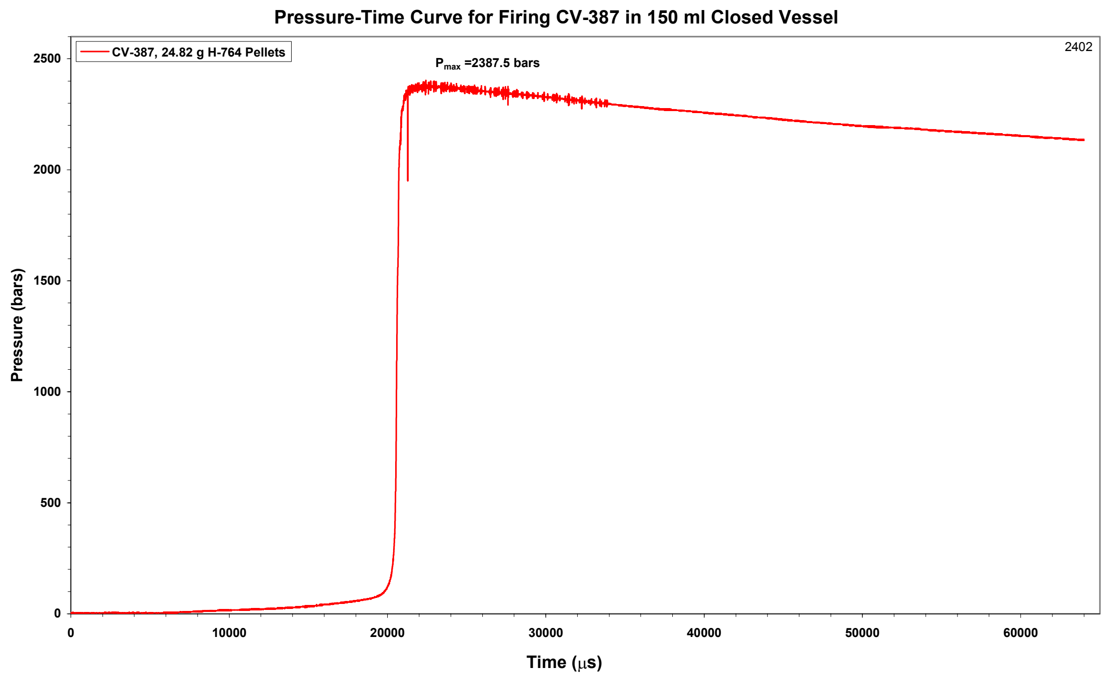

Figure 3.13 Obtained pressure-time curve for firing CV-387 containing H-764 pressed pellets.

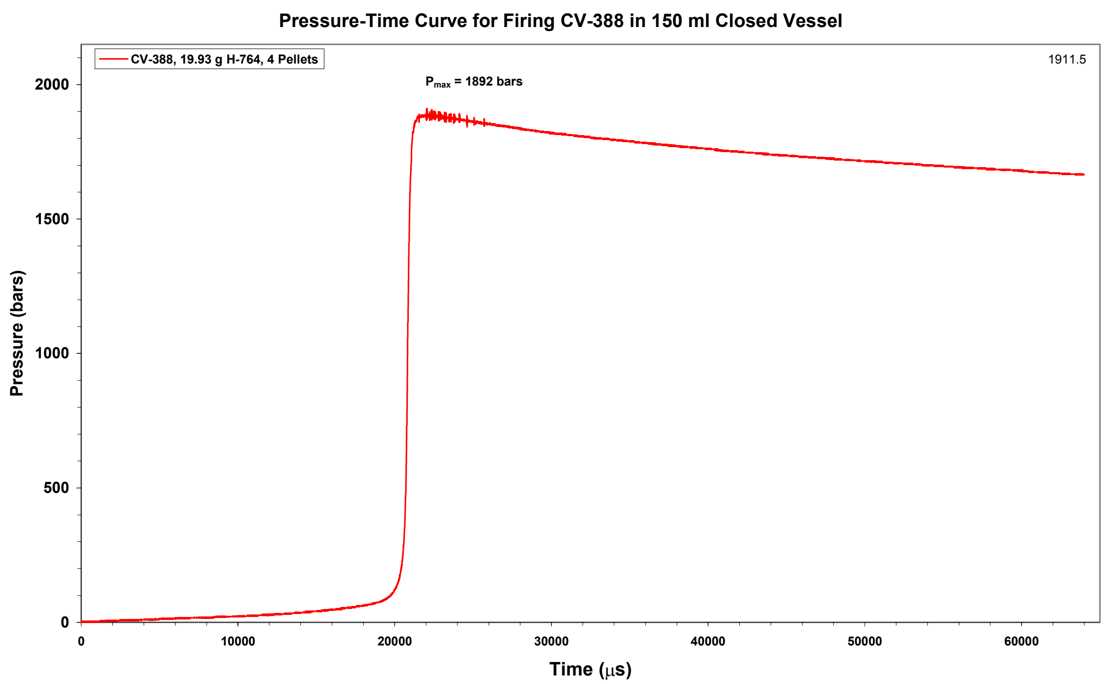

Figure 3.14 Obtained pressure-time curve for firing CV-388 containing H-764 pressed pellets.

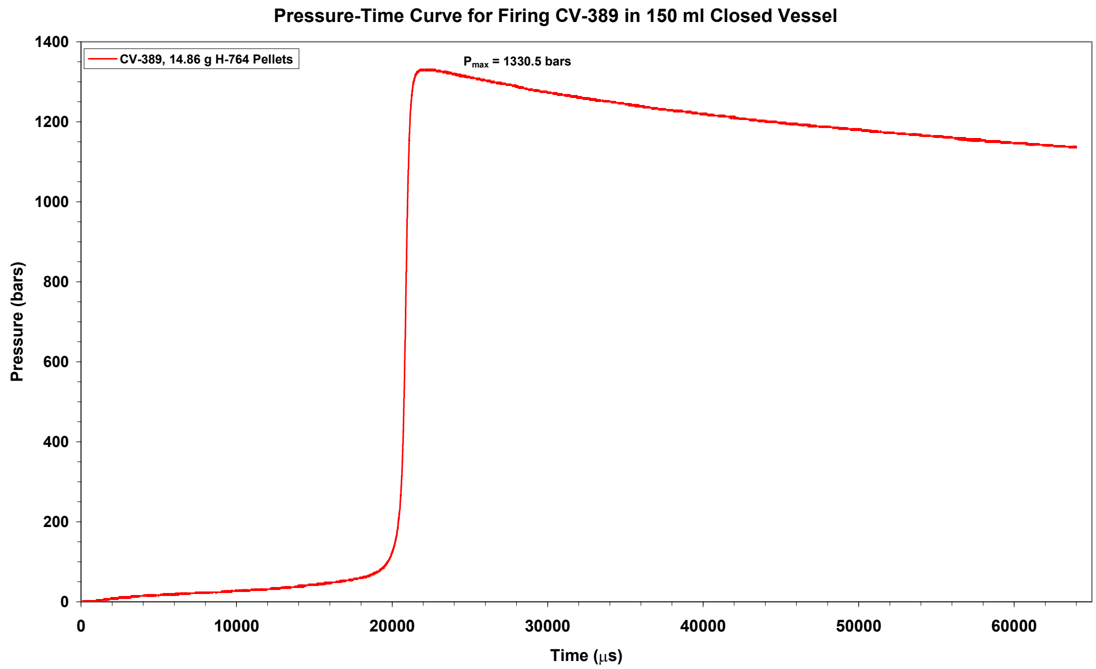

Figure 3.15 Obtained pressure-time curve for firing CV-389 containing H-764 3 pressed pellets.

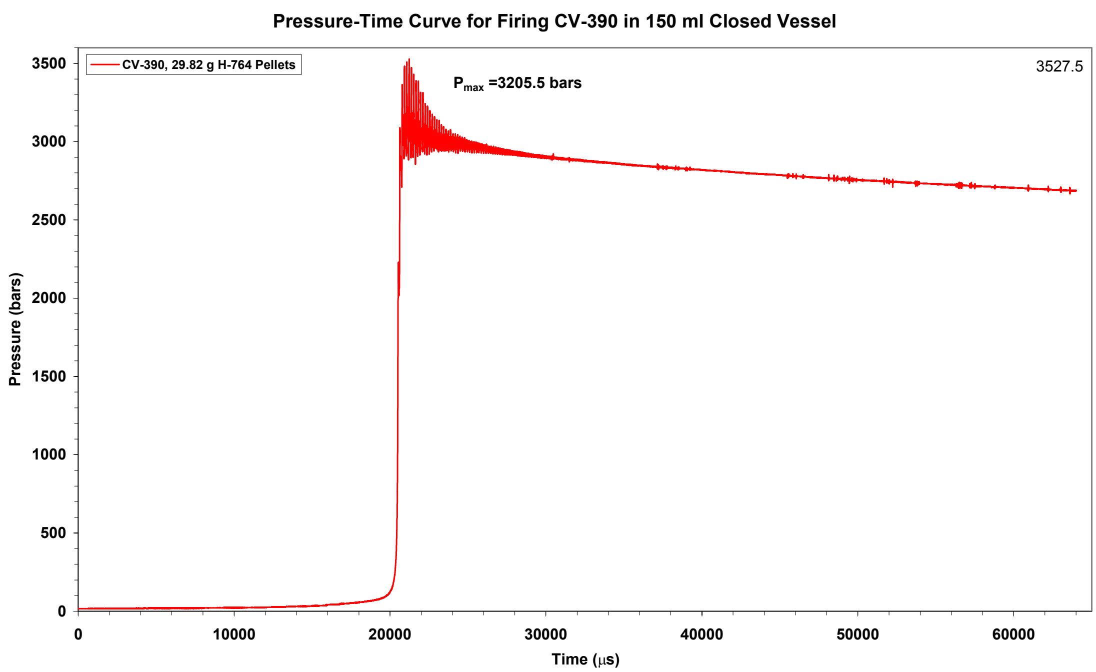

Figure 3.16 Obtained pressure-time curve for firing CV-390 containing H-764 6 pressed pellets.

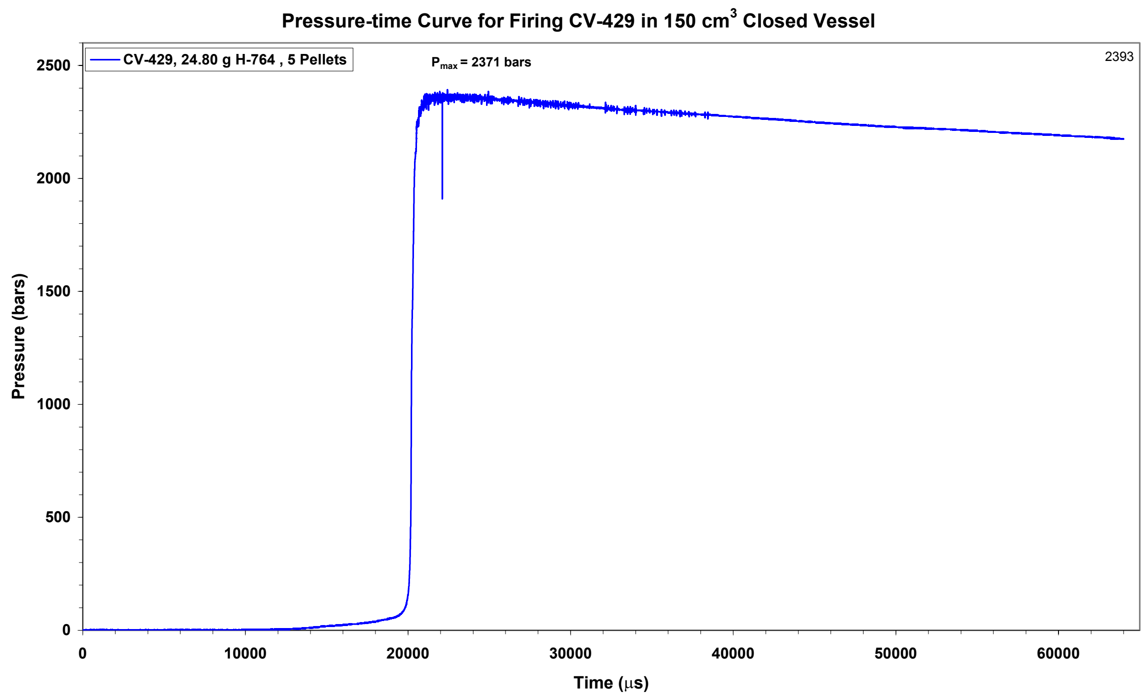

Figure 3.17 Obtained pressure-time curve for firing CV-429 containing H-764 6 pressed pellets.

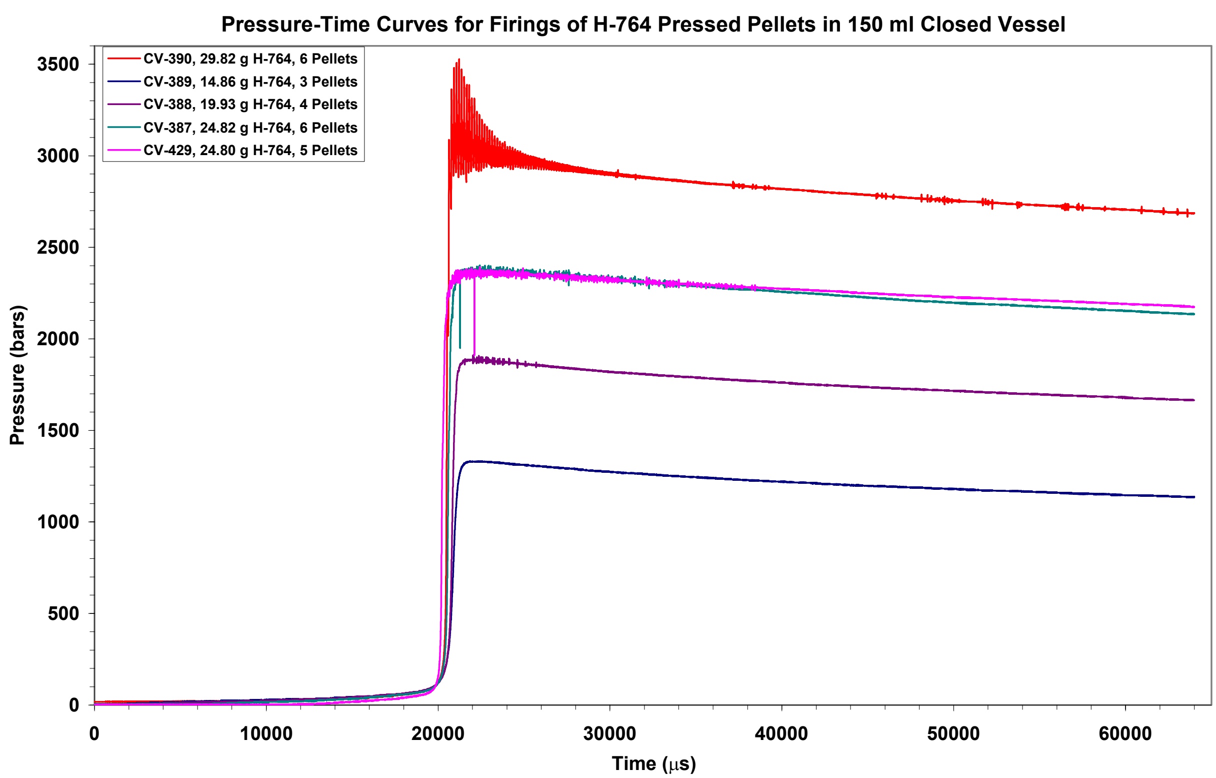

Figure 3.18 Obtained pressure-time curves for firings containing H-764 pellets with density of 1.656 g/cm^3.

Firing No.	Weight (g)	Load Density (g/cm^3)	Pressure (MPa)	P_{max}/LD ($MPa/g/cm^3$)
CV-389	14.86	0.0991	133.05	1343.03
CV-388	19.93	0.1329	189.2	1423.98
CV-387	24.82	0.1655	237.5	1435.33
CV-390	29.82	0.1988	303.5	1526.66
CV-429	24.80	0.1653	237.1	1434.07

Table 3.3 Obtained properties of CV-firings with H-764 pellets pressed to a density of 1.656 g/cm^3.

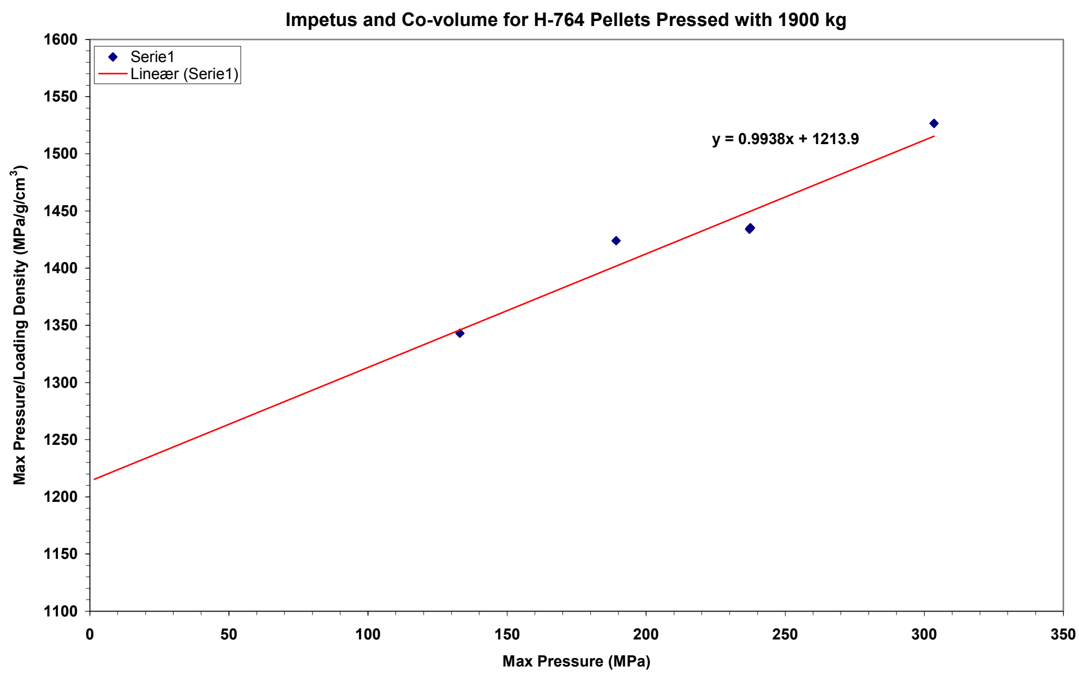

Figure 3.19 Plot of impetus and co-volume of firings with pellets of H-764.

By plotting the properties obtained in table 3.3, figure 3.19 gives the following results for impetus and co-volume, co-volume equal to 0.9938 cm^3/g and impetus equal to 1214 J/g.

3.1.3 H-764 pellets pressed with 5700 kg

Twenty-two pellets of H-764 were pressed to a density of 1.749 g/cm^3. The weight and dimensions of each pellet is given in table 3.4 together with calculated volume and density. Five firing with four different loading densities have been carried out. In figure 3.20 to 3.24 is single pressure-time curves given, while figure 3.25 contains pressure-time curves for all firings.

Pellet No.	Weight (g)	Height (mm)	Volume (cm^3)	Density (g/cm^3)	Firing No. Weight
1	5.00	10.47	2.8526	1.7578	
2	4.99	10.47	2.8526	1.7528	CV-407
3	5.00	10.48	2.8553	1.7511	14.97 g
4	4.98	10.45	2.8472	1.7526	
5	4.97	10.47	2.8526	1.7458	CV-405
6	4.99	10.50	2.8526	1.7493	19.90 g
7	5.00	10.48	2.8608	1.7478	
8	4.96	10.48	2.8553	1.7406	
9	4.99	10.53	2.8553	1.7476	CV-406
10	4.99	10.47	2.8690	1.7393	24.91 g
11	4.98	10.48	2.8526	1.7458	
12	4.98	10.39	2.8553	1.7371	
13	5.01	10.40	2.8308	1.7698	
14	4.98	10.46	2.8335	1.7575	
15	4.99	10.46	2.8499	1.7509	CV-408
16	4.98	10.47	2.8499	1.7474	29.90 g
17	4.98	10.46	2.8526	1.7423	
18	4.97	10.44	2.8499	1.7474	
19	4.98	10.41	2.8444	1.7508	
20	4.99	10.49	2.8363	1.7594	CV-409
21	4.97	10.45	2.8581	1.7389	19.91 g
22	4.98	10.47	2.8472	1.7491	
*Diameter 18.63 mm		**Average density**		**1.7489**	

Table 3.4 Properties of H-764 pellets pressed with 5700 kg.

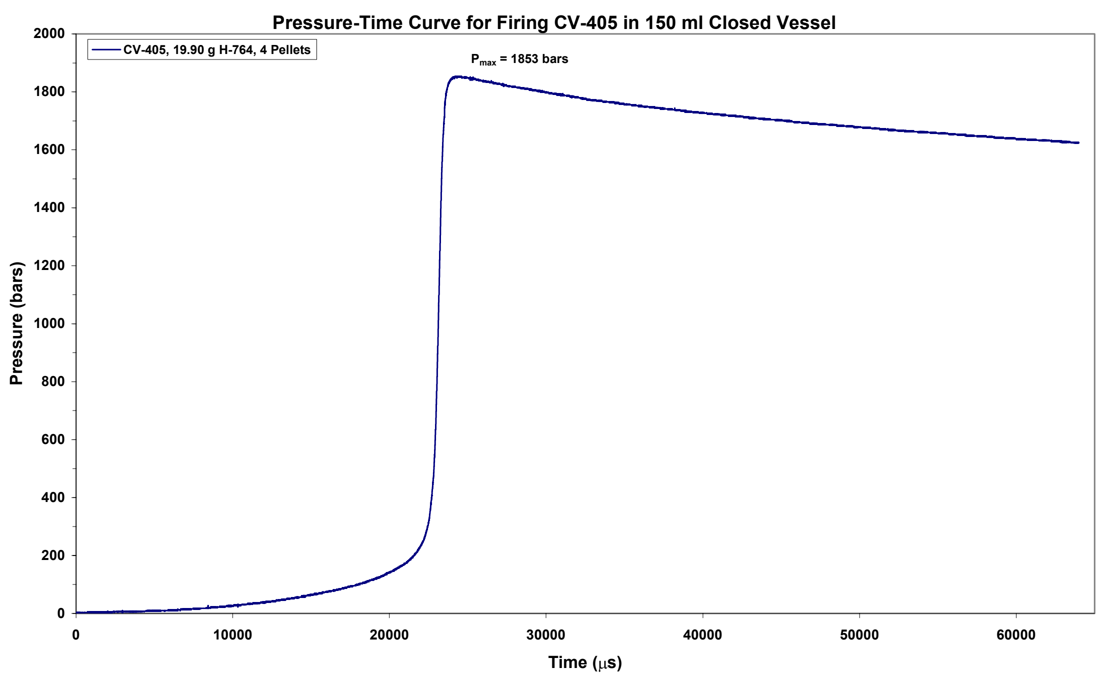

Figure 3.20 Obtained pressure-time curve for firing CV-405 containing H-764 pellets with density 1.749 g/cm³.

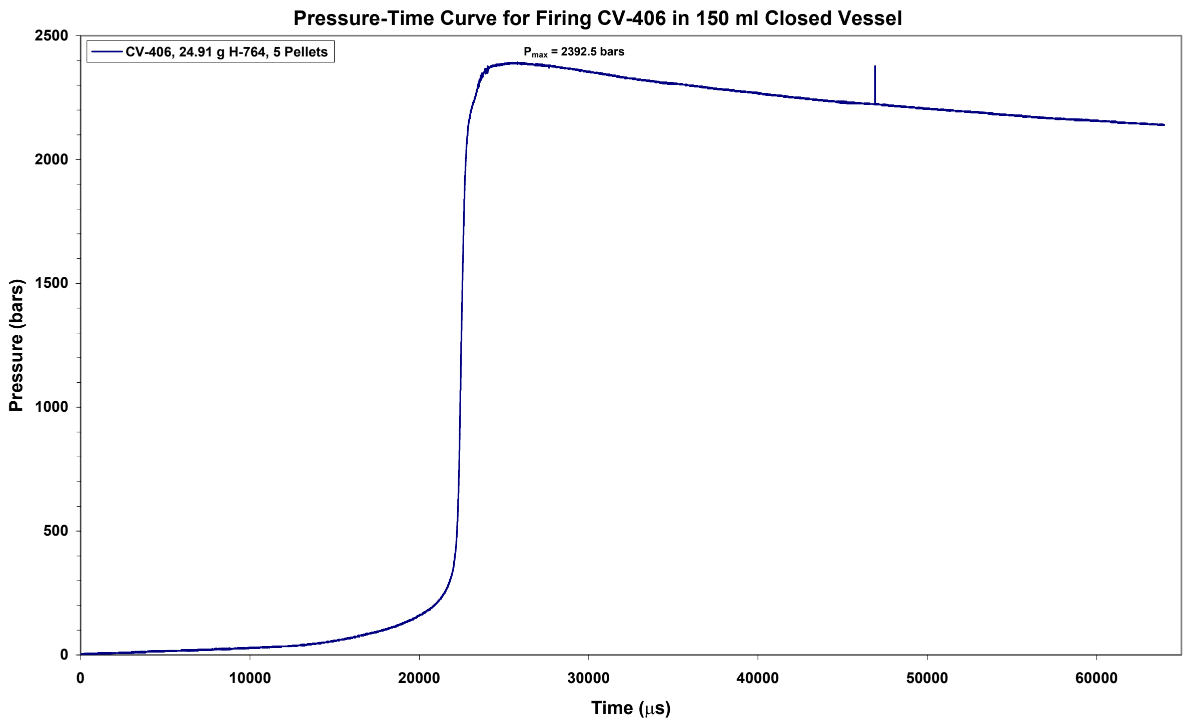

Figure 3.21 Obtained pressure-time curve for firing CV-406 containing H-764 pellets with density 1.749 g/cm³.

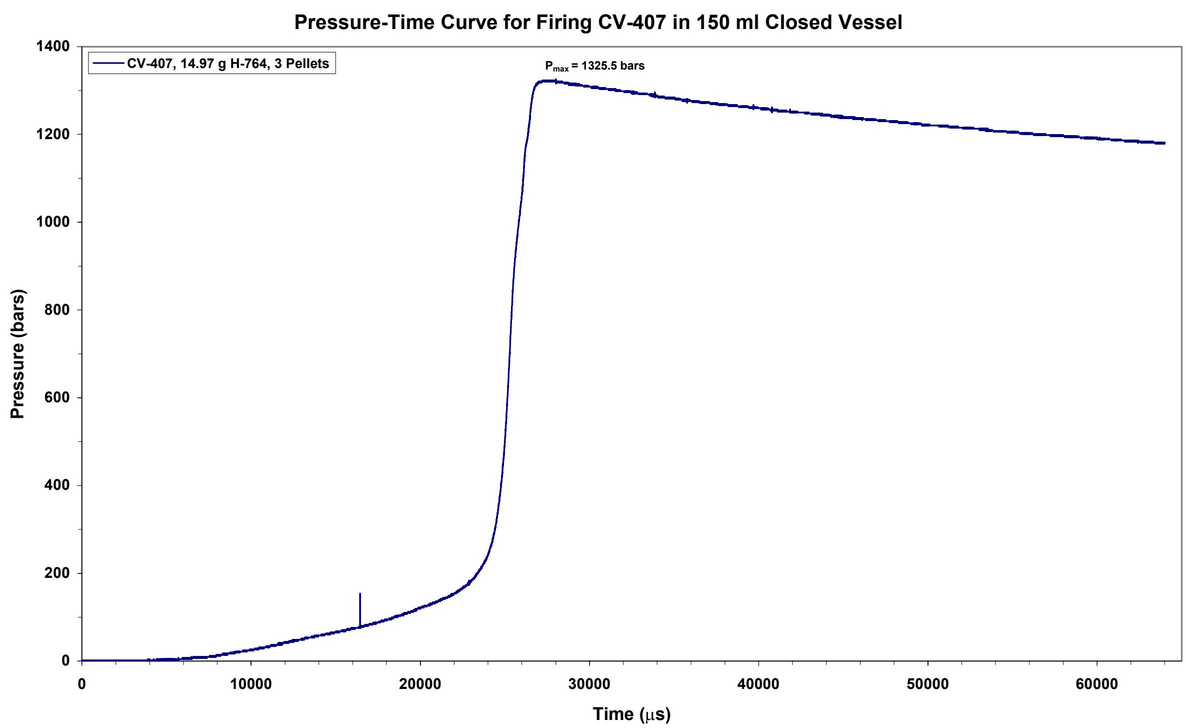

Figure 3.22 Obtained pressure-time curve for firing CV-407 containing H-764 pellets with density 1.749 g/cm³.

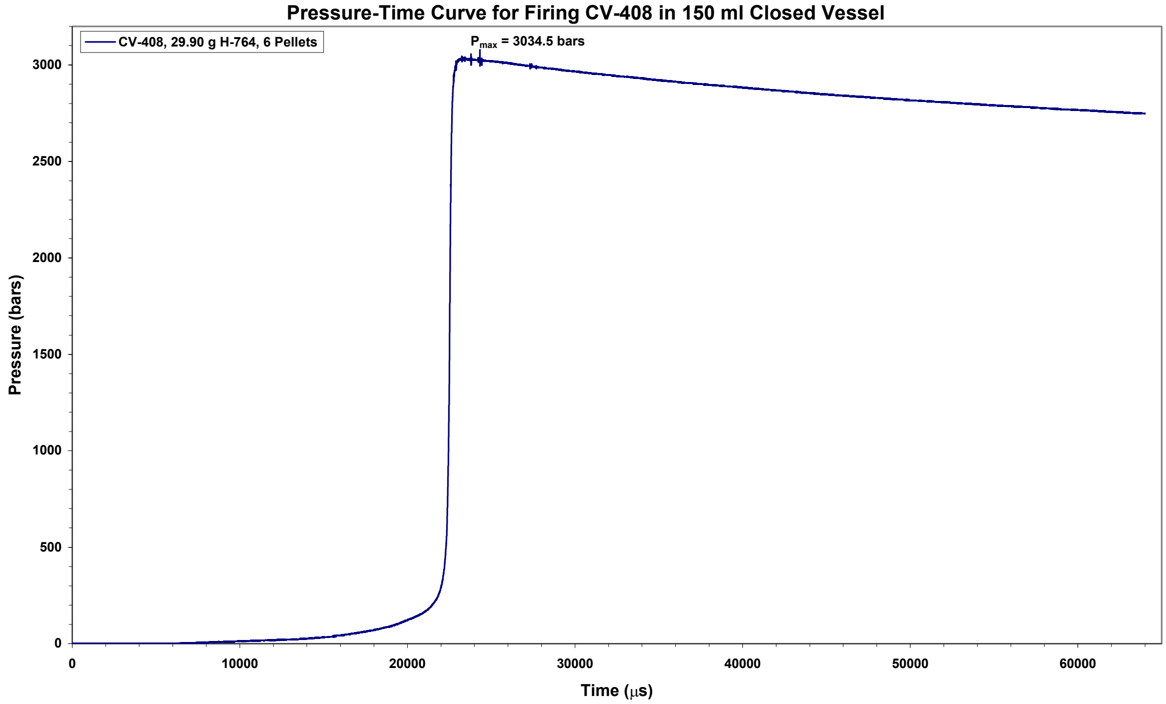

Figure 3.23 Obtained pressure-time curve for firing CV-408 containing H-764 pellets with density 1.749 g/cm^3.

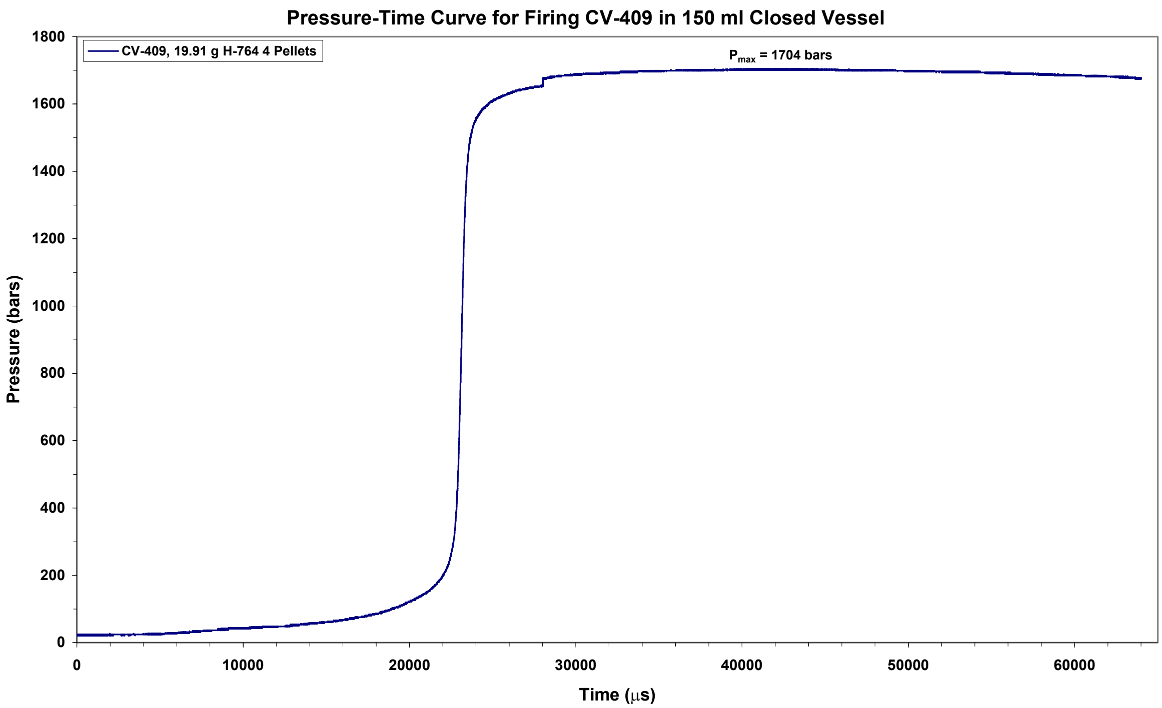

Figure 3.24 Obtained pressure-time curve for firing CV-409 containing H-764 pellets with density 1.749 g/cm^3.

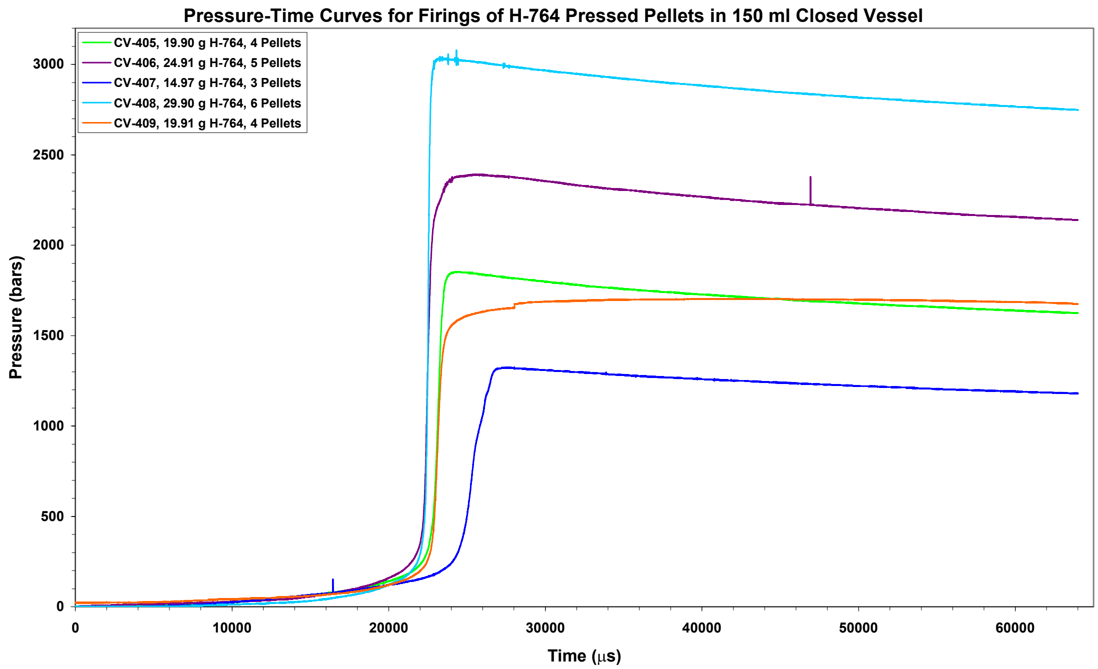

Figure 3.25 All obtained pressure-time curves for firings containing H-764 pellets with density 1.749 g/cm³.

For all firings except firing CV-409 the obtained pressure-time curves have an expected form. We have not a good explanation for why the pressure-time curve for firing CV-409 has an unexpected form. It may be that the ignition is different, since the maximum pressure is reached much later than for the other firings, but we prefer to interpret the slower pressure increase to have something to do with the registration of the pressure and thereby the pressure gauge.

Firing No.	Weight (g)	Loading Density (g/cm^3)	Pressure (MPa)	Pmax/LD (MPa/g/cm^3)
CV-409	19.91	0.1327	170.40	1283.78
CV-408	29.90	0.1993	303.45	1522.32
CV-407	14.97	0.0998	132.50	1327.66
CV-406	24.91	0.1661	239.25	1440.67
CV-405	19.90	0.1327	185.30	1396.73

Table 3.5 Obtained results for firings of H-764 pellets with density 1.749 g/cm³.

In figure 3.26 are the results given in table 3.5 are plotted. This gives two different results for impetus and co-volume if we include all firings or leave out CV-409 since it has a different form of the pressure-time curve. In the last case we get an impetus equal to 1183 J/g and a co-volume equal to 1.109 cm^3/g. These results are as expected, since one by comparing the pressure-time curves given in figure 3.25 with the curves of powder or the lower density pellets, we will see a slower pressure increase after ignition for the firings in figure 3.25.

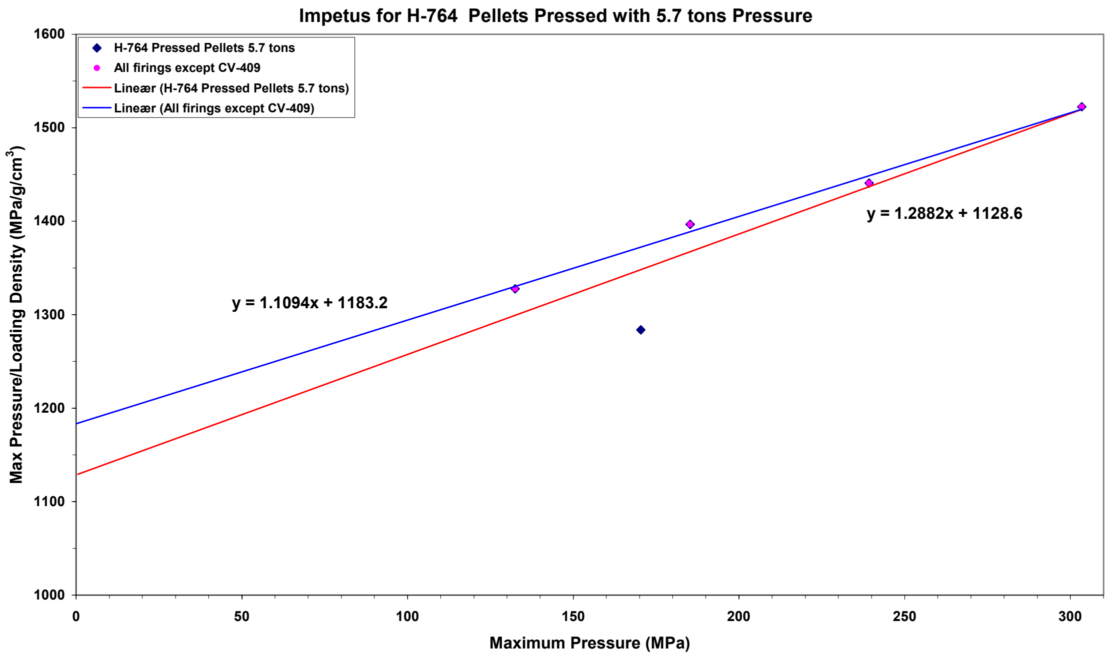

Figure 3.26 Obtained impetus and co-volume for pellets pressed with a pressure of 2092.1 kg/cm^2.

3.1.4 H-764 pellets pressed with 1 GPa pressure

In an attempt to get pellets with density as high as possible we used a 50 tons press and another tool, figure 2.3 for pellet preparation. However, the pellets we were able to produce had lower density than TMD (theoretical maximum density), and therefore must contain some air or pores. The obtained properties of the pellets are given in table 3.6. We did carry out three firings of different loading density with these pellets. The pressure-time curves for these firings are given in figure 3.27 to 3.29.

Pellet No.	Weight (g)	Height (mm)	Volume (cm^3)	Density (g/cm^3)	Firing No. Weight
1	3.6717	8.85	2.0457	1.7948	
2	3.6764	8.89	2.0545	1.7890	CV-423
3	3.6760	8.90	2.0573	1.7868	14.70 g
4	3.6778	8.92	2.0619	1.7837	
1	3.7000	8.89	2.0550	1.8005	
2	3.6848	8.92	2.0619	1.7871	CV-427
3	3.6708	8.91	2.0596	1.7823	18.39 g
4	3.6767	8.87	2.0503	1.7932	
5	3.6801	8.94	2.0665	1.7808	
6	3.6750	8.93	2.0642	1.7803	
7	3.6777	8.91	2.0596	1.7856	
8	3.6709	8.96	2.0712	1.7723	CV-428
9	3.6790	8.96	2.0712	1.7763	22.06 g
10	3.6705	8.88	2.0527	1.7882	
11	3.6830	8.96	2.0712	1.7782	
*Diameter 17.16 mm		**Average density**		**1.7853**	

Table 3.6 Properties of H-764 pellets pressed with a pressure of 1 GPa.

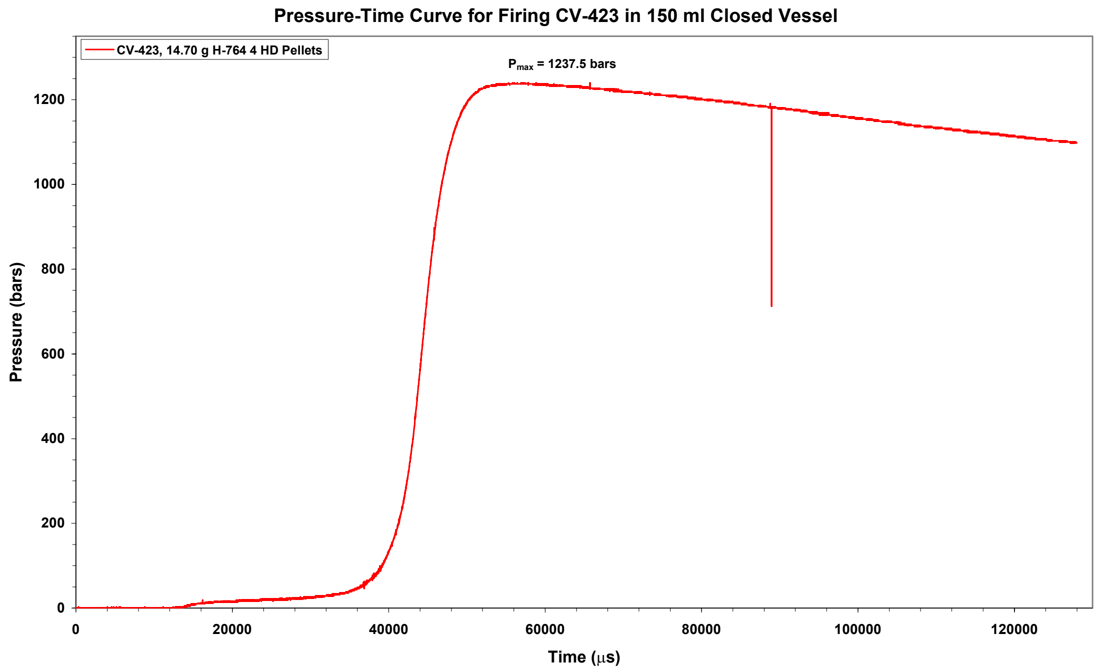

Figure 3.27 Obtained pressure-time curve for CV-323 firing containing pellets with density of 1.785 g/cm^3.

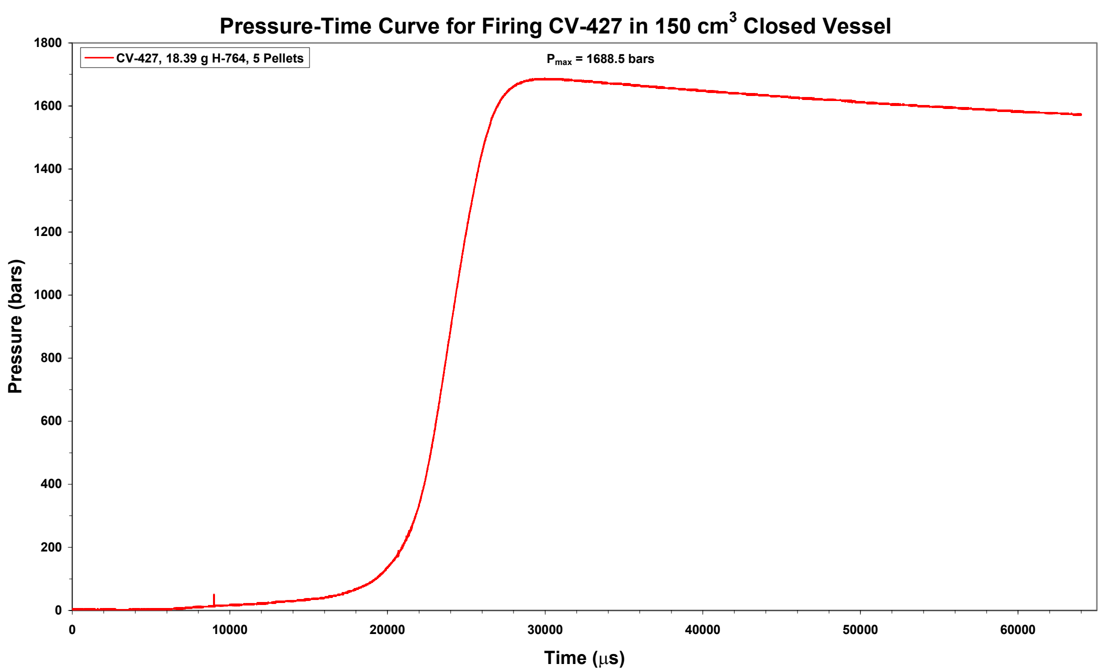

Figure 3.28 Obtained pressure-time curve for CV-327 firing containing pellets with density of 1.785 g/cm^3.

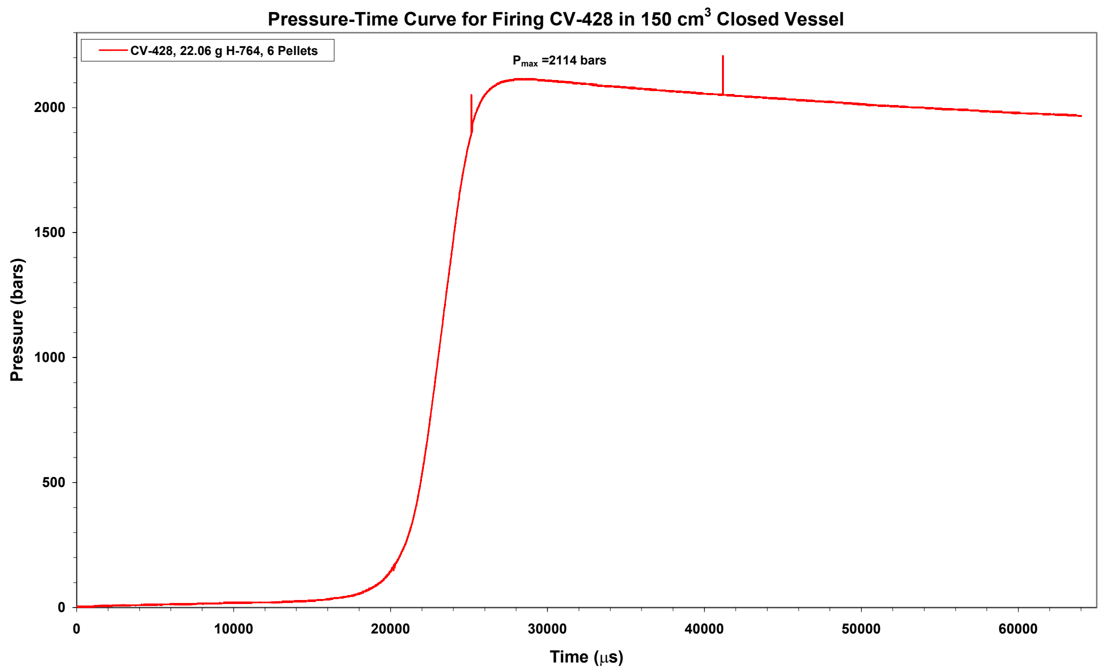

Figure 3.29 Obtained pressure-time curve for CV-328 firing containing pellets with density of 1.785 g/cm^3.

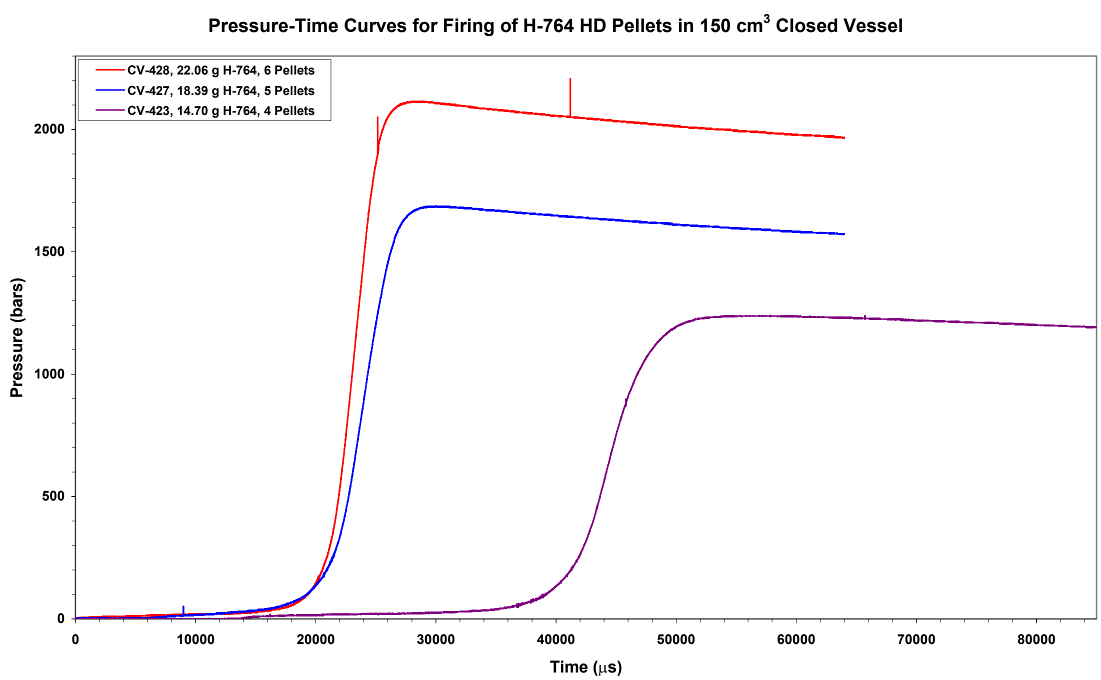

Figure 3.30 Comparison of obtained pressure-time curves for firings containing H-764 pellets with density of 1.785 g/cm^3.

In figure 3.30 is all pressure-time curves given in the same plot. Table 3.7 gives the results for maximum pressure and P_{max}/LD for the firings in figure 3.30. In figure 3.31 has the results in table 3.7 been plotted and impetus and co-volume calculated.

Firing No.	Weight (g)	Loading Density (g/cm^3)	Maximum Pressure (MPa)	P_{max}/LD ($MPa/g/cm^3$)
CV-428	22.06	0.1471	211.40	1437.44
CV-427	18.39	0.1226	168.85	1377.24
CV-423	14.70	0.0980	123.75	1262.76

Table 3.7 Properties of the CV-firings with H-764 pellets with density of 1.785 g/cm^3.

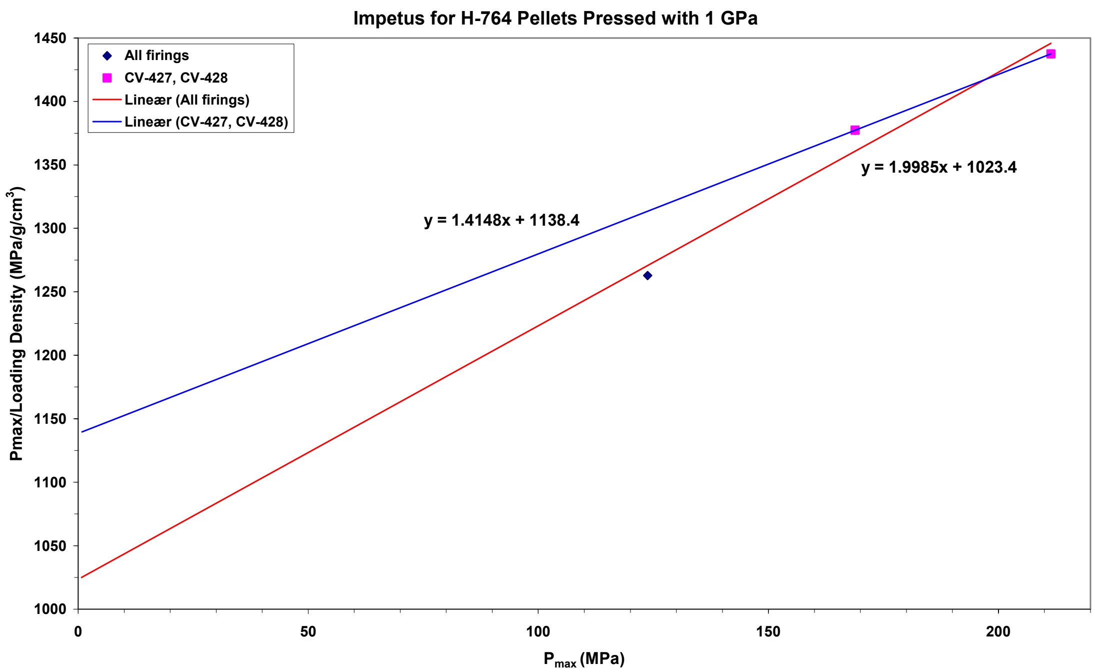

Figure 3.31 Plot of maximum pressure as function of maximum pressure divided by the loading density for the CV-firings of pellets with density of 1.785 g/cm^3.

From figure 3.31 we get an impetus of 1138.4 J/g and a co-volume of 1.4148 cm^3/g if take in to consideration only the two highest loading densities.

3.2 PETN

3.2.1 Powder PETN

PETN in form of crystals was packed in a plastic bag. The ignition was by a squib and black powder and was placed in the center of the PETN powder. Figure 3.32 gives a picture of the tested unit. In figure 3.33 is given a picture of PETN crystals taken by light microscope and figure 3.34 gives a SEM (Scanning Electron Microscope) picture of some PETN crystals. Five different loading densities of powder PETN has been tested in CV. Totally have 8 firings with powder been performed, and figure 3.35 to 3.42 gives pressure-time curves for each firing. Figure 3.43 gives curves for all firings. As figure 3.43 shows there are some minor differences in the maximum pressure for the firing with equal amount of PETN powder.

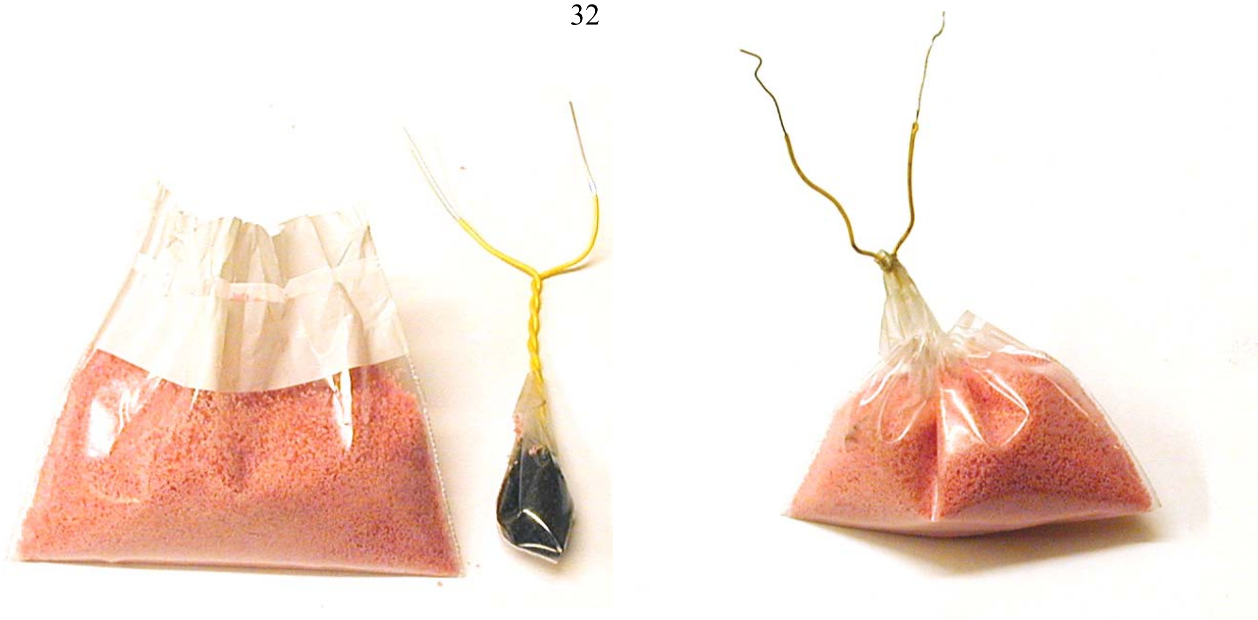

Figure 3.32 Picture of how the PETN powder is packed for testing in closed vessel.

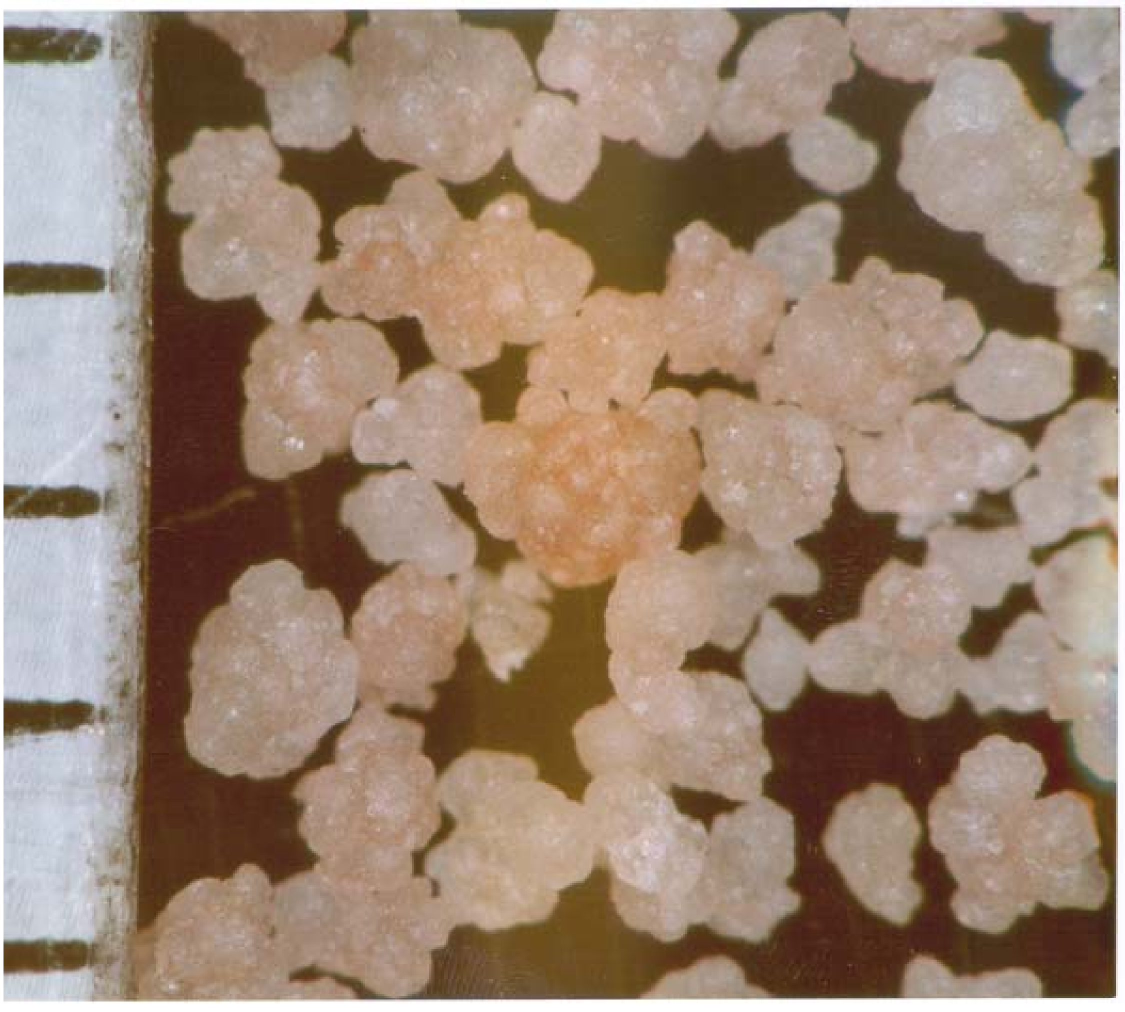

Figure 3.33 Picture of PETN crystal in light microscope.

Figure 3.34 SEM picture of PETN crystals

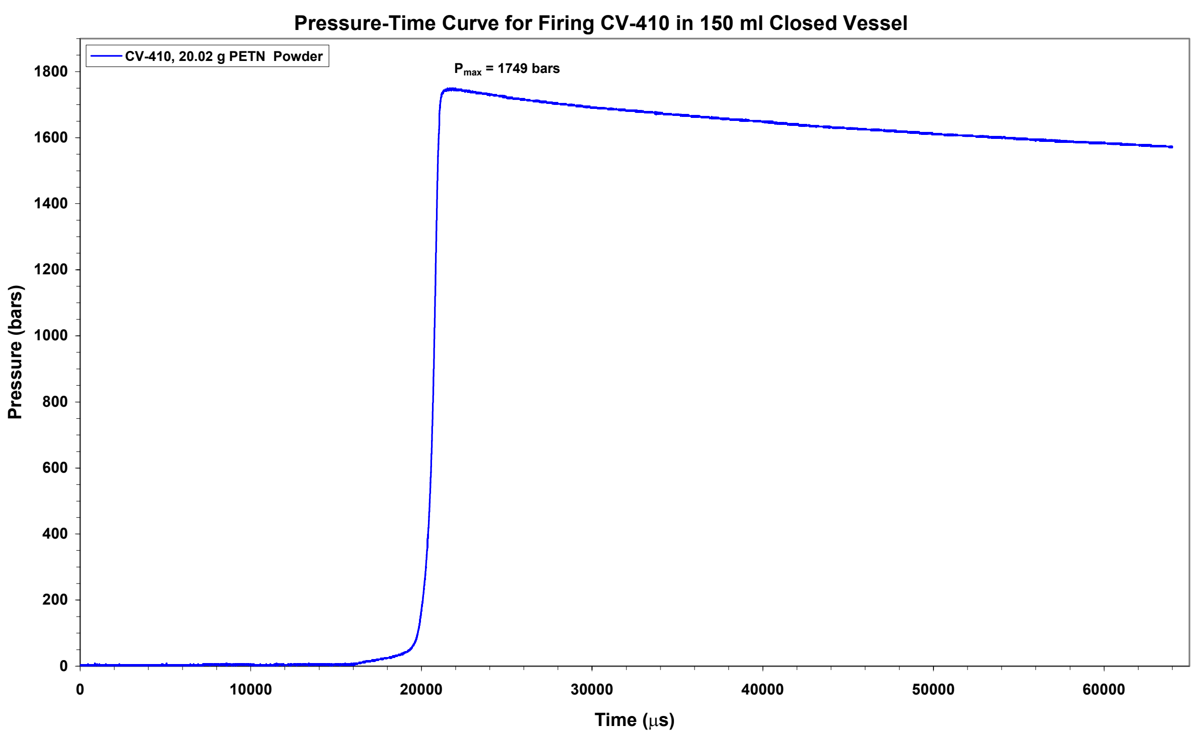

Figure 3.35 Obtained pressure-time curve for firing CV-410 with PETN powder.

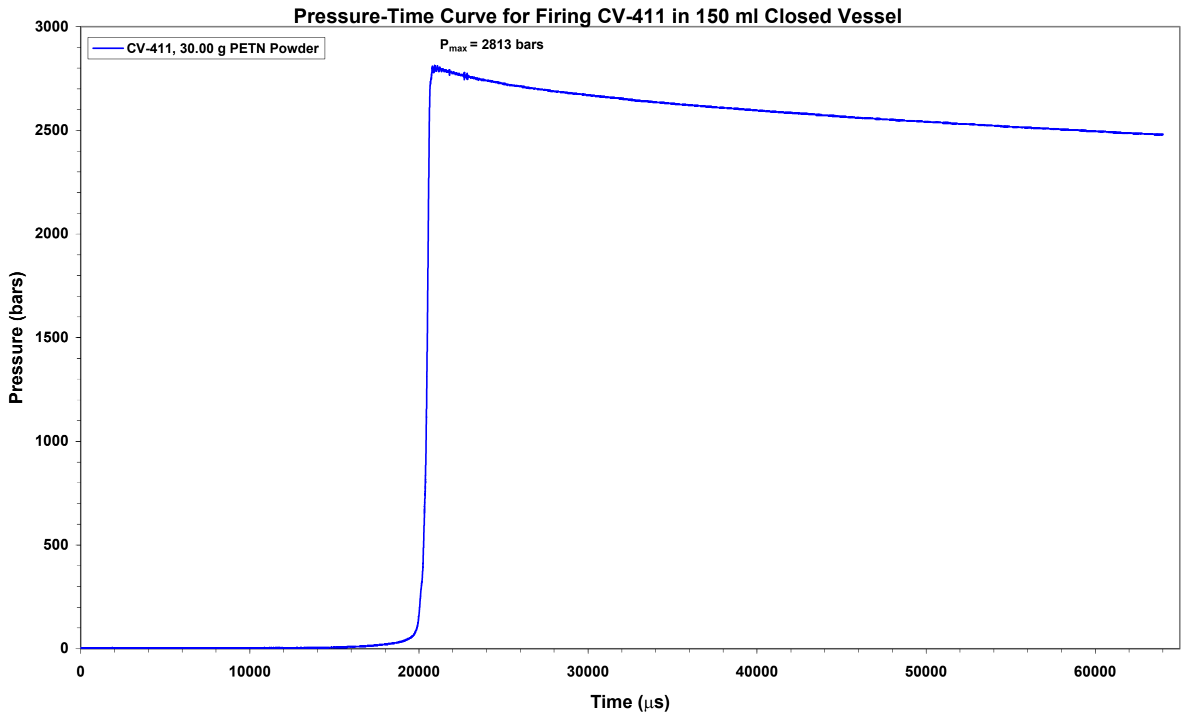

Figure 3.36 Obtained pressure-time curve for firing CV-411 with PETN powder.

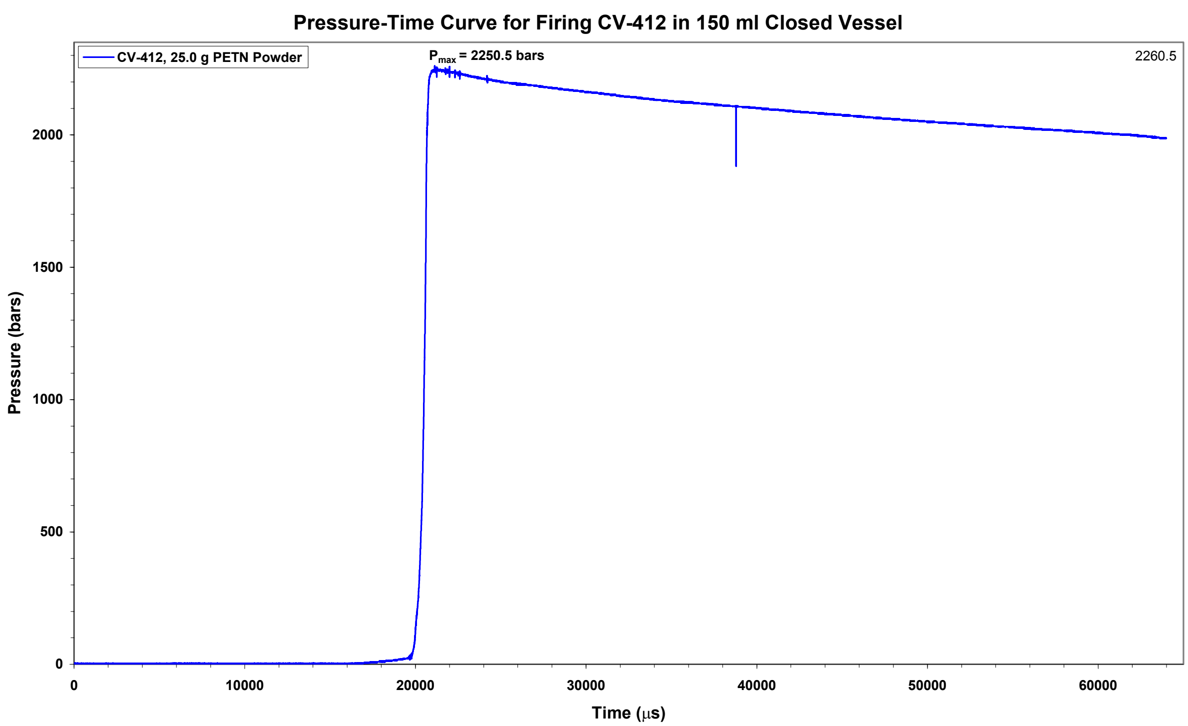

Figure 3.37 Obtained pressure-time curve for firing CV-412 with PETN powder.

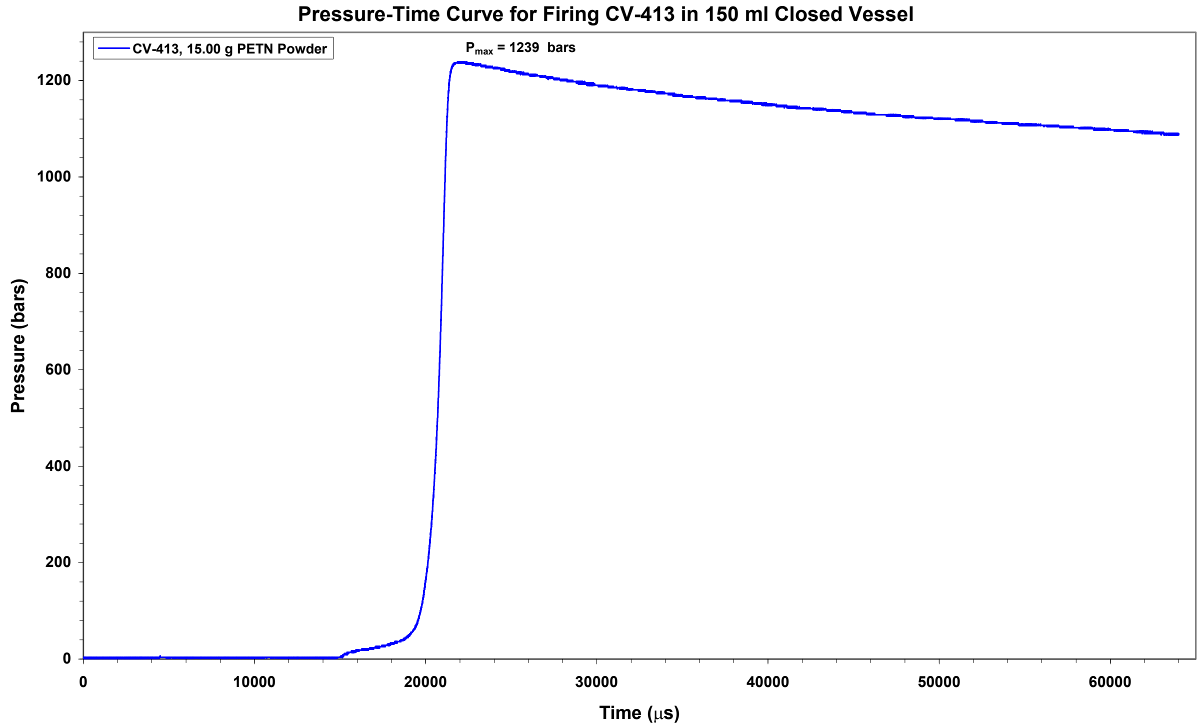

Figure 3.38 Obtained pressure-time curve for firing CV-413 with PETN powder.

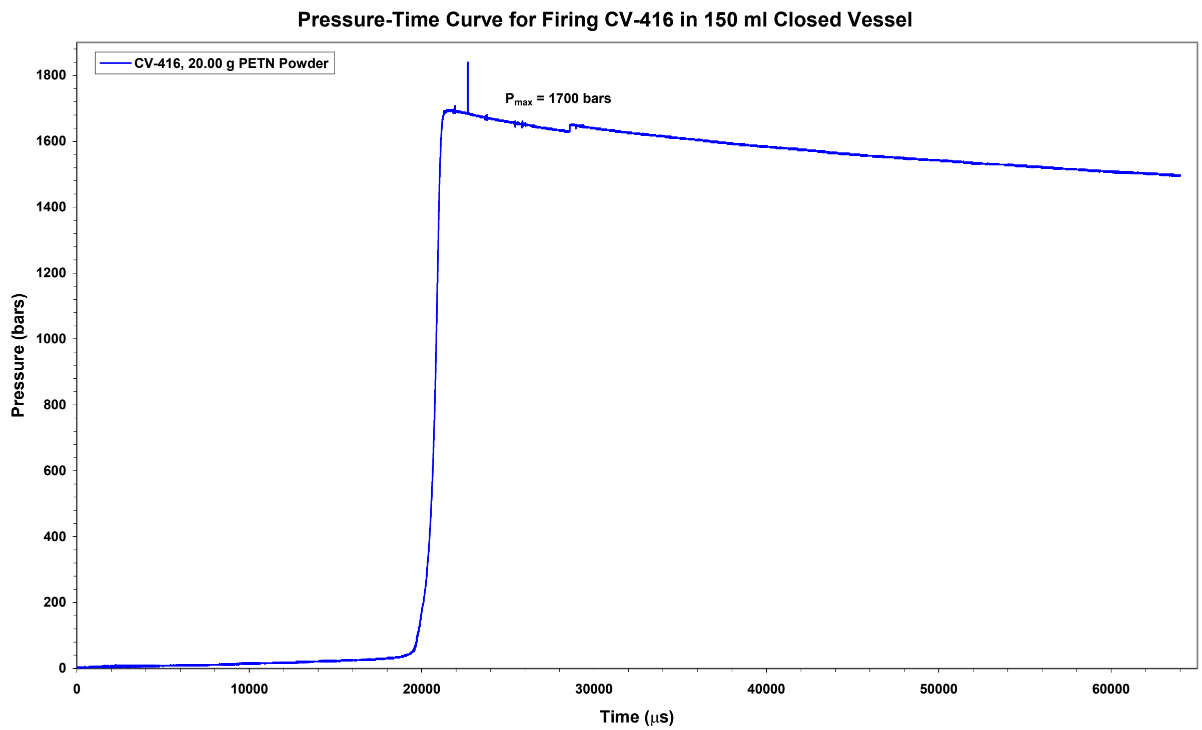

Figure 3.39 Obtained pressure-time curve for firing CV-416 with PETN powder.

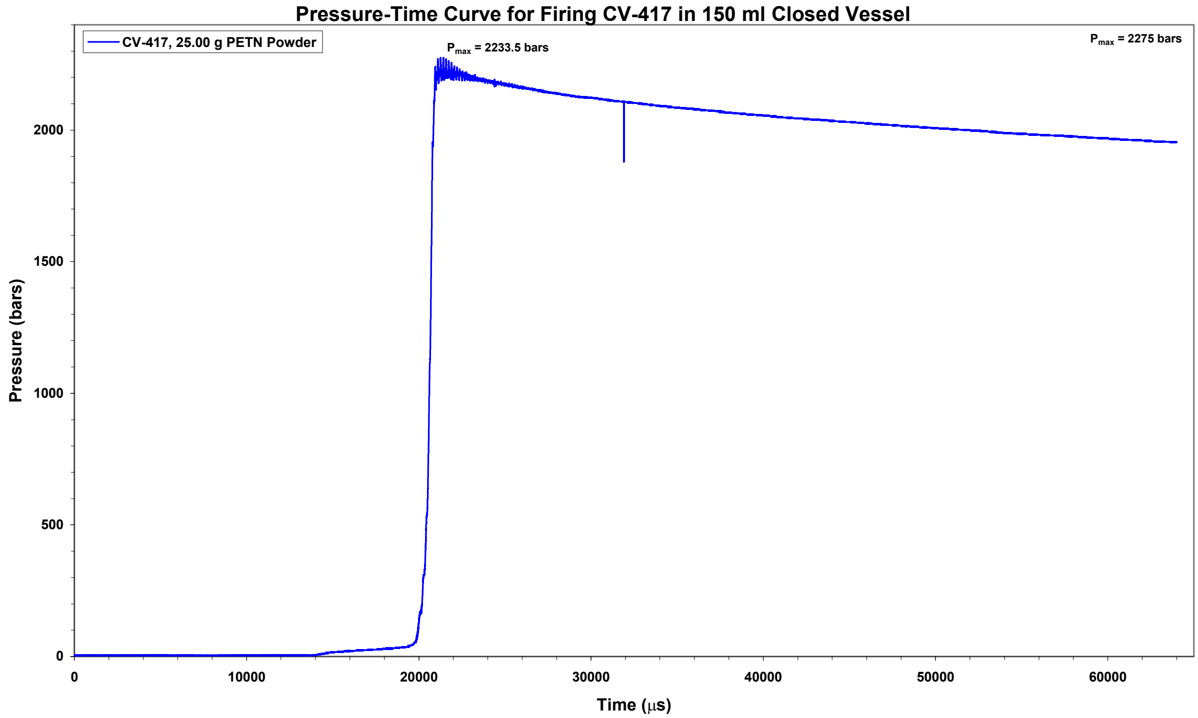

Figure 3.40   Obtained pressure-time curve for firing CV-417 with PETN powder.

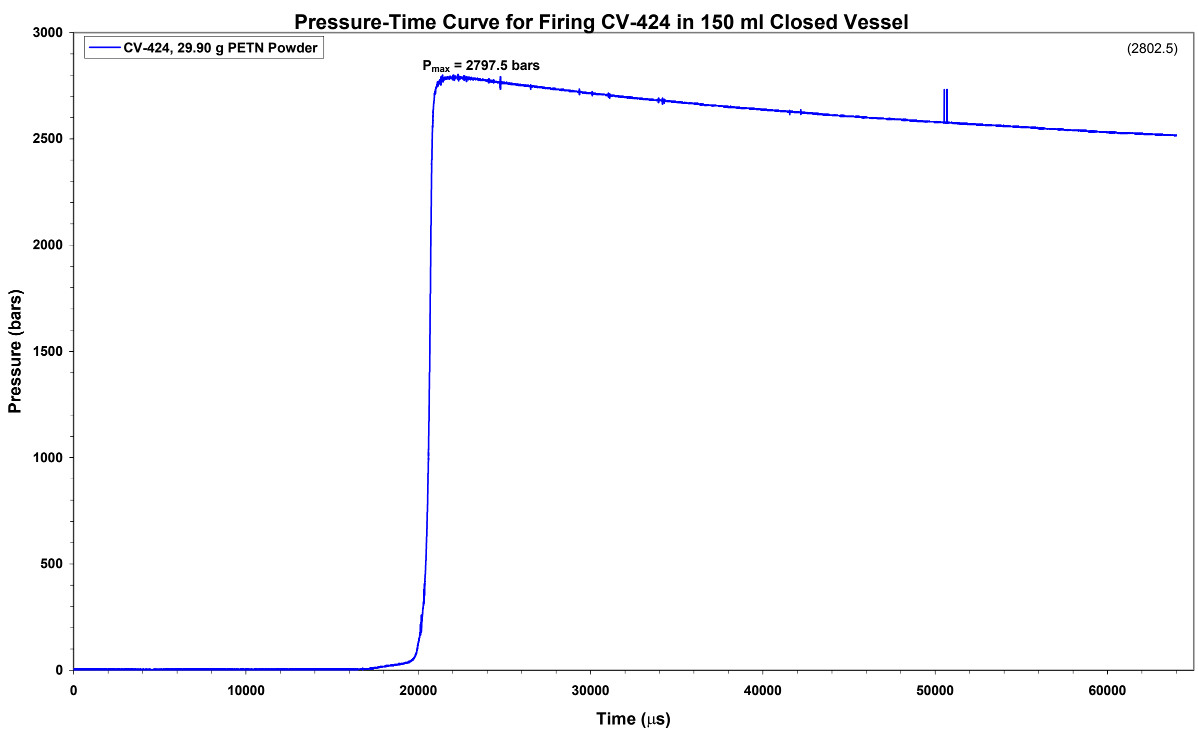

Figure 3.41   Obtained pressure-time curve for firing CV-424 with PETN powder.

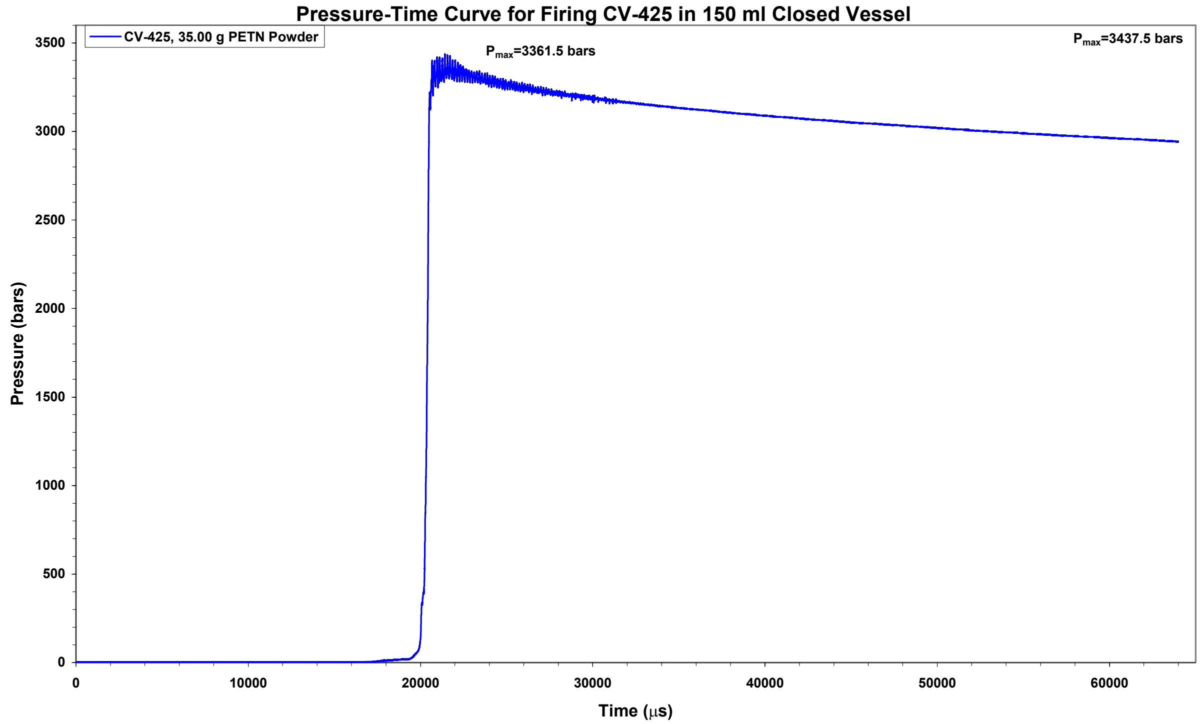

Figure 3.42 Obtained pressure-time curve for firing CV-425 with PETN powder.

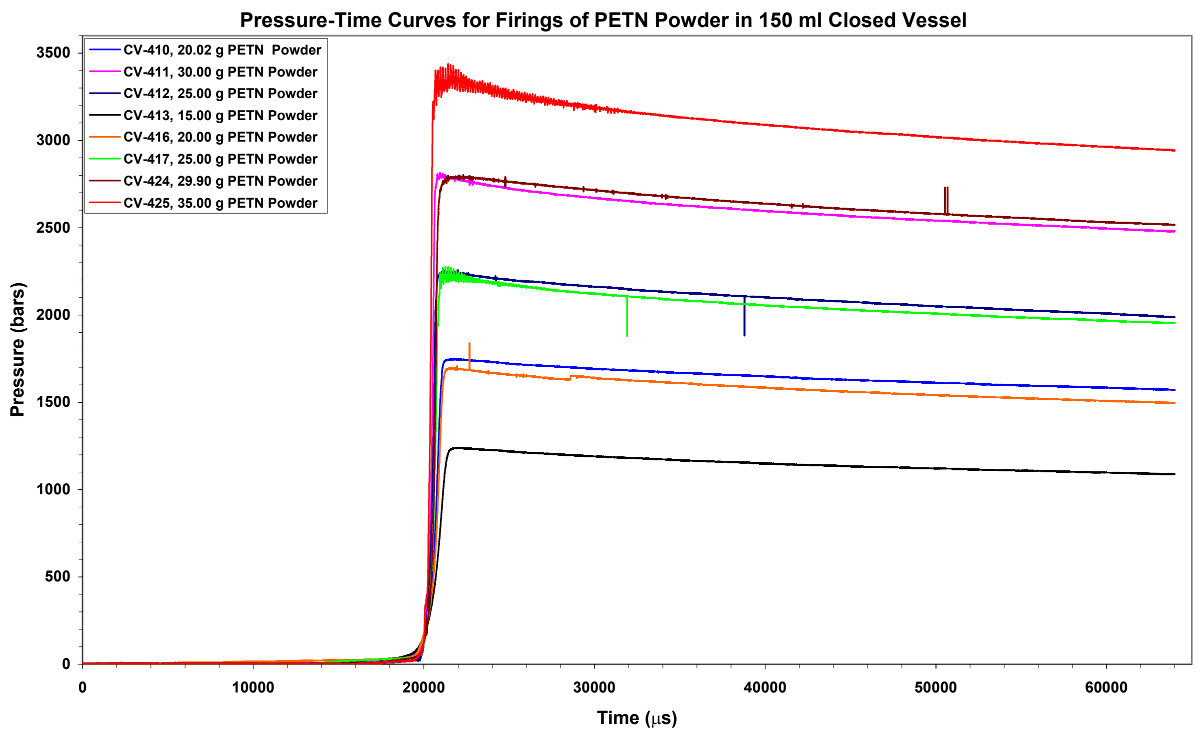

Figure 3.43 Obtained pressure-time curves for all CV firing with PETN powder.

Table 3.8 summaries the experimentally measured maximum pressures for all firings with powder PETN. In addition table 3.8 gives calculated values for P_{max}/LD. In figure 3.44 is

Firing No.	Weight (g)	Loading Density (g/cm^3)	Maximum Pressure (MPa)	P_{max}/LD ($MPa/g/cm^3$)
CV-410	20.02	0.1335	174.90	1310.44
CV-411	30.00	0.2000	281.30	1406.50
CV-412	25.00	0.1667	225.05	1350.30
CV-413	15.00	0.1000	123.90	1239.00
CV-416	20.00	0.1333	170.00	1275.00
CV-417	25.00	0.1667	223.35	1340.10
CV-424	29.90	0.1993	279.75	1403.43
CV-425	35.00	0.2333	336.15	1440.64

Table 3.8 Properties of the CV-firings with PETN powder.

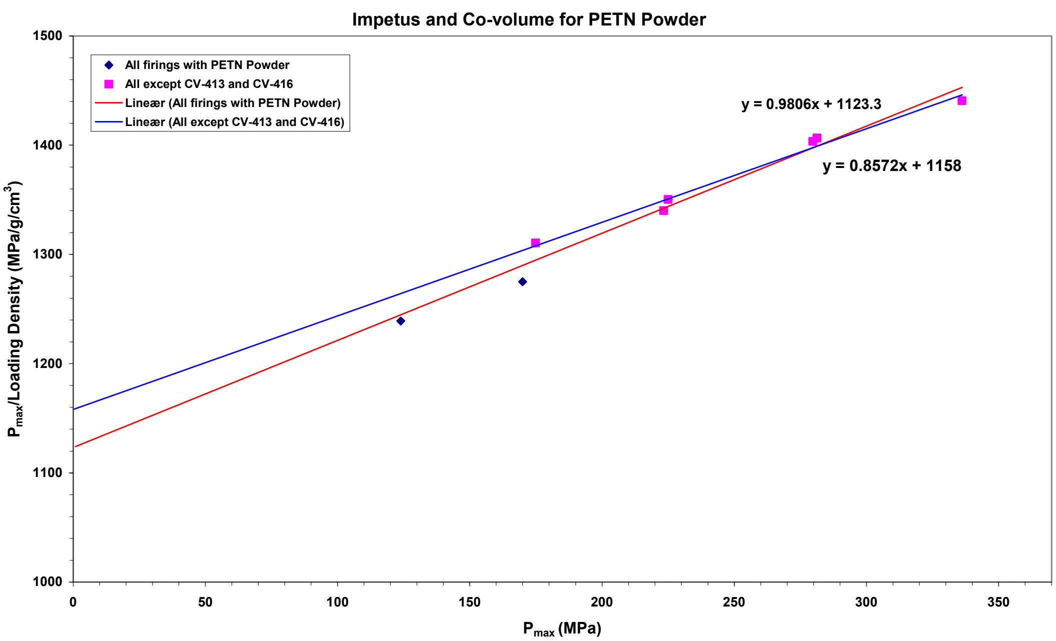

Figure 3.44 Maximum pressure plotted as function of maximum pressure divided by the loading density for PETN powder.

the results in table 3.8 plotted. Including all firings gives an impetus of 1123.3 J/g and a co-volume of 0.9806 cm^3/g. Excluding firing CV-416 due to irregular form of the curve, and firing CV-413 with the lowest loading density, we obtain an impetus of 1158 J/g and a co-volume of 0.8572 cm^3/g.

3.2.2 PETN pellets pressed with 1 GPa

Table 3.9 gives the weight and dimensions of the pellets of PETN that have been pressed with a pressure of 1 GPa. Figure 3.45 shows how the pellets were packed before testing. Figure 3.46 to 3.48 give the pressure-time curves obtained from the firings. Due to the low burn rate or more correctly the low surface area of the pellets of PETN, we lost the maximum pressure for the first firing. The used sampling time of 1 μs was to fast.

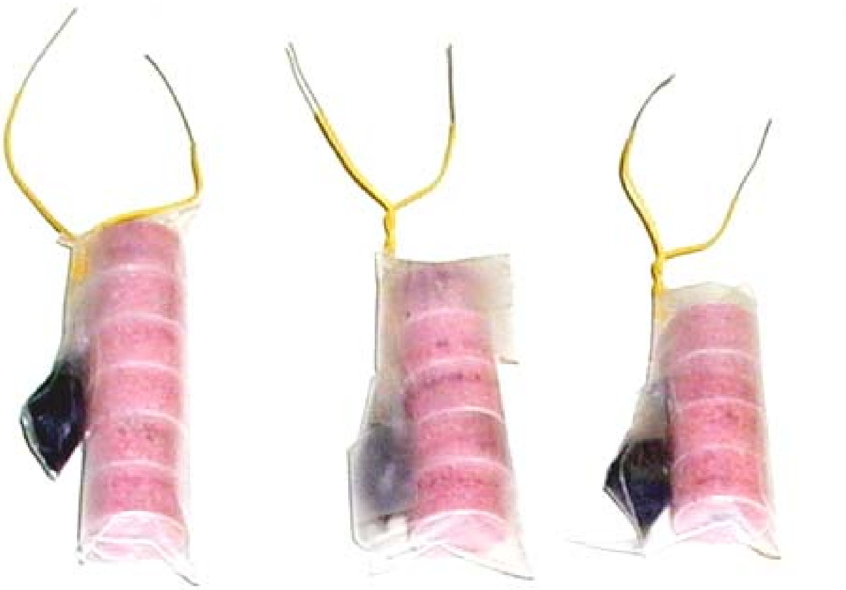

Figure 3.45 Picture of how the high density pellets of PETN were packed for testing in the Closed Vessel.

Pellet No.	Weight (g)	Height (mm)	Volume (cm^3)	Density (g/cm^3)	Firing No. Weight (g)
1	3.7309	9.915	2.2919	1.6279	
2	3.7320	9.900	2.2884	1.6308	CV-434, 18.69
3	3.7310	9.920	2.2931	1.6271	(1-5)
4	3.7354	9.920	2.2931	1.6290	
5	3.7320	9.930	2.2954	1.6259	
6	3.7354	9.860	2.2792	1.6389	
7	3.7346	9.920	2.2931	1.6287	CV-436, 14.94
8	3.7348	9.860	2.2792	1.6387	(6-9)
9	3.7400	9.870	2.2815	1.6393	
10	3.7307	9.920	2.2931	1.6270	
11	3.7319	9.910	2.2907	1.6291	CV-435, 22.42
12	3.7350	9.910	2.2907	1.6305	(10-15)
13	3.7356	9.850	2.2769	1.6407	
14	3.7327	9.900	2.2884	1.6311	
15	3.7389	9.900	2.2884	1.6338	
16	3.7292	9.810	2.2676	1.6445	
17	3.7353	9.830	2.2723	1.6439	CV-441, 18.68
18	3.7334	9.855	2.2780	1.6389	(16-20)
19	3.7334	9.835	2.2734	1.6422	
20	3.7338	9.785	2.2619	1.6508	
Average	3.7338	9.88			
*Diameter 17.16 mm		Average Density		1.6349	

Table 3.9 Properties of PETN pellets pressed with 1 GPa.

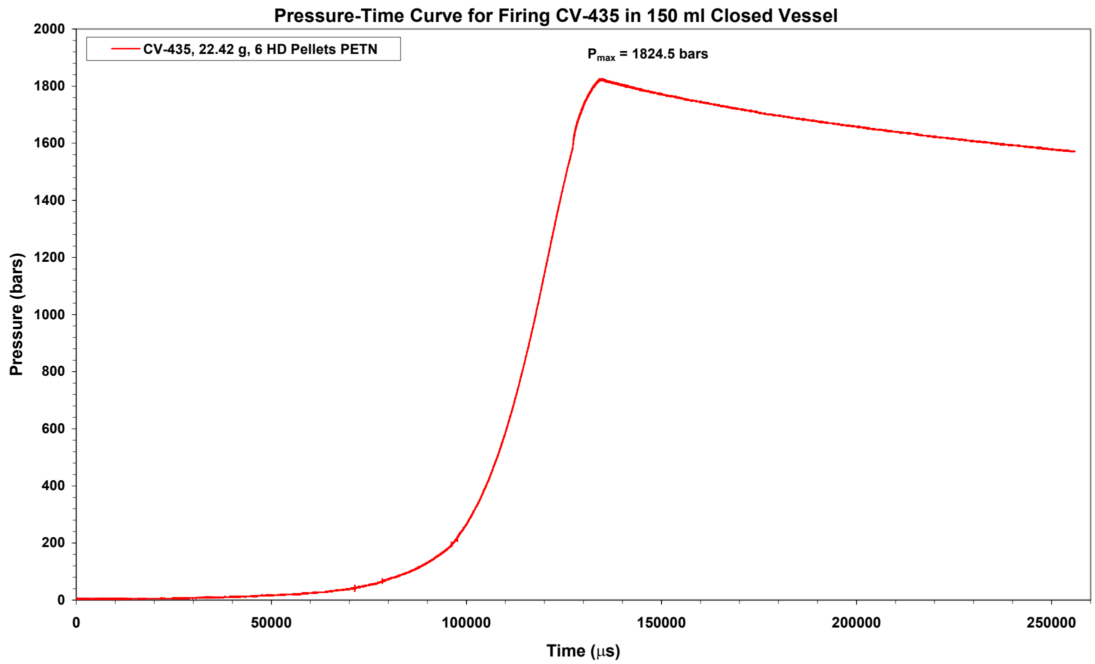

Figure 3.46 Obtained pressure-time curve for firing CV-435 containing PETN pellets.

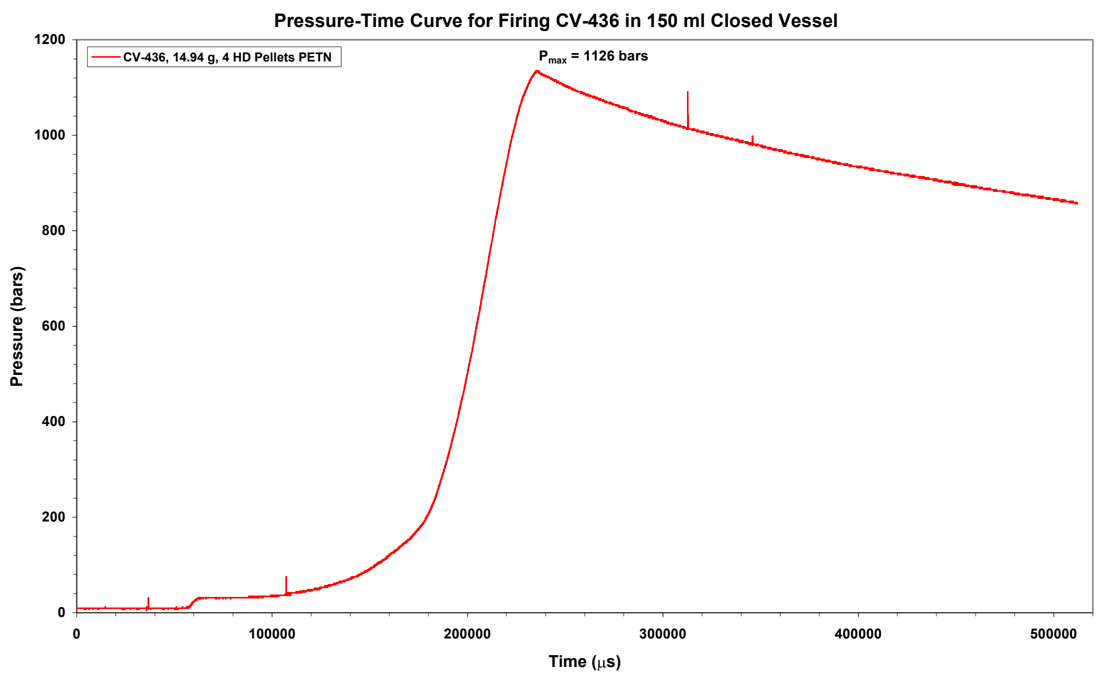

Figure 3.47 Obtained pressure-time curve for firing CV-436 containing PETN pellets.

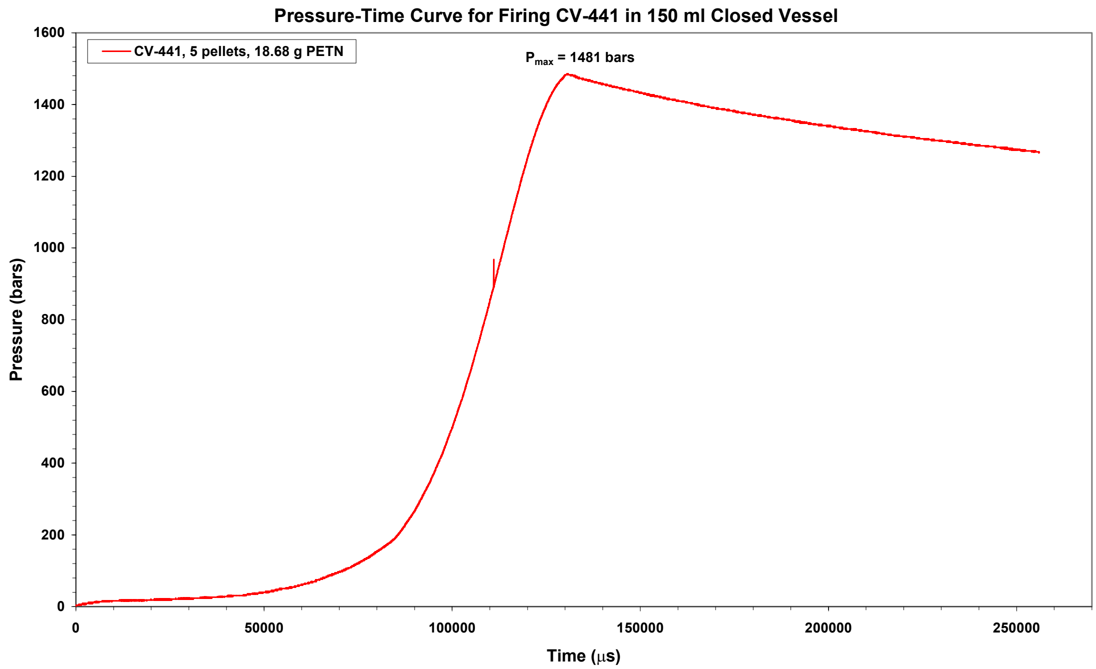

Figure 3.48 Obtained pressure-time curve for firing CV-441 containing PETN pellets.

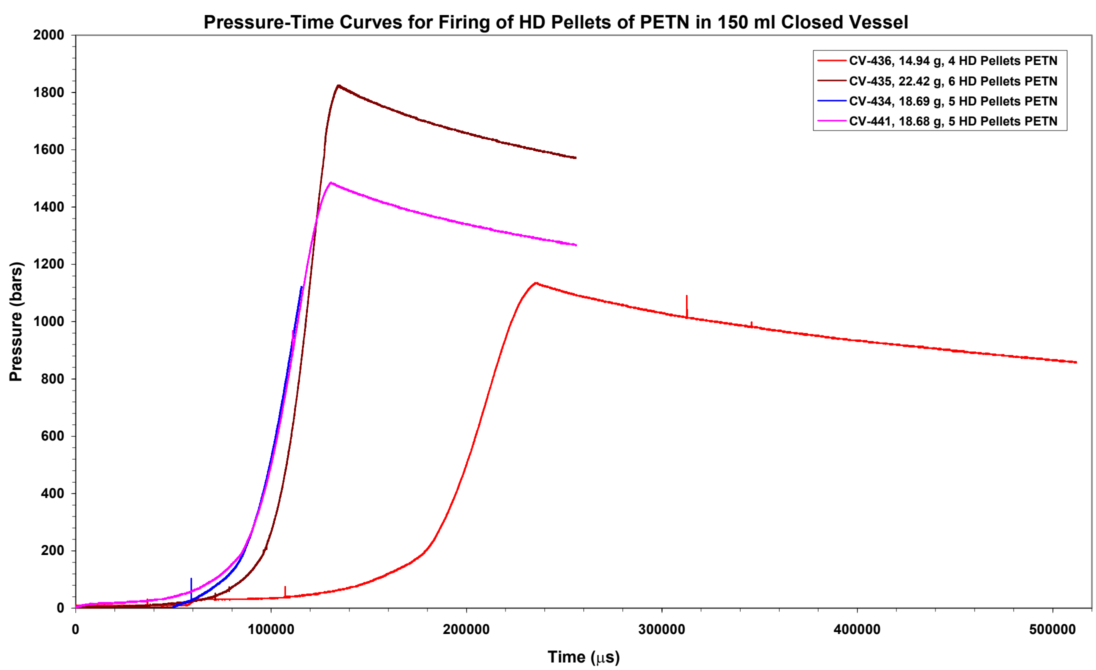

Figure 3.49 Obtained pressure-time curves for firing containing PETN pellets.

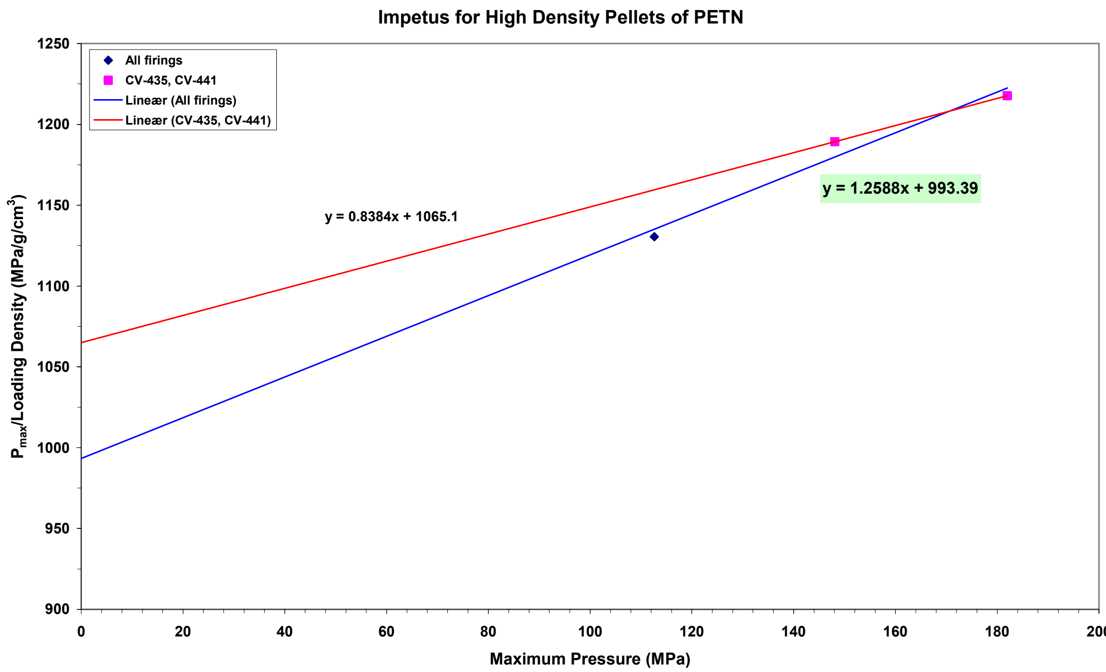

Figure 3.50 Plot of maximum pressure as function of maximum pressure divided by loading density for PETN pellets with high density.

Table 3.10 gives a summary of experimentally measure maximum pressure for the firings given in figure 3.49. In addition table 3.10 gives calculated values for P_{max}/LD. In figure 3.50 is the results in table 3.10 plotted. For impetus we get 1065.1 J/g and co-volume equal to 0.8384 cm^3/g if we use only the two highest loading densities. Due to the slow gas production for the lowest loading density, we have a large heat loss and thereby a lower maximum pressure than expected.

Firing No.	Weight (g)	Loading Density (g/cm^3)	Maximum Pressure (MPa)	P_{max}/LD ($MPa/g/cm^3$)
CV-435	22.42	0.1495	182.0	1217.66
CV-436	14.94	0.0996	112.6	1130.52
CV-441	18.68	0.1245	148.1	1189.24

Table 3.10 Properties of firings of PETN pellets with high density.

3.3 Theoretical calculation by use of CHEETAH

3.3.1 H-764

The thermochemical code CHEETAH 2.0 (1) has been used to calculate theoretical properties of the H-764 composition. Table 3.11 gives a summary of the properties for loading densities up to 1.0 g/cm^3. Table 3.12 gives a summary of obtained experimentally properties for impetus and co-volume from 3.1. The obtained experimentally results show a decreasing impetus as the density of the pellets increase and the surface area decrease. The obtained experimentally impetus is lower than the theoretical calculated. For the co-volume the experimentally results observed have an opposite trend.

In figure 3.51 has experimentally measured pressures for H-764 powder and theoretical calculated pressures been plotted as function of loading density. All experimentally pressures are as expected lower than the theoretical calculated ones.

Rho g/cc	Temperature K	Pressure MPa	Impetus J/g	Mol Wt. Gas	Covol cc/g	Frozen Cp/Cv	Phi
0.05	3810.9	71.1	1342.43	23.603	1.128	1.238	1.060
0.10	3870.4	152.6	1357.18	23.712	1.105	1.236	1.124
0.15	3902.0	244.3	1364.58	23.776	1.081	1.235	1.194
0.20	3922.8	347.1	1369.11	23.824	1.056	1.235	1.268
0.25	3937.9	462.0	1372.04	23.864	1.030	1.237	1.347
0.30	3949.4	589.7	1373.87	23.902	1.003	1.239	1.431
0.35	3958.4	731.0	1374.85	23.939	0.976	1.242	1.519
0.40	3965.4	886.8	1375.05	23.978	0.949	1.245	1.612
0.45	3971.0	1057.6	1374.51	24.021	0.922	1.249	1.710
0.50	3975.2	1243.8	1373.20	24.070	0.896	1.259	1.811
0.55	3978.3	1445.7	1371.03	24.127	0.870	1.259	1.917
0.60	3980.3	1663.2	1367.94	24.193	0.844	1.265	2.026
0.65	3981.3	1895.8	1363.80	24.273	0.819	1.271	2.138
0.70	3981.4	2142.8	1358.51	24.368	0.794	1.277	2.253
0.75	3980.6	2403.0	1351.98	24.481	0.771	1.282	2.370
0.80	3978.8	2674.9	1344.14	24.613	0.747	1.288	2.487
0.85	3976.2	2956.8	1334.99	24.765	0.725	1.294	2.605
0.90	3972.8	3246.7	1324.53	24.939	0.703	1.299	2.723
0.95	3968.5	3542.8	1312.85	25.134	0.682	1.304	2.840
1.00	3963.4	3843.1	1300.06	25.348	0.662	1.308	2.956

Table 3.11 Theoretical calculated properties of H-764 by use of the CHEETAH code.

Condition	Density (g/cm^3)	Impetus (J/g)	Co-volume (cm^3/g)
Powder		1304.4	0.7634
Pellets	1.6558	1213.9	0.9938
Pellets	1.7489	1183.2	1.1094
Pellets	1.7853	1138.4	1.4148

Table 3.12 Experimentally determined impetus and co-volumes for H-764 at different conditions of the material.

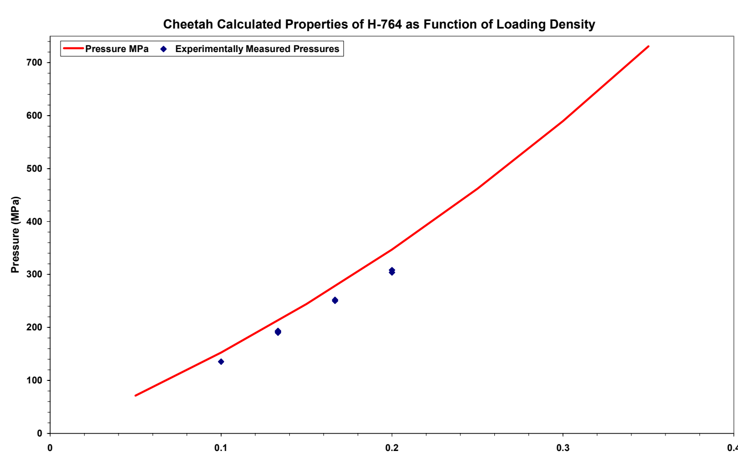

Figure 3.51 In figure 3.51 are experimentally measure pressures for powder and theoretical calculated by Cheetah given as function of loading density.

3.3.2 PETN

Table 3.13 gives theoretical properties calculated by use of the CHEETAH code. Table 3.14 gives the experimentally determined impetus and co-volume for powder and pellets of PETN. Figure 3.52 gives experimentally determined and theoretically calculated pressures as function of loading density for powder PETN .

Rho g/cc	Temperature K	Pressure MPa	Impetus J/g	Mol Wt. Gas	Covolume cc/g	Frozen Cp/Cv	Phi
0.05	3856.8	62.4	1186.90	27.018	0.980	1.207	1.052
0.10	3963.8	133.8	1209.35	27.253	0.963	1.205	1.107
0.15	4030.0	213.7	1222.93	27.400	0.945	1.204	1.165
0.20	4079.4	302.7	1232.94	27.510	0.926	1.204	1.227
0.25	4119.7	401.3	1241.00	27.602	0.907	1.204	1.293
0.30	4154.3	510.2	1247.80	27.682	0.888	1.206	1.363
0.35	4184.8	630.3	1253.74	27.753	0.868	1.207	1.436
0.40	4212.4	762.1	1259.00	27.819	0.848	1.210	1.513
0.45	4237.6	906.4	1263.73	27.881	0.828	1.213	1.594
0.50	4260.9	1063.8	1267.99	27.941	0.808	1.216	1.678
0.55	4282.6	1235.0	1271.83	27.998	0.788	1.219	1.766
0.60	4302.9	1420.6	1275.27	28.055	0.769	1.223	1.857
0.65	4321.8	1621.2	1278.31	28.111	0.750	1.227	1.951
0.70	4339.4	1837.2	1280.93	28.168	0.731	1.232	2.049
0.75	4355.9	2069.0	1283.11	28.226	0.713	1.237	2.150
0.80	4371.1	2316.9	1284.80	28.288	0.695	1.242	2.254
0.85	4385.0	2580.8	1285.93	28.353	0.678	1.247	2.361
0.90	4397.6	2860.6	1286.44	28.423	0.661	1.252	2.471
0.95	4408.9	3155.8	1286.23	28.501	0.645	1.258	2.583
1.00	4418.7	3465.7	1285.21	28.587	0.629	1.263	2.697

Table 3.13 Theoretical calculated properties of PETN by use of the CHEETAH code.

Condition	Density (g/cm^3)	Impetus (J/g)	Co-volume (cm^3/g)
Powder		1158.0	0.8572
Pellets	1.6328	1065.1	0.8384

Table 3.14 Experimentally determined impetus and co-volume for PETN.

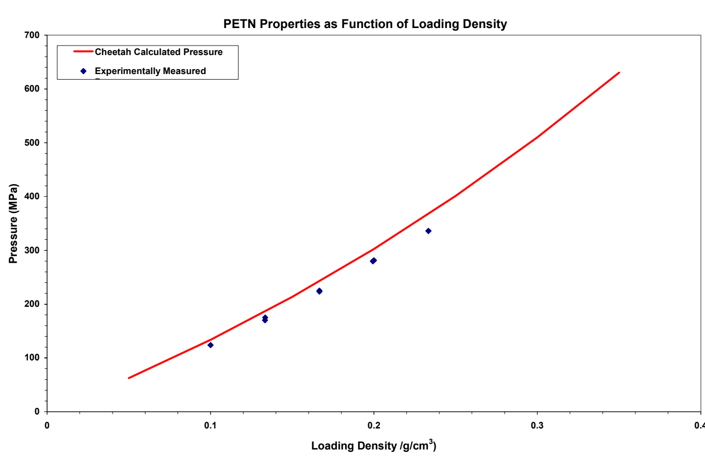

Figure 3.52 Comparison between theoretically calculated and experimentally measured pressures for PETN.

3.4 Burn rate determination

3.4.1 H-764

3.4.1.1 H-764 Powder

Burn rate has been calculated for several firings of powder H-764. From figure 3.2 and figure 3.3 one can see that the H-764 powder consist of the crystals used to produce granulate. There are, as normally observed for many compositions for press filling, no agglomeration of the crystals to build grains. The coating is on the surface of single crystals and not on the surface of agglomerated crystals. This makes it easier to determining the surface area available for the burning, which we needed to know to calculate the burn rate. Table 3.15 summaries the most important properties used for the firings we have calculated the burn rates.

Property	CV-378	CV-378b	CV-388	CV-405	CV-428
Test date	23/4-02	23/4-02	25/4-02	3/5-02	1/6-02
Test temperature (°C)	20	20	20	20	20
H-764, Press pressure	Powder	Powder	1900 kg	5700 kg	1 GPa
Loading density (g/cm^3)	0.1471	0.1471	0.1329	0.1327	0.1471
Ignited with squib +	1 g BK	1 g BK	1 g BK	1 g BK	1 g BK
Density (g/cm^3)	1.90	1.90	1.710	1.790	1.790
Co-volume (cm^3/g)	1.00	1.00	1.00	1.00	1.00
Geometry	Powder	Powder	Cylinder	Cylinder	Cylinder
Diameter (mm)	*	0.300	18.63	18.63	17.16
Length (mm)		0.300	11.03	10.46	8.89
Calibration factor	500	500	500	500	500
Sampling time (μs)	1	1	1	1	1
Averaging time (μs)	4	4	20	20	20
P_{max} (bars)	1928	1928	1888	1832	2092

*See table below

Table 3.15 Properties for firings calculated burn rate for.

Diameter (μm)	**Weight %**	**Form factor**		
		a_1	**a_2**	**a_3**
500	40	120	-4800	64000
340	20	176.471	-10380.62	203541.6
200	20	300	-30000	1000000
100	10	600	-120000	8000000
20	10	3000	-3000000	1000000000

Table 3.16 Form factors used for burn rate calculations for H-764 powder.

Table 3.16 gives the crystal distribution obtained from the sieve analysis given by the producer, and which have been used to determining the form factors. In figure 3.53 has this particle distribution and the form factors given in table 3.16 been used to calculate the burn rate for firing CV-378 with H-764 powder. As the figure shows this gives more or less a straight line. We did first try to use only on particle size 300μm, with the properties given in the second column in table 3.15. The burn rate curve we then obtained is given in figure 3.54. This curve is not straight and do give too low burn rate at high pressure. Figure 3.55 gives a comparison between the two different ways for calculation of the burn rate. We did select to use the multi-modal crystal distribution for the determinations of the burn rate for H-764 powder firings. In figure 3.56 to 3.61 is burn rate curves of different firings of H-764 powder given.

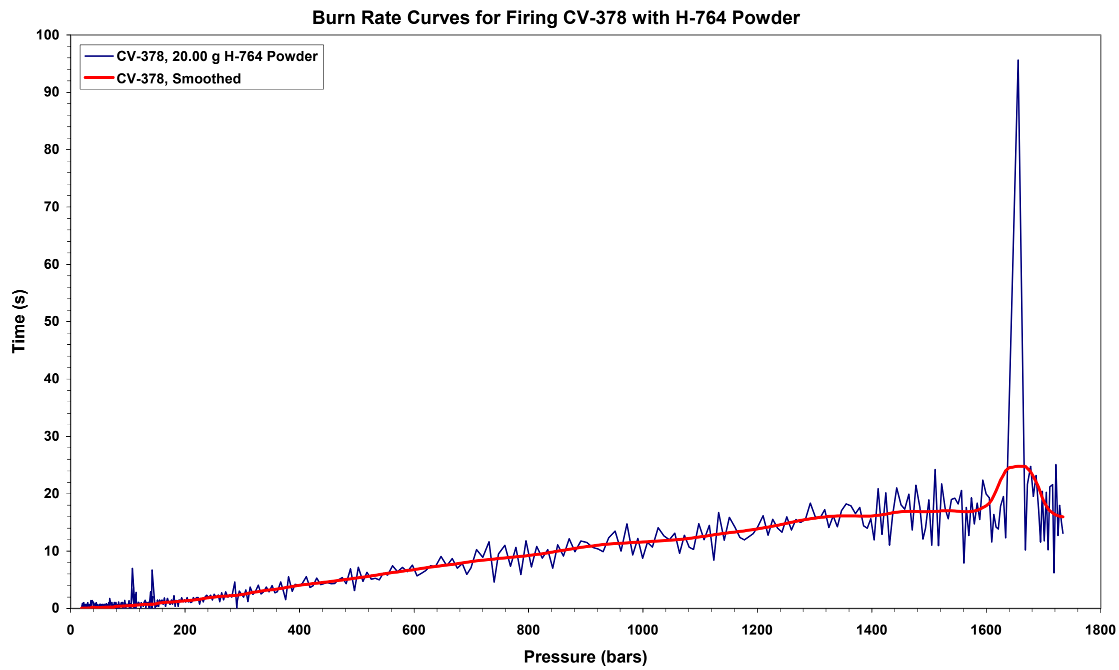

Figure 3.53 Burn rate curves for firing CV-378.

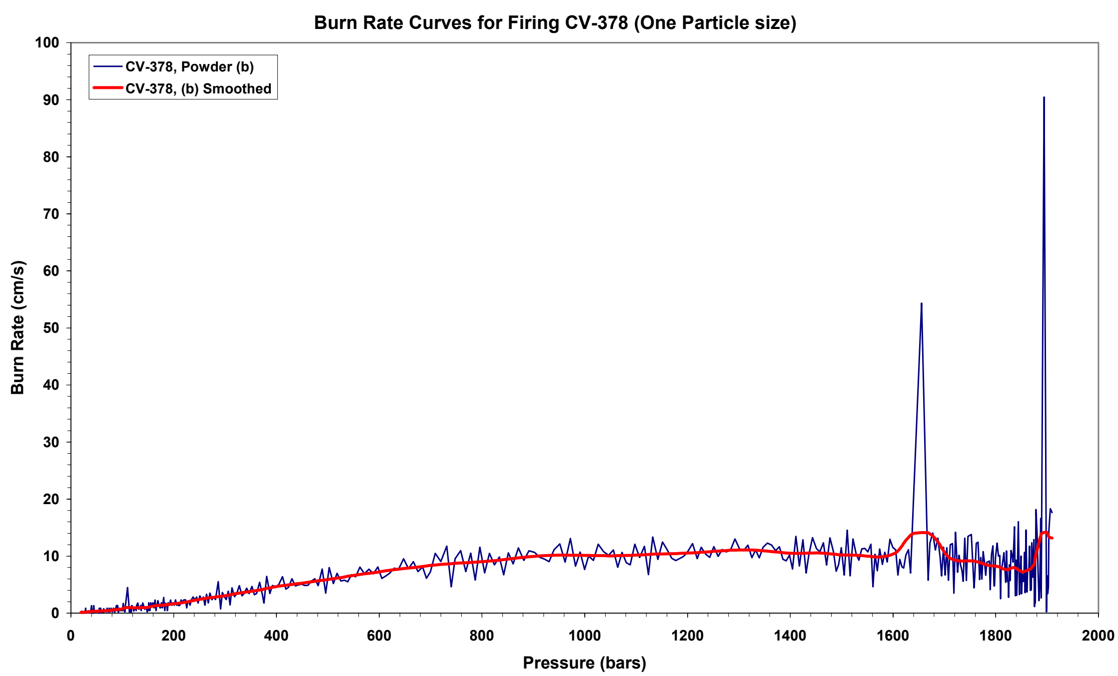

Figure 3.54 Burn rate calculated with CV-378b properties.

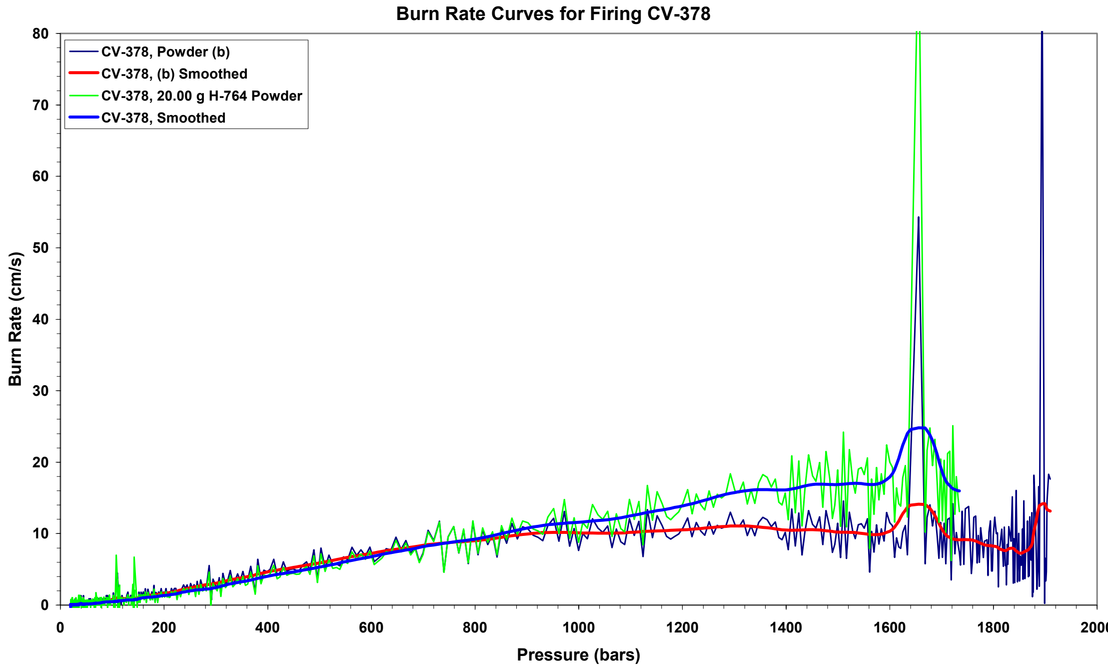

Figure 3.55 Burn rate curves for CV-378 from different powder size.

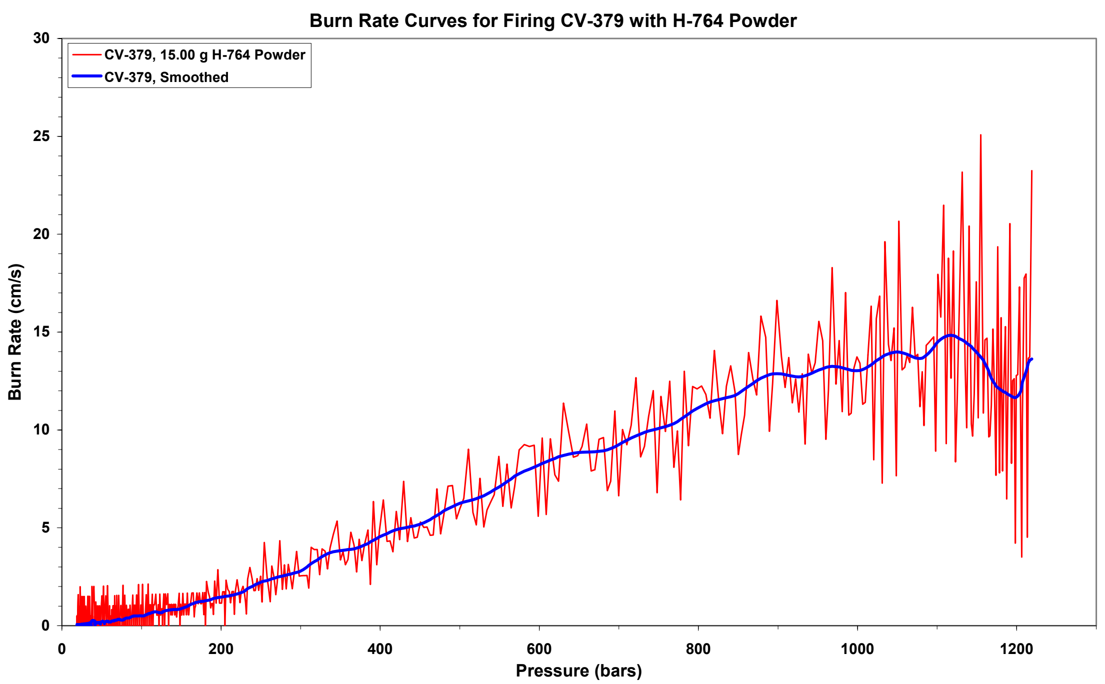

Figure 3.56 Burn rate curves for firing CV-379.

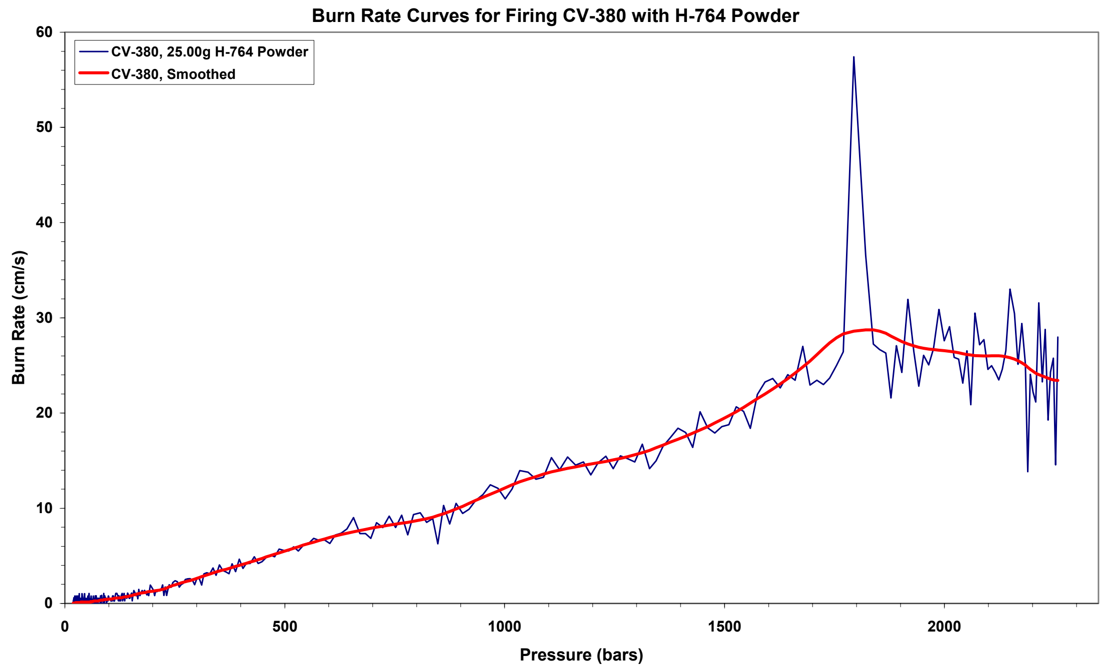

Figure 3.57 Burn rate curves for firing CV-380.

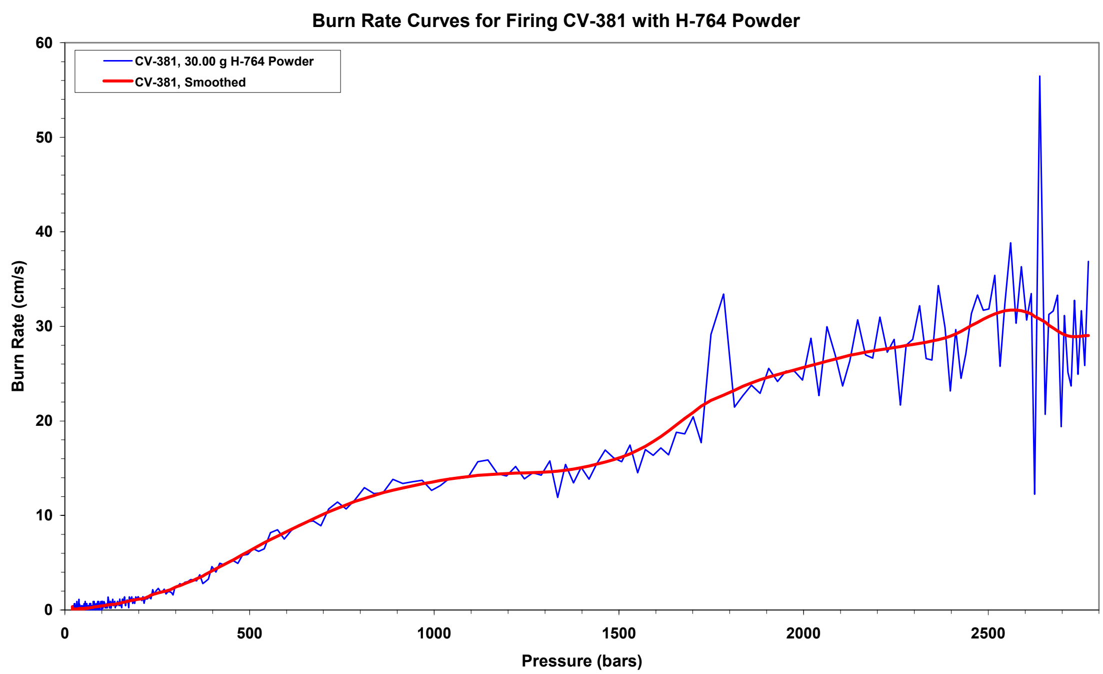

Figure 3.58 Burn rate curves for firing CV-381.

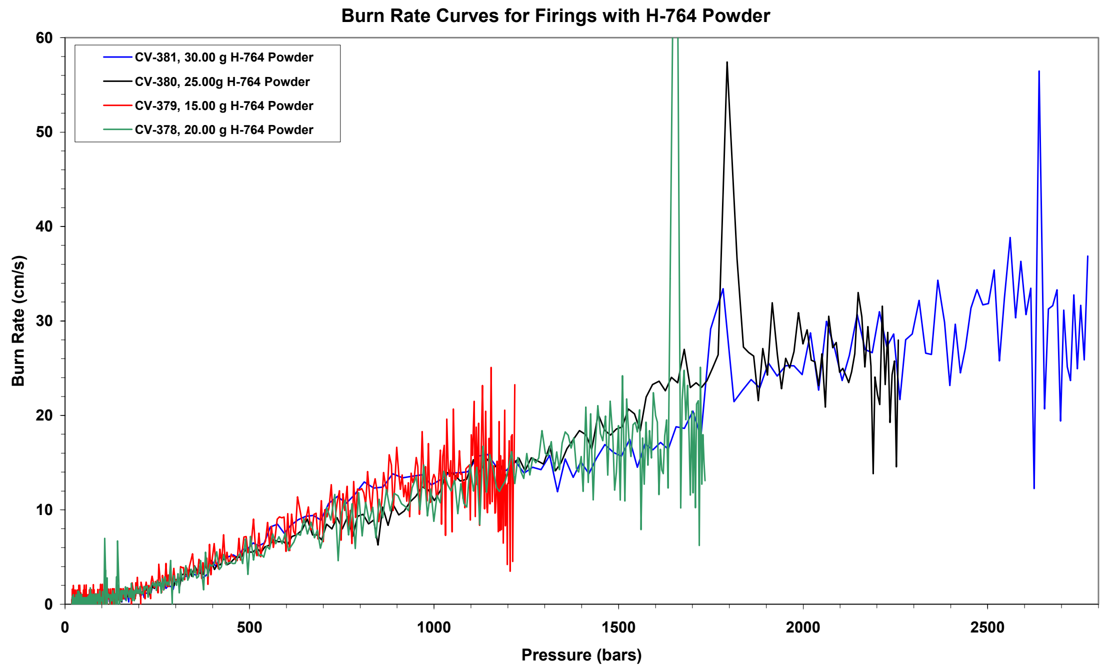

Figure 3.59 Burn rate curves for firings of different loading densities of H-764 powder.

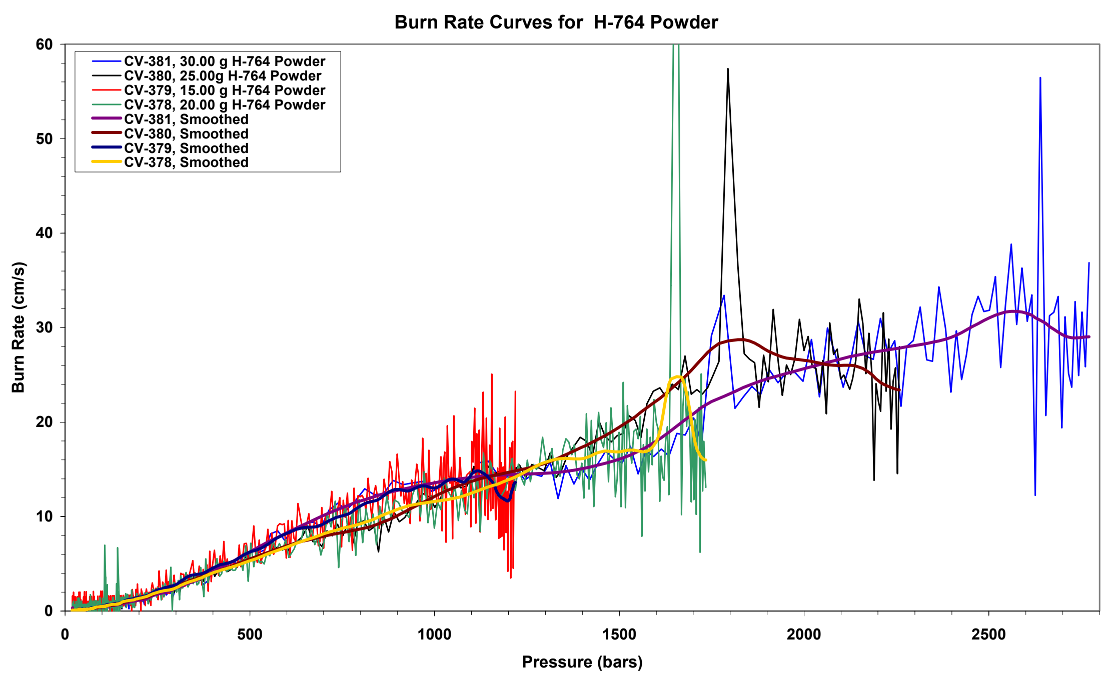

Figure 3.60 Burn rate curves for firings of different loading densities of H-764 powder.

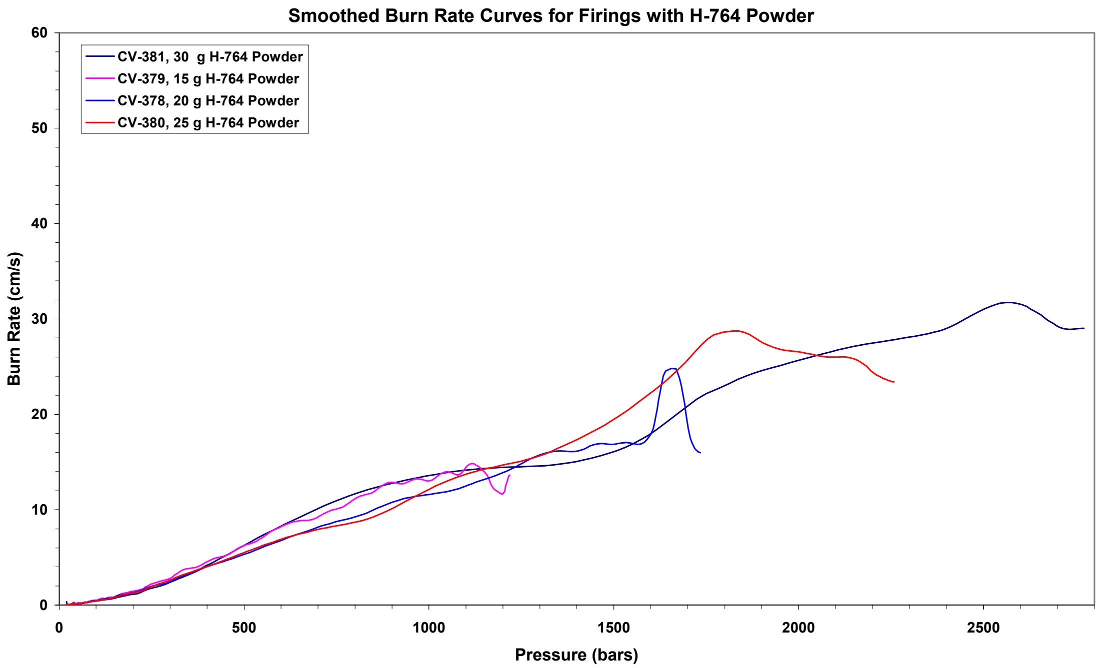

Figure 3.61 Smoothed burn rate curves for firings of different loading densities of H-764 powder.

3.4.1.2 H-764 pellets pressed with 1900kg

Figure 3.62 gives the burn rate curves for firing CV-388, where the surface area is calculated by the properties given in table 3.15. As the figure shows the obtained burn rate curves have not the form of a straight line. The burning take place on a much greater surface area then obtained from the cylindrical pellets. Very soon after ignition the majority of the crystals will have ignited.

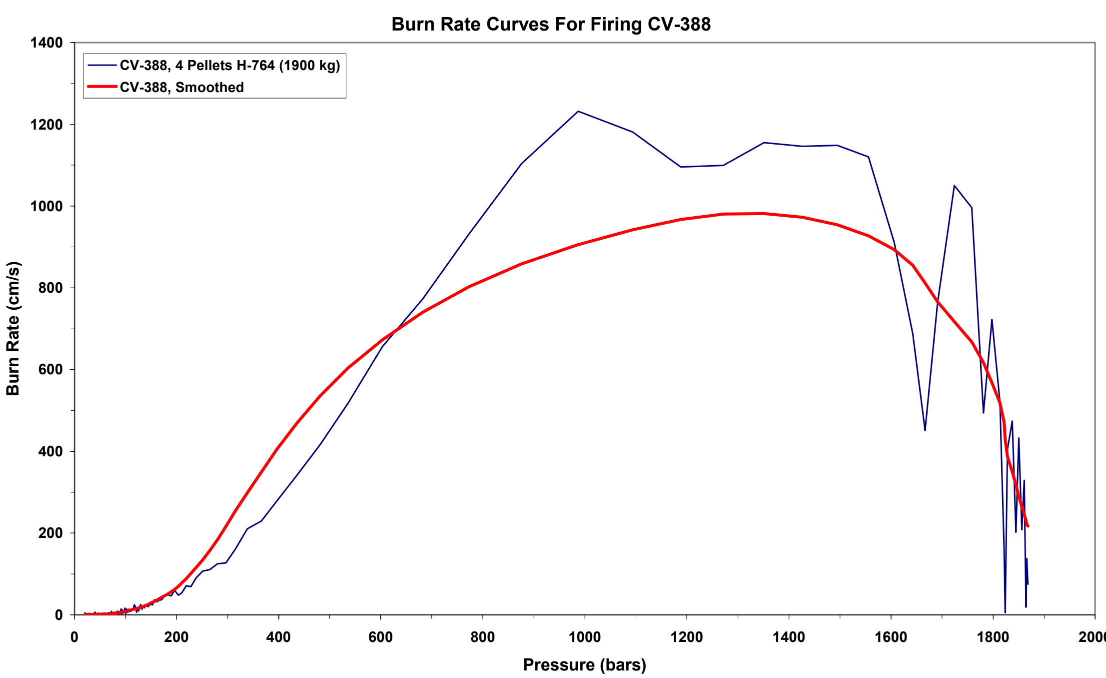

Figure 3.62 Burn rate curves for firing CV-388.

3.4.1.3 H-764 pellets pressed with 5900 kg

In figure 3.63 is given the burn rate curves for pellets pressed with 5900 kg. Compared with the burn rate calculated in figure 3.62 the results are more or less equal. However, it take a bit longer time before every crystals have ignited.

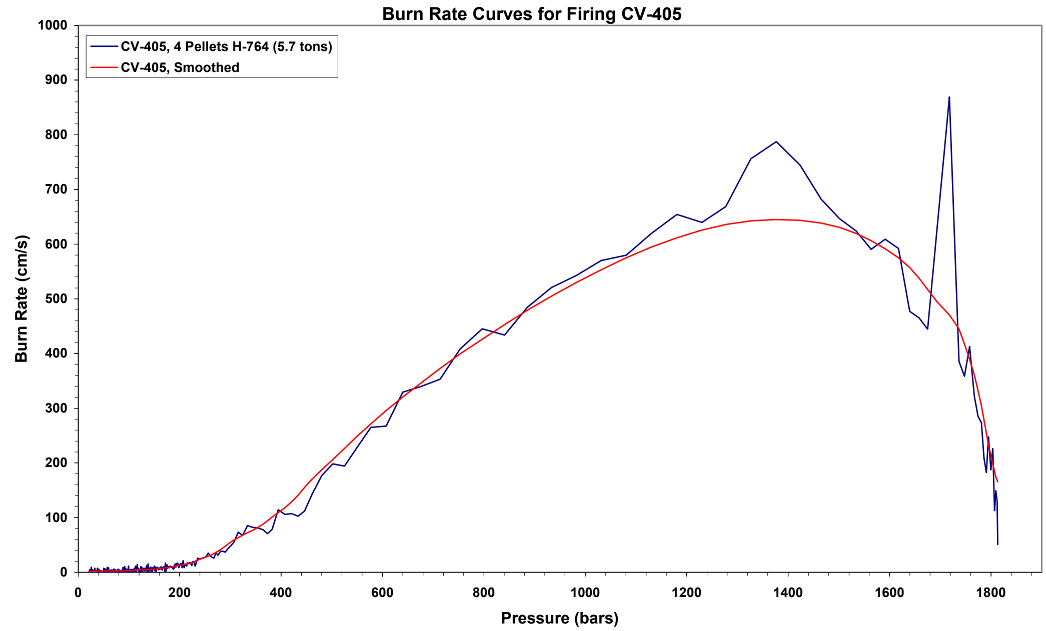

Figure 3.63 Burn rate curves for firing CV-405.

3.4.1.4 H-764 pellets pressed with 1 GPa

Figure 3.64 to 3.66 gives burn rate curves for firings of pellets pressed with a pressure of 1

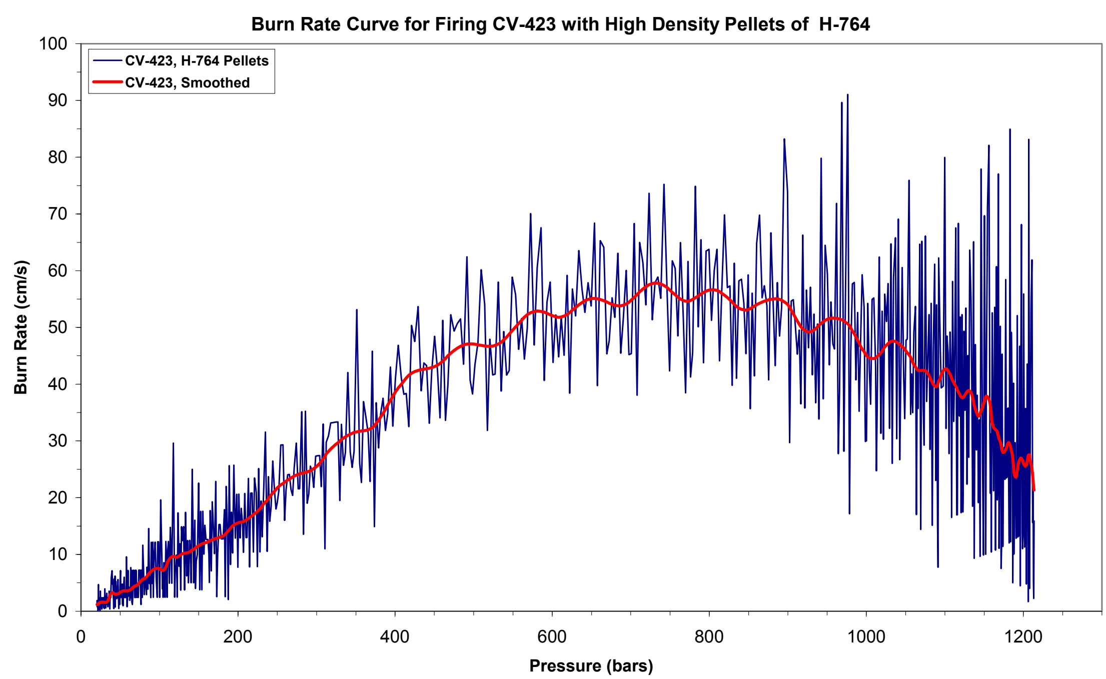

Figure 3.64 Burn rate curve for firing CV-423.

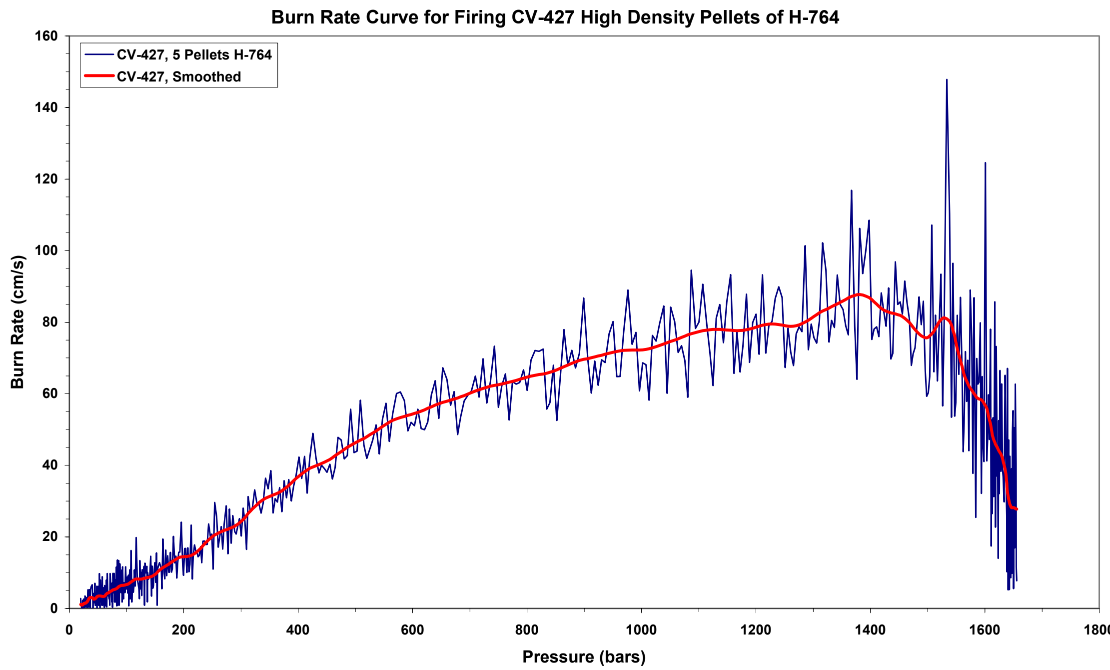

Figure 3.65 Burn rate curve for firing CV-427.

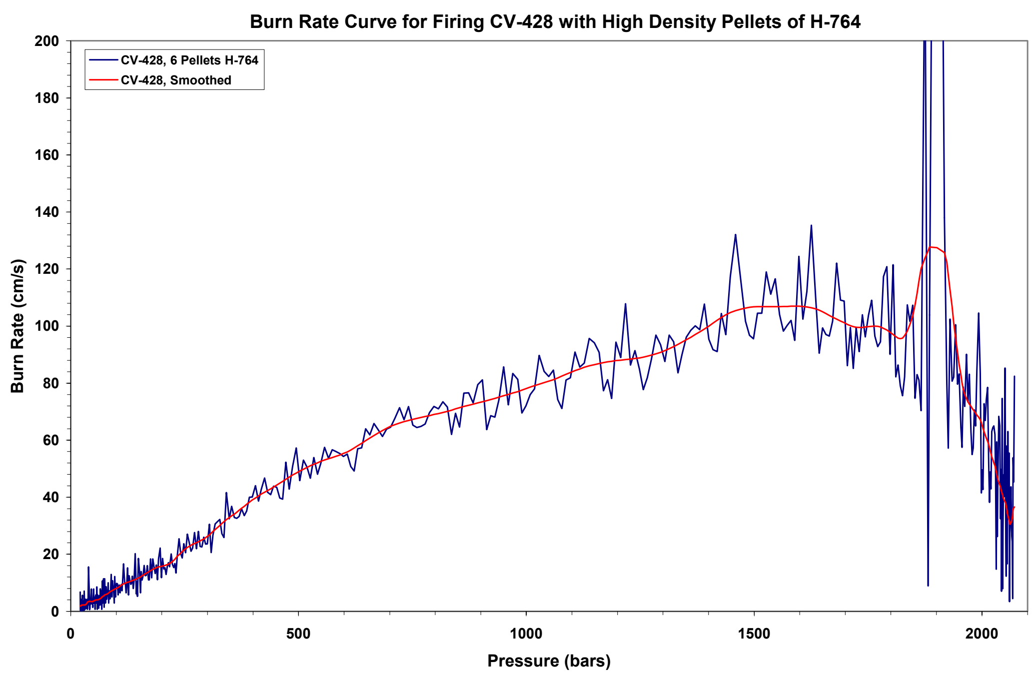

Figure 3.66 Burn rate curve for firing CV-428.

GPa. Compared with the burn rate curves of looser pressed pellets given in figure 3.62 and 363 we see that the burning now follow closer to a straight line, but still not completely and as the pressure increase the curve get flat. There are two interpretations of the obtained burn rate curves, either that the obtained burn rate is too high or the used surface area is too low. The obtained curves in figures 3.64 to 3.66 indicate that both cases can be the situation. The pellets are burning on more than the surface.

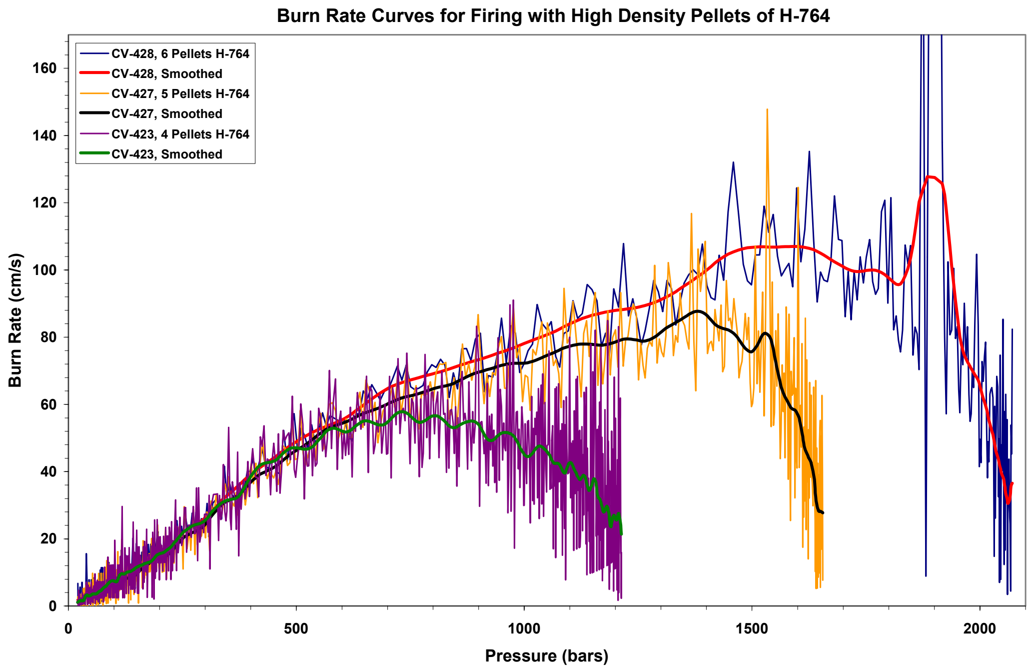

Figure 3.67 Burn rate curves for all firings with H-764 pellets pressed with 1 GPa pressure.

3.4.1.5 Comparison of burn rates for powder and pellets of different densities

Figure 3.68 gives burn rate curves for all different pellet densities and powder. For the pellets pressed with the two lowest press pressure the used dimensions or surface area are clearly wrong and too low. For the samples pressed with 1 GPa we have probably to high burn rate

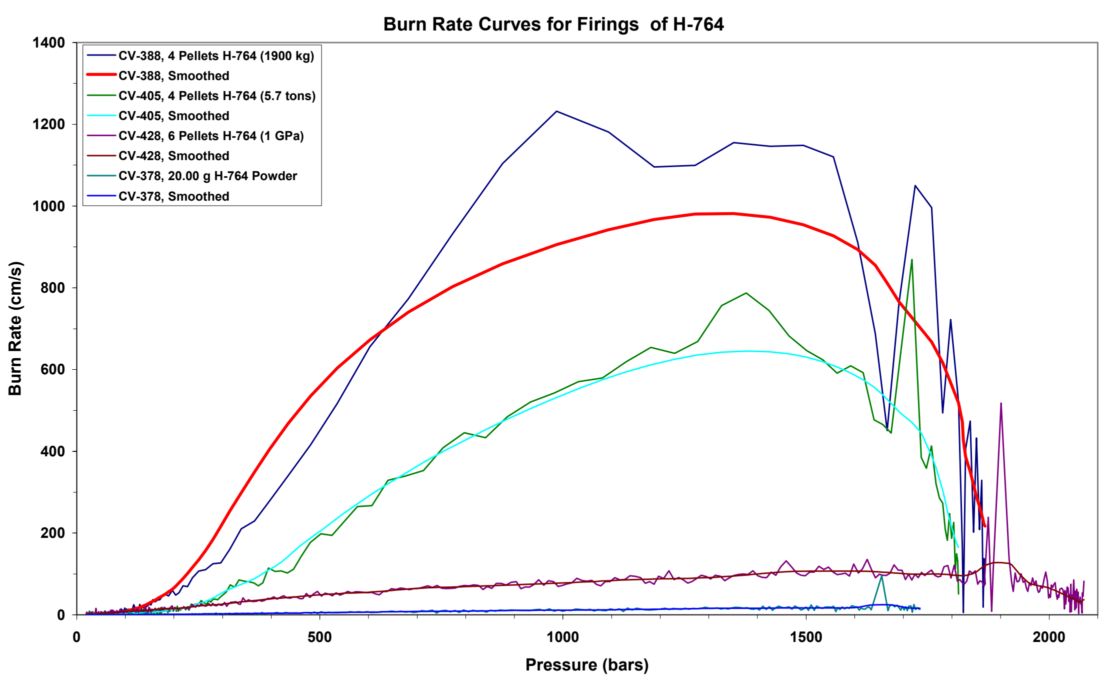

Figure 3.68 Burn rate curves for different pellet densities and powder of H-764.

due to burning also inside the pellets. However as seen from figure 3.68 this contribution is significant lower than for the two lowest densities. The real burn rate for H-764 is most probably what we observe for powder.

3.4.2 PETN

3.4.2.1 Powder

For the powder of PETN we have no sieve analysis, but from the pictures given in figure 3.33 and 3.34 one can see that the particles are relative large. However, they seems not to consist of single crystals but been build up of many small particles. To calculate the burn rate we have used one single particle size 300 µm. Table 3.17 gives all data used in the calculations. The obtained burn rate curve given in figure 3.69, have a slightly too low burn rate in the lower pressure region and a too high burn rate in the upper pressure region. However the obtained burn rate at different pressures are not very different from the burn rate obtained for pellets. A better agreement can be obtained by using a combination of several particle sizes.

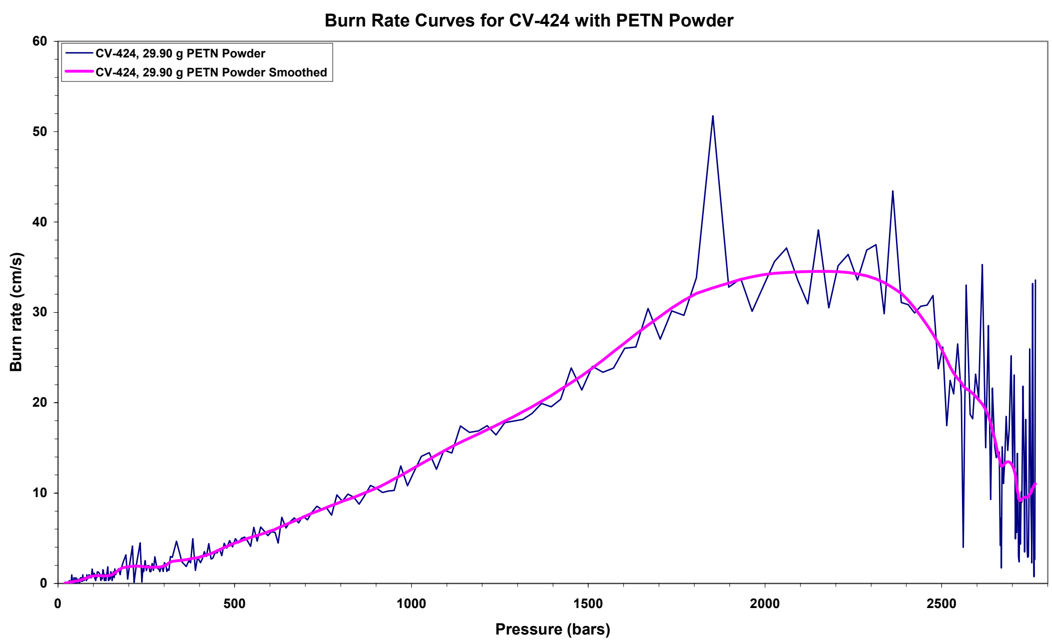

Figure 3.69 Burn rate curve for firing CV-424 with PETN powder.

3.4.2.2 PETN high density pellets

For the pellets of density 1.6349 g/cm^3 are the burn rate curves given in figure 3.70 to 3.72. The properties used to calculate the burn rates are given in table 3.17. From figure 3.70 to 3.72 one will see that the obtained burn rate curves are very straight, indicating that the used surface area of the pellets is correct, and therefore the burning only take place on the surface of the pellets and not on the surface of individual particles.

The burn rate for PETN is not very different from the burn rate of H-764 or HMX under the test conditions we have used.

Property		CV-424	CV-435	CV-436	CV-441
Test date		8/5-02	21/8-02	21/8-02	29/8-02
Test temperature	(^oC)	25	25	25	25
PETN, Press pressure		Powder	1 GPa	1 GPa	1 GPa
Loading density	(g/cm^3)	0.1993	0.1499	0.0996	0.1245
Ignited by squib +		1 g BK	1 g BK	1 g BK	1 g BK
Density	(g/cm^3)	1.76	1.63	1.63	1.63
Co-volume	(cm^3/g)	1.00	1.00	1.00	1.00
Geometry		Cylinder	Cylinder	Cylinder	Cylinder
Diameter	(mm)	0.300	17.16	17.16	17.16
Length	(mm)	0.300	9.91	9.91	9.91
Calibration factor		500	500	500	500
Sampling time	(µs)	1	4	8	4
Averaging time	(µs)	4	80	80	80
P_{max}	(bars)	2795	1820	1126	1481
Form factor	a_1	200	4.349	4.349	4.349
	a_2	-13333.33	-6.063	-6.063	-6.063
	a_3	296296.3	2.742	2.742	2.742
Web	(mm)	0.300	9.91	9.91	9.91

Table 3.17 Properties used in the calculation of burn rate for different firings with PETN.

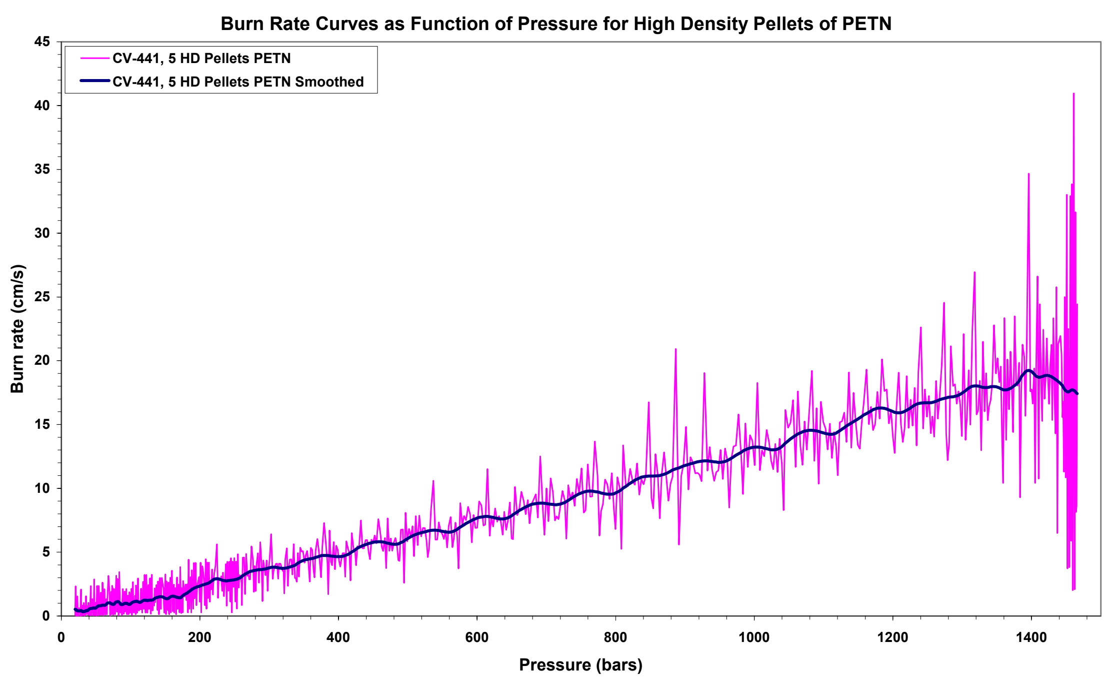

Figure 3.70 Burn rate curves for firing CV-441.

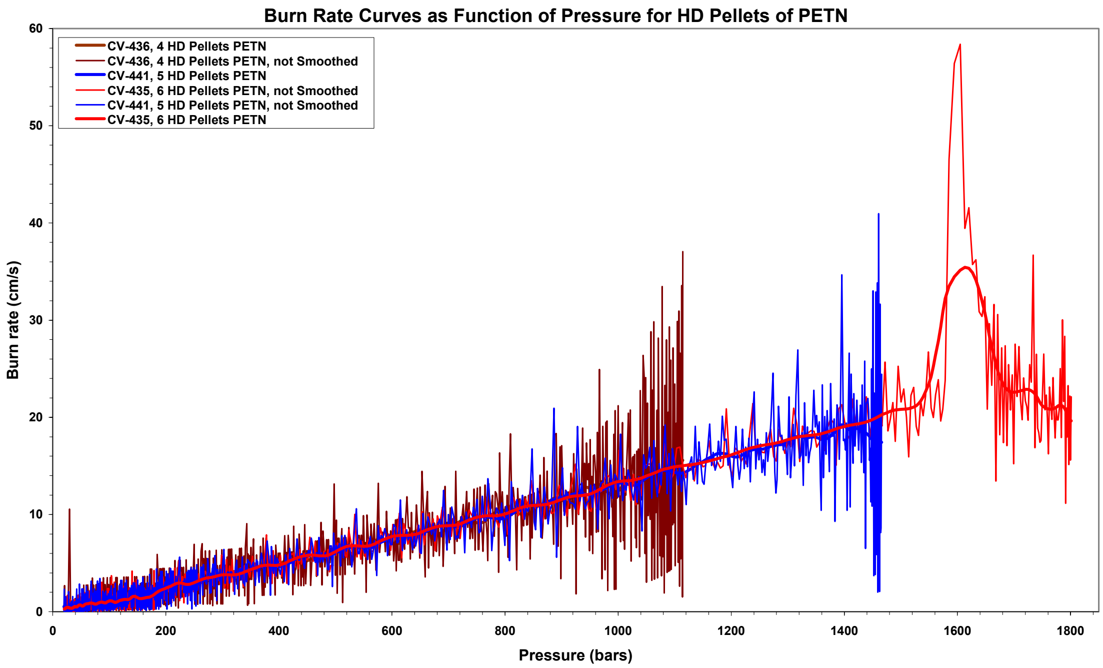

Figure 3.71 Burn rates curves for pellets with high density of PETN.

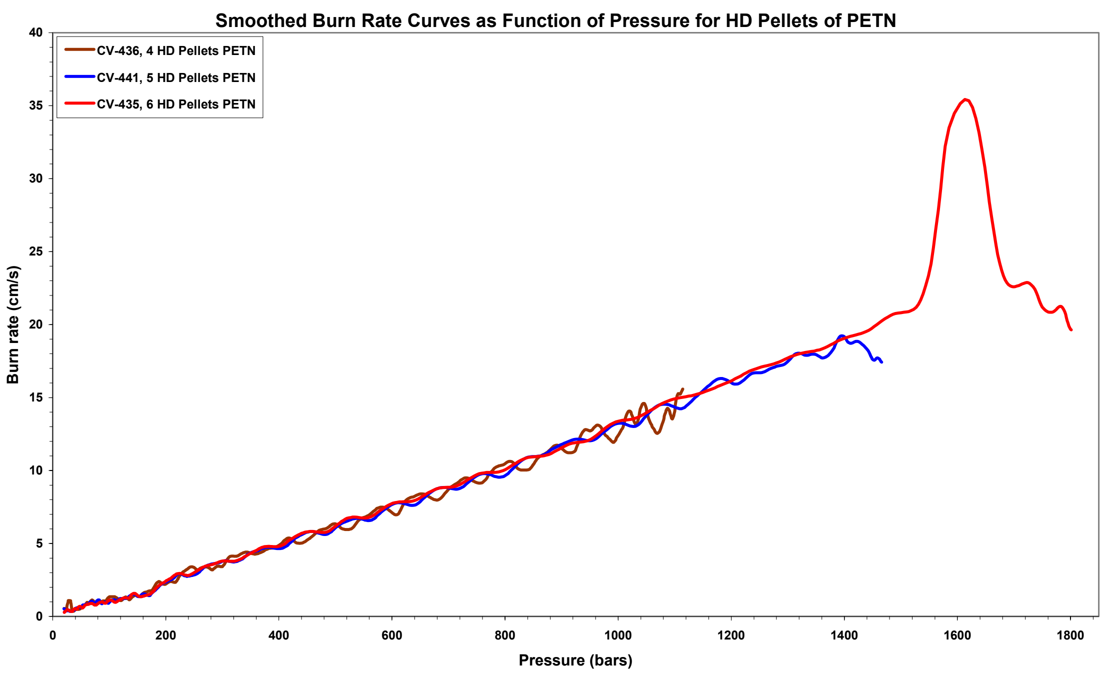

Figure 3.72 Smoothed burn rates curves for pellets with high density of PETN.

3.4.2.3 Comparison of burn rates of PETN

In figure 3.73 is given a comparison between power and pellet burn rates of PETN. As explained in 3.4.2.1 the curve for powder can bee optimised by using several particle sizes. However we can conclude that the burn rate is the same for both test conditions.

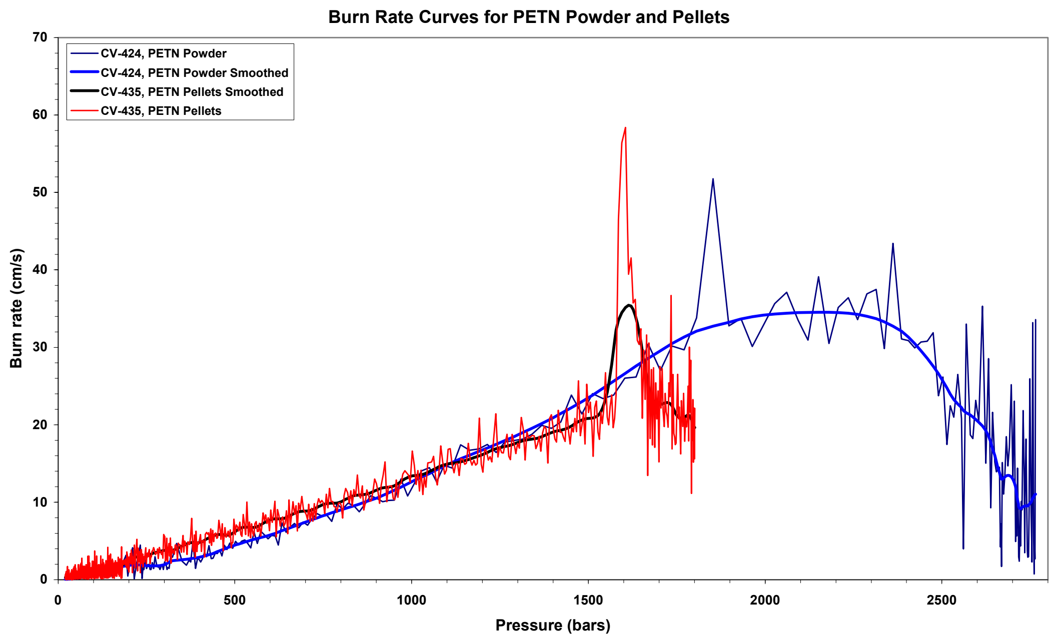

Figure 3.73 Burn rate curves for powder and pellets of PETN.

4 SUMMARY

H-764 and PETN have been studied in closed vessel for determination of burning properties. For both compositions have in addition to powder also pellets of different densities been tested. For H.764 has three different pellet densities been tested with the purpose to see if it was possible to say anything about how the pellets do burn. Did they burning only on the surface or did the fire also spread to inside the pellets. For PETN only one pellet density was tested. In addition to burning properties has impetus and co-volume been determined experimentally for both H-764 and PETN.

H-764 powder has a burn rate as expected for HMX. Due to it contains relative small crystals and thereby has a relative large surface area, we obtain a relative fast consumption of the material and thereof pressure rise in the bomb. For pellets with increasing density the burning time increase. For the pellets of lowest density it take very short time for the flame to ignite every crystal also those inside the pellets. For the highest pellet density we have initially only burning on the surface of the pellets, but after some time it also spread to inside the pellets. Since H-764 contain relatively small amount of binder it's very difficult to press pellets with density close to the TMD, therefore pellets of H-764 will normally contain pores and voids. In practical filling of MP-ammunition it may be difficult to get a void or pore free filling.

PETN pellets pressed to a density of 1.63 g/cm^3 burn in the closed vessel only on the surface of the pellets. The burn rate of PETN is slightly lower than for H-764 (HMX).

For both H-764 and PETN the experimentally determined pressure, impetus and co-volume are lower than theoretically calculated. The difference between experimentally determined properties and theoretically calculated increase as the density of pellets increase. The explanation for this observation is mainly heat loss to the closed vessel due to longer burn time.

Appendix

A CONTROL REPORT FOR H-764

DYNO
Forsvarsprodukter

KONTROLLRAPPORT B
etter 10204 - 3.1 B

Kjøper/Mottaker Forsvarets Forkningsinstitutt Avd. for våpen og matriell Postboks 25, 2007 Kjeller	Bestillingsnummer Etter avtale Bestillingsdato 05.04.02	Rapport nummer 159 Kontroll dato 09.04.02
Produsent Dyno Nobel ASA N-3476 Sætre NORGE	Produksjonsdato 13.03.02	Offentlig oppdragsnummer
Lot nummer	Mengde 2 kg	
Sprengstofftype **H-764**	Leveringsbetingelser/Teknisk underlag Dyno Spesifikasjon 366-K-146, utgave 1	

Analyseresultater for loten

	Sammensetning			Kornfordeling		Fuktighet og flyktige bestanddeler
	HMX	Calciumresinate	Grafitt	Gjennom USSS nr. 18	På USSS nr. 50	
KRAV	≤ 98,0 %	≤ 1,0 %	≤ 1,0 %	100 %	Hovedmengde	≤ 0,1 %
RESULTAT 02/02	99,1	0,4	0,5	100	27	0,01

Kvalitetssjef

DYNO
Defence Products
Manager QA

Figure A. 1 Control report for H.764 used in the study.

B THEORETICAL CALCULATIONS

B.1 H-764

```
The Composition

Name      % wt.   % mol% vol.  Heat of  Standard   Standard    Mol.  Formula
                              formation  volume    entropy     wt.
                               (cal/mol) (cc/mol) (cal/K/mol)
hmx        98.00 79.59 97.35    17866     155.46   0.000    296.16  c4h8n8o8
graphite   1.00 20.03  0.90        0       5.72   0.000     12.01  c1
resinat    1.00  0.38  1.75   -23901     580.75   0.000    627.20 c40h58o4mg1

Heat of formation =     58.738 cal/gm
Standard volume   =      0.528 cc/gm
Standard entropy  =      0.000 cal/k/gm
Standard energy   =     58.725 cal/gm

The elements and percent by mole
     c            15.460
     h            28.800
     n            27.828
     o            27.895
     mg            0.017
The average mol. wt. = 240.524 g/mol
Input>composition, HMX, 98, graphite, 1, resinat, 1, weight
                                The Composition

Name      % wt.   % mol% vol. Heat of  Standard   Standard    Mol.   Formula
                             formation  volume     entropy    wt.
                              (cal/mol) (cc/mol)  (cal/K/mol)
hmx        98.00 79.59 97.35  17866     155.46   0.000     296.16  c4h8n8o8
graphite   1.00 20.03  0.90      0       5.72   0.000      12.01  c1
resinat    1.00  0.38  1.75 -23901     580.75   0.000     627.20  c40h58o4mg1

Heat of formation =     58.738 cal/gm
Standard volume   =      0.528 cc/gm
Standard entropy  =      0.000 cal/k/gm
Standard energy   =     58.725 cal/gm

The elements and percent by mole
     c            15.460
     h            28.800
     n            27.828
     o            27.895
     mg            0.017
The average mol. wt. = 240.524 g/mol
Input>gun, 0.050000, 0.050000, 2.500000
GUN calculation:


     Rho     Temp   Pressure  Impetus  Mol Wt.  Covol  Frozen    Phi
     g/cc     K       MPa       J/g     Gas      cc/g  Cp/Cv
 1.)  0.0500  3810.9    71.1  1342.43  23.603   1.128   1.238   1.060
 2.)  0.1000  3870.4   152.6  1357.18  23.712   1.105   1.236   1.124
 3.)  0.1500  3902.0   244.3  1364.58  23.776   1.081   1.235   1.194
 4.)  0.2000  3922.8   347.1  1369.11  23.824   1.056   1.235   1.268
 5.)  0.2500  3937.9   462.0  1372.04  23.864   1.030   1.237   1.347
 6.)  0.3000  3949.4   589.7  1373.87  23.902   1.003   1.239   1.431
 7.)  0.3500  3958.4   731.0  1374.85  23.939   0.976   1.242   1.519
 8.)  0.4000  3965.4   886.8  1375.05  23.978   0.949   1.245   1.612
```

9.)	0.4500	3971.0	1057.6	1374.51	24.021	0.922	1.249	1.710
10.)	0.5000	3975.2	1243.8	1373.20	24.070	0.896	1.254	1.811
11.)	0.5500	3978.3	1445.7	1371.03	24.127	0.870	1.259	1.917
12.)	0.6000	3980.3	1663.2	1367.94	24.193	0.844	1.265	2.026
13.)	0.6500	3981.3	1895.8	1363.80	24.273	0.819	1.271	2.138
14.)	0.7000	3981.4	2142.8	1358.51	24.368	0.794	1.277	2.253
15.)	0.7500	3980.6	2403.0	1351.98	24.481	0.771	1.282	2.370
16.)	0.8000	3978.8	2674.9	1344.14	24.613	0.747	1.288	2.487
17.)	0.8500	3976.2	2956.8	1334.99	24.765	0.725	1.294	2.605
18.)	0.9000	3972.8	3246.7	1324.53	24.939	0.703	1.299	2.723
19.)	0.9500	3968.5	3542.8	1312.85	25.134	0.682	1.304	2.840
20.)	1.0000	3963.4	3843.1	1300.06	25.348	0.662	1.308	2.956
21.)	1.0500	3957.5	4146.0	1286.31	25.582	0.642	1.312	3.069
22.)	1.1000	3950.9	4450.1	1271.73	25.832	0.623	1.316	3.181
23.)	1.1500	3943.6	4754.0	1256.50	26.096	0.605	1.319	3.289
24.)	1.2000	3935.6	5056.7	1240.76	26.374	0.588	1.321	3.396
25.)	1.2500	3927.0	5357.5	1224.66	26.662	0.571	1.323	3.499
26.)	1.3000	3917.9	5655.8	1208.33	26.959	0.556	1.325	3.600
27.)	1.3500	3908.2	5951.1	1191.91	27.263	0.540	1.327	3.698
28.)	1.4000	3898.1	6243.4	1175.49	27.573	0.526	1.328	3.793
29.)	1.4500	3887.6	6532.4	1159.16	27.886	0.512	1.329	3.886
30.)	1.5000	3876.8	6818.4	1143.02	28.201	0.499	1.329	3.976
31.)	1.5500	3865.7	7101.3	1127.11	28.517	0.486	1.330	4.064
32.)	1.6000	3854.4	7381.6	1111.51	28.833	0.474	1.330	4.150
33.)	1.6500	3842.9	7659.5	1096.25	29.147	0.463	1.330	4.233
34.)	1.7000	3831.3	7935.3	1081.36	29.459	0.452	1.330	4.315
35.)	1.7500	3820.2	8209.2	1067.10	29.767	0.441	1.330	4.395
36.)	1.8000	3808.5	8482.1	1053.04	30.071	0.431	1.330	4.474
37.)	1.8500	3796.7	8754.1	1039.42	30.371	0.422	1.330	4.552
38.)	1.9000	3785.0	9025.9	1026.24	30.666	0.413	1.330	4.628
39.)	1.9500	3773.3	9297.8	1013.52	30.955	0.404	1.330	4.704
40.)	2.0000	3761.7	9570.5	1001.24	31.238	0.395	1.330	4.779
41.)	2.0500	3750.1	9844.5	989.42	31.515	0.387	1.330	4.853
42.)	2.1000	3738.7	10120.4	978.05	31.784	0.380	1.331	4.927
43.)	2.1500	3727.4	10398.7	967.12	32.046	0.372	1.331	5.000
44.)	2.2000	3716.3	10680.1	956.63	32.301	0.365	1.331	5.074
45.)	2.2500	3705.3	10965.1	946.57	32.547	0.358	1.331	5.148
46.)	2.3000	3694.4	11254.6	936.92	32.786	0.352	1.332	5.222
47.)	2.3500	3683.7	11549.0	927.69	33.016	0.345	1.332	5.297
48.)	2.4000	3673.1	11849.0	918.85	33.238	0.339	1.333	5.372
49.)	2.4500	3662.7	12155.1	910.38	33.452	0.333	1.334	5.449
50.)	2.5000	3652.3	12467.9	902.28	33.656	0.328	1.335	5.527

Product concentrations (mol/kg)

Name		1.)	2.)	3.)	4.)	5.)	6.)
n2	Gas	1.315e+001	1.316e+001	1.317e+001	1.317e+001	1.317e+001	1.316e+001
co	Gas	1.216e+001	1.214e+001	1.213e+001	1.213e+001	1.213e+001	1.212e+001
h2o	Gas	8.430e+000	8.614e+000	8.729e+000	8.817e+000	8.892e+000	8.958e+000
h2	Gas	4.673e+000	4.617e+000	4.567e+000	4.517e+000	4.464e+000	4.407e+000
co2	Gas	2.540e+000	2.554e+000	2.552e+000	2.542e+000	2.529e+000	2.513e+000
h	Gas	5.851e-001	4.319e-001	3.493e-001	2.930e-001	2.506e-001	2.166e-001
oh	Gas	5.832e-001	4.567e-001	3.829e-001	3.305e-001	2.897e-001	2.563e-001
no	Gas	1.608e-001	1.302e-001	1.113e-001	9.754e-002	8.662e-002	7.757e-002
o	Gas	4.160e-002	2.448e-002	1.691e-002	1.249e-002	9.556e-003	7.475e-003
o2	Gas	2.819e-002	1.670e-002	1.149e-002	8.423e-003	6.387e-003	4.945e-003
cho	Gas	5.032e-003	8.329e-003	1.155e-002	1.494e-002	1.866e-002	2.282e-002
nh3	Gas	3.010e-003	6.591e-003	1.095e-002	1.630e-002	2.289e-002	3.102e-002
hcn	Gas	1.728e-003	3.887e-003	6.626e-003	1.012e-002	1.459e-002	2.031e-002
nh2	Gas	1.364e-003	2.240e-003	3.053e-003	3.867e-003	4.712e-003	5.609e-003
n	Gas	7.663e-004	6.605e-004	5.880e-004	5.319e-004	4.855e-004	4.456e-004
hno	Gas	7.203e-004	8.906e-004	1.006e-003	1.100e-003	1.184e-003	1.261e-003
formac	Gas	7.024e-004	1.661e-003	2.917e-003	4.558e-003	6.702e-003	9.508e-003
nh	Gas	6.156e-004	7.474e-004	8.319e-004	8.965e-004	9.501e-004	9.967e-004
ho2	Gas	5.772e-004	5.223e-004	4.745e-004	4.336e-004	3.977e-004	3.659e-004
hnco	Gas	5.693e-004	1.353e-003	2.408e-003	3.825e-003	5.730e-003	8.295e-003

ch2o	Gas	5.577e-004	1.270e-003	2.175e-003	3.328e-003	4.798e-003	6.677e-003
h2o2	Gas	2.405e-004	2.993e-004	3.358e-004	3.626e-004	3.839e-004	4.018e-004
n2o	Gas	1.507e-004	1.924e-004	2.246e-004	2.540e-004	2.832e-004	3.133e-004
no2	Gas	7.948e-005	7.497e-005	7.072e-005	6.706e-005	6.389e-005	6.111e-005
nco	Gas	5.058e-005	9.226e-005	1.367e-004	1.870e-004	2.459e-004	3.159e-004
cn	Gas	4.854e-005	8.640e-005	1.257e-004	1.691e-004	2.187e-004	2.763e-004
hno2	Gas	3.200e-005	4.265e-005	5.038e-005	5.698e-005	6.308e-005	6.901e-005
ch3	Gas	9.855e-006	3.238e-005	6.981e-005	1.272e-004	2.119e-004	3.343e-004
ch4	Gas	3.643e-006	1.533e-005	3.847e-005	7.830e-005	1.424e-004	2.416e-004
ch2	Gas	2.904e-006	7.225e-006	1.288e-005	2.012e-005	2.933e-005	4.096e-005
ch2oh	Gas	1.031e-006	3.653e-006	8.236e-006	1.552e-005	2.662e-005	4.312e-005
c	Gas	4.642e-007	6.196e-007	7.297e-007	8.205e-007	9.006e-007	9.738e-007
ketene	Gas	4.148e-007	2.073e-006	5.987e-006	1.391e-005	2.884e-005	5.583e-005
ch4o	Gas	2.963e-007	1.427e-006	3.950e-006	8.766e-006	1.731e-005	3.183e-005
c2h2	Gas	2.814e-007	1.384e-006	3.943e-006	9.037e-006	1.847e-005	3.522e-005
c2h4	Gas	6.705e-010	6.204e-009	2.585e-008	7.808e-008	1.984e-007	4.529e-007
ch3cn	Gas	4.532e-010	4.738e-009	2.221e-008	7.565e-008	2.179e-007	5.672e-007
mgo2h2	Gas	6.368e-012	8.169e-012	9.420e-012	1.046e-011	1.142e-011	1.236e-011
mgo	liquid	1.594e-002	1.594e-002	1.594e-002	1.594e-002	1.594e-002	1.594e-002
c(s)	solid	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000
mgo	solid	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000
Total Gas		4.237e+001	4.217e+001	4.206e+001	4.198e+001	4.190e+001	4.184e+001
Total Cond.		1.594e-002	1.594e-002	1.594e-002	1.594e-002	1.594e-002	1.594e-002

Product concentrations (mol/kg)

Name		7.)	8.)	9.)	10.)	11.)	12.)
n2	Gas	1.316e+001	1.315e+001	1.313e1.311e+001	1.309e+001	1.306e+001	
co	Gas	1.212e+001	1.211e+001	1.209e+001	1.206e+001	1.202e+001	1.195e+001
h2o	Gas	9.019e+000	9.076e+000	9.129e+000	9.179e+000	9.225e+000	9.268e+000
h2	Gas	4.343e+000	4.273e+000	4.193e+000	4.101e+000	3.997e+000	3.878e+000
co2	Gas	2.495e+000	2.478e+000	2.460e+000	2.444e+000	2.430e+000	2.420e+000
oh	Gas	2.281e-001	2.038e-001	1.825e-001	1.638e-001	1.473e-001	1.326e-001
h	Gas	1.884e-001	1.644e-001	1.437e-001	1.256e-001	1.096e-001	9.553e-002
no	Gas	6.986e-002	6.317e-002	5.731e-002	5.215e-002	4.759e-002	4.358e-002
nh3	Gas	4.105e-002	5.340e-002	6.856e-002	8.705e-002	1.094e-001	1.361e-001
hcn	Gas	2.763e-002	3.698e-002	4.887e-002	6.390e-002	8.270e-002	1.059e-001
cho	Gas	2.751e-002	3.285e-002	3.893e-002	4.586e-002	5.370e-002	6.251e-002
formac	Gas	1.319e-002	1.801e-002	2.433e-002	3.261e-002	4.344e-002	5.754e-002
hnco	Gas	1.175e-002	1.640e-002	2.265e-002	3.105e-002	4.227e-002	5.718e-002
ch2o	Gas	9.076e-003	1.214e-002	1.603e-002	2.095e-002	2.713e-002	3.480e-002
nh2	Gas	6.569e-003	7.604e-003	8.721e-003	9.921e-003	1.120e-002	1.255e-002
o	Gas	5.929e-003	4.748e-003	3.828e-003	3.103e-003	2.527e-003	2.067e-003
o2	Gas	3.881e-003	3.077e-003	2.458e-003	1.977e-003	1.601e-003	1.306e-003
hno	Gas	1.336e-003	1.411e-003	1.485e-003	1.561e-003	1.639e-003	1.720e-003
nh	Gas	1.038e-003	1.075e-003	1.108e-003	1.137e-003	1.162e-003	1.182e-003
ch3	Gas	5.083e-004	7.523e-004	1.090e-003	1.550e-003	2.167e-003	2.976e-003
h2o2	Gas	4.175e-004	4.317e-004	4.449e-004	4.577e-004	4.705e-004	4.836e-004
n	Gas	4.103e-004	3.784e-004	3.494e-004	3.226e-004	2.977e-004	2.745e-004
nco	Gas	3.999e-004	5.015e-004	6.247e-004	7.743e-004	9.558e-004	1.175e-003
ch4	Gas	3.910e-004	6.108e-004	9.282e-004	1.377e-003	1.998e-003	2.835e-003
n2o	Gas	3.454e-004	3.801e-004	4.182e-004	4.606e-004	5.081e-004	5.620e-004
cn	Gas	3.435e-004	4.224e-004	5.149e-004	6.229e-004	7.479e-004	8.910e-004
ho2	Gas	3.373e-004	3.114e-004	2.881e-004	2.671e-004	2.482e-004	2.316e-004
ketene	Gas	1.034e-004	1.855e-004	3.252e-004	5.592e-004	9.450e-004	1.569e-003
hno2	Gas	7.498e-005	8.117e-005	8.771e-005	9.478e-005	1.026e-004	1.112e-004
ch2oh	Gas	6.725e-005	1.021e-004	1.518e-004	2.221e-004	3.199e-004	4.540e-004
c2h2	Gas	6.412e-005	1.130e-004	1.939e-004	3.256e-004	5.355e-004	8.618e-004
no2	Gas	5.868e-005	5.656e-005	5.472e-005	5.319e-005	5.198e-005	5.112e-005
ch4o	Gas	5.586e-005	9.483e-005	1.570e-004	2.546e-004	4.053e-004	6.338e-004
ch2	Gas	5.556e-005	7.377e-005	9.627e-005	1.237e-004	1.567e-004	1.955e-004
ch3cn	Gas	1.382e-006	3.212e-006	7.207e-006	1.570e-005	3.332e-005	6.883e-005
c	Gas	1.042e-006	1.105e-006	1.163e-006	1.215e-006	1.259e-006	1.294e-006
c2h4	Gas	9.613e-007	1.935e-006	3.733e-006	6.949e-006	1.251e-005	2.179e-005

mgo2h2	Gas	1.332e-011	1.432e-011	1.538e-011	1.654e-011	1.781e-011	1.920e-011
mgo	liquid	1.594e-002	1.594e-002	1.594e-002	1.594e-002	1.594e-002	1.594e-002
c(s)	solid	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000
mgo	solid	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000
Total	Gas	4.177e+001	4.170e+001	4.163e+001	4.155e+001	4.145e+001	4.133e+001
Total	Cond.	1.594e-002	1.594e-002	1.594e-002	1.594e-002	1.594e-002	1.594e-002

Name		43.)	44.)	45.)	46.)	47.)	48.)
n2	Gas	1.053e+001	1.047e+001	1.041e+001	1.036e+001	1.031e+001	1.026e+001
h2o	Gas	5.467e+000	5.305e+000	5.147e+000	4.995e+000	4.849e+000	4.707e+000
hnco	Gas	4.437e+000	4.602e+000	4.761e+000	4.912e+000	5.056e+000	5.190e+000
formac	Gas	4.395e+000	4.573e+000	4.747e+000	4.917e+000	5.084e+000	5.247e+000
co2	Gas	2.491e+000	2.427e+000	2.362e+000	2.294e+000	2.225e+000	2.154e+000
co	Gas	2.268e+000	2.063e+000	1.871e+000	1.692e+000	1.525e+000	1.370e+000
nh3	Gas	4.819e-001	4.616e-001	4.412e-001	4.208e-001	4.005e-001	3.804e-001
hcn	Gas	3.382e-001	3.124e-001	2.873e-001	2.628e-001	2.392e-001	2.166e-001
ch2o	Gas	2.017e-001	1.905e-001	1.792e-001	1.679e-001	1.567e-001	1.456e-001
h2	Gas	1.515e-001	1.331e-001	1.168e-001	1.023e-001	8.943e-002	7.800e-002
ketene	Gas	1.484e-001	1.385e-001	1.282e-001	1.177e-001	1.071e-001	9.664e-002
cho	Gas	1.070e-001	1.002e-001	9.345e-002	8.690e-002	8.055e-002	7.442e-002
ch3cn	Gas	5.086e-002	4.732e-002	4.358e-002	3.971e-002	3.579e-002	3.191e-002
ch4o	Gas	2.634e-002	2.480e-002	2.321e-002	2.160e-002	1.999e-002	1.839e-002
n2o	Gas	2.146e-002	2.416e-002	2.727e-002	3.088e-002	3.510e-002	4.004e-002
nco	Gas	2.144e-002	2.179e-002	2.212e-002	2.241e-002	2.267e-002	2.290e-002
no	Gas	1.729e-002	1.725e-002	1.724e-002	1.728e-002	1.735e-002	1.747e-002
oh	Gas	1.188e-002	1.116e-002	1.051e-002	9.901e-003	9.340e-003	8.821e-003
nh2	Gas	8.677e-003	8.128e-003	7.606e-003	7.110e-003	6.638e-003	6.190e-003
c2h2	Gas	5.633e-003	4.752e-003	3.970e-003	3.282e-003	2.685e-003	2.172e-003
ch2oh	Gas	5.294e-003	4.925e-003	4.560e-003	4.202e-003	3.853e-003	3.515e-003
hno	Gas	4.684e-003	4.790e-003	4.907e-003	5.035e-003	5.177e-003	5.334e-003
hno2	Gas	3.411e-003	3.814e-003	4.279e-003	4.819e-003	5.450e-003	6.192e-003
ch3	Gas	3.093e-003	2.632e-003	2.226e-003	1.869e-003	1.558e-003	1.290e-003
ch4	Gas	1.765e-003	1.441e-003	1.167e-003	9.372e-004	7.459e-004	5.882e-004
h2o2	Gas	1.235e-003	1.263e-003	1.296e-003	1.332e-003	1.372e-003	1.418e-003
cn	Gas	1.166e-003	1.074e-003	9.852e-004	9.007e-004	8.203e-004	7.442e-004
h	Gas	7.105e-004	6.090e-004	5.217e-004	4.466e-004	3.818e-004	3.260e-004
no2	Gas	5.180e-004	5.768e-004	6.450e-004	7.247e-004	8.185e-004	9.294e-004
nh	Gas	2.249e-004	2.080e-004	1.923e-004	1.779e-004	1.644e-004	1.520e-004
ho2	Gas	1.742e-004	1.766e-004	1.796e-004	1.832e-004	1.875e-004	1.927e-004
o2	Gas	1.546e-004	1.533e-004	1.525e-004	1.523e-004	1.527e-004	1.537e-004
ch2	Gas	5.052e-005	4.225e-005	3.514e-005	2.905e-005	2.387e-005	1.949e-005
o	Gas	4.750e-005	4.395e-005	4.075e-005	3.786e-005	3.525e-005	3.289e-005
c2h4	Gas	3.427e-005	2.597e-005	1.943e-005	1.434e-005	1.043e-005	7.480e-006
n	Gas	1.705e-005	1.569e-005	1.446e-005	1.333e-005	1.230e-005	1.136e-005
c	Gas	2.733e-008	2.236e-008	1.823e-008	1.481e-008	1.197e-008	9.635e-009
mgo2h2	Gas	5.743e-011	5.568e-011	5.397e-011	5.228e-011	5.063e-011	4.901e-011
mgo	solid	1.594e-002	1.594e-002	1.594e-002	1.594e-002	1.594e-002	1.594e-002
mgo	liquid	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000
c(s)	solid	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000
Total	Gas	3.120e+001	3.096e+001	3.072e+001	3.050e+001	3.029e+001	3.009e+001
Total	Cond.	1.594e-002	1.594e-002	1.594e-002	1.594e-002	1.594e-002	1.594e-002

Product concentrations (mol/kg)

Name		49.)	50.)
n2	Gas	1.021e+001	1.017e+001
formac	Gas	5.406e+000	5.561e+000
hnco	Gas	5.315e+000	5.430e+000
h2o	Gas	4.571e+000	4.440e+000
co2	Gas	2.083e+000	2.012e+000

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       co  Gas   1.226e+000  1.094e+000
      nh3  Gas   3.604e-001  3.408e-001
      hcn  Gas   1.951e-001  1.748e-001
     ch2o  Gas   1.347e-001  1.241e-001
   ketene  Gas   8.645e-002  7.666e-002
      cho  Gas   6.852e-002  6.286e-002
       h2  Gas   6.787e-002  5.890e-002
      n2o  Gas   4.587e-002  5.276e-002
    ch3cn  Gas   2.814e-002  2.453e-002
      nco  Gas   2.310e-002  2.326e-002
       no  Gas   1.763e-002  1.784e-002
     ch4o  Gas   1.681e-002  1.529e-002
       oh  Gas   8.339e-003  7.891e-003
     hno2  Gas   7.069e-003  8.111e-003
      nh2  Gas   5.765e-003  5.362e-003
      hno  Gas   5.507e-003  5.699e-003
    ch2oh  Gas   3.191e-003  2.882e-003
     c2h2  Gas   1.738e-003  1.374e-003
     h2o2  Gas   1.470e-003  1.528e-003
      no2  Gas   1.061e-003  1.219e-003
      ch3  Gas   1.059e-003  8.629e-004
       cn  Gas   6.723e-004  6.048e-004
      ch4  Gas   4.594e-004  3.554e-004
        h  Gas   2.779e-004  2.365e-004
      ho2  Gas   1.988e-004  2.058e-004
       o2  Gas   1.554e-004  1.577e-004
       nh  Gas   1.404e-004  1.296e-004
        o  Gas   3.075e-005  2.879e-005
      ch2  Gas   1.580e-005  1.272e-005
        n  Gas   1.049e-005  9.687e-006
     c2h4  Gas   5.284e-006  3.676e-006
        c  Gas   7.714e-009  6.142e-009
   mgo2h2  Gas   4.741e-011  4.584e-011
      mgo  solid 1.594e-002  1.594e-002
      mgo liquid 0.000e+000  0.000e+000
     c(s)  solid 0.000e+000  0.000e+000

     Total Gas   2.989e+001  2.971e+001

     Total Cond. 1.594e-002  1.594e-002
```

B.2 PETN

```
Reactant library title:# Version 2.0 by P. Clark Souers

                                The Composition

Name      % wt. % mol % vol. Heat of  Standard   Standard   Mol.   Formula
                             formation  volume    entropy    wt.
                             (cal/mol) (cc/mol)  (cal/K/mol)
petn    100.00 100.00 100.00 -125956  177.80      0.000    316.13  c5h8n4o12

Heat of formation =   -398.425 cal/gm
Standard volume   =      0.562 cc/gm
Standard entropy  =      0.000 cal/k/gm
Standard energy   =   -398.438 cal/gm

The elements and percent by mole
     c            17.241
     h            27.586
     n            13.793
     o            41.379
The average mol. wt. = 316.135 g/mol
Input>composition, petn, 100, weight
                                The Composition
```

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
petn	100.00	100.00	100.00	-125956	177.80	0.000	316.13	c5h8n4o12

```
Heat of formation =   -398.425 cal/gm
Standard volume   =      0.562 cc/gm
Standard entropy  =      0.000 cal/k/gm
Standard energy   =   -398.438 cal/gm

The elements and percent by mole
     c            17.241
     h            27.586
     n            13.793
     o            41.379
The average mol. wt. = 316.135 g/mol
Input>gun, 0.050000, 0.050000, 2.500000
GUN calculation:
```

	Rho g/cc	Temp K	Pressure MPa	Impetus J/g	Mol Wt. Gas	Covol cc/g	Frozen Cp/Cv	Phi
1.)	0.0500	3856.8	62.4	1186.90	27.018	0.980	1.207	1.052
2.)	0.1000	3963.8	133.8	1209.35	27.253	0.963	1.205	1.107
3.)	0.1500	4030.0	213.7	1222.93	27.400	0.945	1.204	1.165
4.)	0.2000	4079.4	302.7	1232.94	27.510	0.926	1.204	1.227
5.)	0.2500	4119.7	401.3	1241.00	27.602	0.907	1.204	1.293
6.)	0.3000	4154.3	510.2	1247.80	27.682	0.888	1.206	1.363
7.)	0.3500	4184.8	630.3	1253.74	27.753	0.868	1.207	1.436
8.)	0.4000	4212.4	762.1	1259.00	27.819	0.848	1.210	1.513
9.)	0.4500	4237.6	906.4	1263.73	27.881	0.828	1.213	1.594
10.)	0.5000	4260.9	1063.8	1267.99	27.941	0.808	1.216	1.678
11.)	0.5500	4282.6	1235.0	1271.83	27.998	0.788	1.219	1.766
12.)	0.6000	4302.9	1420.6	1275.27	28.055	0.769	1.223	1.857
13.)	0.6500	4321.8	1621.2	1278.31	28.111	0.750	1.227	1.951
14.)	0.7000	4339.4	1837.2	1280.93	28.168	0.731	1.232	2.049
15.)	0.7500	4355.9	2069.0	1283.11	28.226	0.713	1.237	2.150
16.)	0.8000	4371.1	2316.9	1284.80	28.288	0.695	1.242	2.254
17.)	0.8500	4385.0	2580.8	1285.93	28.353	0.678	1.247	2.361
18.)	0.9000	4397.6	2860.6	1286.44	28.423	0.661	1.252	2.471
19.)	0.9500	4408.9	3155.8	1286.23	28.501	0.645	1.258	2.583
20.)	1.0000	4418.7	3465.7	1285.21	28.587	0.629	1.263	2.697
21.)	1.0500	4426.9	3789.1	1283.26	28.684	0.614	1.269	2.812
22.)	1.1000	4433.5	4124.4	1280.29	28.793	0.599	1.274	2.929
23.)	1.1500	4438.3	4469.8	1276.21	28.916	0.584	1.280	3.046
24.)	1.2000	4441.4	4823.3	1270.96	29.056	0.570	1.285	3.163
25.)	1.2500	4442.7	5182.7	1264.53	29.212	0.556	1.289	3.279
26.)	1.3000	4442.2	5545.9	1256.92	29.386	0.543	1.294	3.394
27.)	1.3500	4439.9	5910.9	1248.20	29.576	0.530	1.298	3.508
28.)	1.4000	4436.1	6276.2	1238.46	29.782	0.517	1.302	3.620
29.)	1.4500	4430.6	6640.5	1227.84	30.003	0.505	1.305	3.730
30.)	1.5000	4423.8	7003.0	1216.48	30.237	0.493	1.308	3.838
31.)	1.5500	4415.6	7363.2	1204.51	30.481	0.482	1.311	3.944
32.)	1.6000	4406.2	7720.8	1192.08	30.733	0.471	1.313	4.048
33.)	1.6500	4395.7	8075.9	1179.30	30.992	0.460	1.316	4.150
34.)	1.7000	4384.2	8428.6	1166.30	31.256	0.450	1.318	4.251
35.)	1.7500	4371.6	8779.0	1153.15	31.521	0.440	1.320	4.350
36.)	1.8000	4358.1	9127.3	1139.93	31.788	0.431	1.322	4.448
37.)	1.8500	4343.6	9473.6	1126.70	32.054	0.422	1.323	4.545
38.)	1.9000	4328.1	9817.9	1113.48	32.319	0.413	1.325	4.641
39.)	1.9500	4311.6	10160.2	1100.30	32.581	0.405	1.327	4.736
40.)	2.0000	4294.0	10500.3	1087.19	32.840	0.396	1.328	4.829
41.)	2.0500	4275.5	10837.8	1074.13	33.096	0.389	1.330	4.922
42.)	2.1000	4256.0	11172.5	1061.15	33.348	0.381	1.331	5.014
43.)	2.1500	4235.4	11503.8	1048.23	33.596	0.374	1.333	5.105

44.)	2.2000	4213.8	11831.3	1035.38	33.840	0.367	1.334	5.194
45.)	2.2500	4191.3	12154.4	1022.59	34.080	0.360	1.336	5.283
46.)	2.3000	4167.9	12472.8	1009.88	34.316	0.354	1.337	5.370
47.)	2.3500	4143.6	12786.0	997.23	34.549	0.348	1.339	5.456
48.)	2.4000	4118.6	13093.7	984.68	34.778	0.341	1.340	5.541
49.)	2.4500	4092.9	13395.6	972.21	35.004	0.336	1.342	5.624
50.)	2.5000	4066.7	13691.6	959.85	35.228	0.330	1.343	5.706

Product concentrations (mol/kg)

Name		1.)	2.)	3.)	4.)	5.)	6.)
h2o	Gas	1.046e+001	1.067e+001	1.080e+001	1.091e+001	1.099e+001	1.107e+001
co	Gas	8.018e+000	7.730e+000	7.550e+000	7.416e+000	7.307e+000	7.214e+000
co2	Gas	7.796e+000	8.081e+000	8.258e+000	8.390e+000	8.496e+000	8.585e+000
n2	Gas	6.035e+000	6.039e+000	6.044e+000	6.049e+000	6.054e+000	6.059e+000
oh	Gas	1.562e+000	1.401e+000	1.294e+000	1.209e+000	1.137e+000	1.073e+000
h2	Gas	1.240e+000	1.142e+000	1.078e+000	1.026e+000	9.823e-001	9.426e-001
o2	Gas	7.443e-001	6.070e-001	5.236e-001	4.623e-001	4.132e-001	3.720e-001
no	Gas	5.782e-001	5.666e-001	5.541e-001	5.418e-001	5.299e-001	5.181e-001
h	Gas	3.291e-001	2.553e-001	2.144e-001	1.859e-001	1.640e-001	1.460e-001
o	Gas	2.352e-001	1.779e-001	1.468e-001	1.256e-001	1.096e-001	9.663e-002
ho2	Gas	7.865e-003	9.464e-003	1.049e-002	1.126e-002	1.189e-002	1.242e-002
cho	Gas	1.806e-003	2.930e-003	3.994e-003	5.084e-003	6.244e-003	7.506e-003
h2o2	Gas	1.593e-003	2.406e-003	3.084e-003	3.705e-003	4.300e-003	4.886e-003
no2	Gas	1.430e-003	1.865e-003	2.199e-003	2.496e-003	2.778e-003	3.056e-003
hno	Gas	1.335e-003	1.925e-003	2.417e-003	2.873e-003	3.319e-003	3.767e-003
n	Gas	6.215e-004	6.358e-004	6.384e-004	6.370e-004	6.337e-004	6.290e-004
formac	Gas	5.740e-004	1.305e-003	2.216e-003	3.353e-003	4.775e-003	6.555e-003
n2o	Gas	3.661e-004	5.631e-004	7.453e-004	9.306e-004	1.128e-003	1.342e-003
hno2	Gas	2.859e-004	4.905e-004	6.884e-004	8.928e-004	1.111e-003	1.348e-003
nh3	Gas	2.743e-004	5.312e-004	8.077e-004	1.115e-003	1.461e-003	1.855e-003
nh2	Gas	2.628e-004	4.295e-004	5.821e-004	7.323e-004	8.854e-004	1.045e-003
nh	Gas	2.472e-004	3.310e-004	3.941e-004	4.482e-004	4.974e-004	5.437e-004
hnco	Gas	1.313e-004	2.910e-004	4.897e-004	7.393e-004	1.055e-003	1.455e-003
ch2o	Gas	9.731e-005	1.984e-004	3.133e-004	4.468e-004	6.040e-004	7.904e-004
hcn	Gas	8.536e-005	1.673e-004	2.581e-004	3.620e-004	4.832e-004	6.257e-004
nco	Gas	2.502e-005	4.846e-005	7.446e-005	1.045e-004	1.399e-004	1.822e-004
cn	Gas	5.179e-006	9.209e-006	1.334e-005	1.782e-005	2.284e-005	2.855e-005
ch3	Gas	1.906e-007	5.079e-007	9.417e-007	1.511e-006	2.244e-006	3.179e-006
ch2	Gas	1.192e-007	2.714e-007	4.531e-007	6.689e-007	9.249e-007	1.229e-006
ch2oh	Gas	9.617e-008	3.051e-007	6.329e-007	1.108e-006	1.773e-006	2.686e-006
c	Gas	8.158e-008	1.208e-007	1.530e-007	1.822e-007	2.101e-007	2.375e-007
ch4	Gas	3.367e-008	1.033e-007	2.072e-007	3.504e-007	5.403e-007	7.874e-007
ch4o	Gas	1.332e-008	5.199e-008	1.233e-007	2.397e-007	4.190e-007	6.870e-007
ketene	Gas	9.980e-009	3.930e-008	9.525e-008	1.904e-007	3.437e-007	5.840e-007
c2h2	Gas	1.470e-009	5.397e-009	1.244e-008	2.384e-008	4.142e-008	6.786e-008
c2h4	Gas	8.779e-013	5.352e-012	1.658e-011	3.909e-011	7.961e-011	1.482e-010
ch3cn	Gas	7.829e-013	5.589e-012	1.983e-011	5.323e-011	1.233e-010	2.616e-010
c(s)	solid	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000
Total Gas		3.701e+001	3.669e+001	3.650e+001	3.635e+001	3.623e+001	3.612e+001
Total Cond.		0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000

Product concentrations (mol/kg)

Name		7.)	8.)	9.)	10.)	11.)	12.)
h2o	Gas	1.114e+001	1.120e+001	1.126e+001	1.131e+001	1.136e+001	1.140e+001
co2	Gas	8.664e+000	8.734e+000	8.797e+000	8.855e+000	8.909e+000	8.960e+000
co	Gas	7.131e+000	7.055e+000	6.985e+000	6.918e+000	6.854e+000	6.791e+000
n2	Gas	6.063e+000	6.067e+000	6.071e+000	6.075e+000	6.079e+000	6.082e+000
oh	Gas	1.015e+000	9.610e-001	9.100e-001	8.616e-001	8.153e-001	7.708e-001
h2	Gas	9.057e-001	8.709e-001	8.376e-001	8.055e-001	7.744e-001	7.439e-001
no	Gas	5.064e-001	4.947e-001	4.830e-001	4.711e-001	4.591e-001	4.469e-001
o2	Gas	3.362e-001	3.045e-001	2.760e-001	2.503e-001	2.268e-001	2.053e-001

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h      Gas 1.308e-001 1.176e-001 1.059e-001 9.545e-002 8.605e-002 7.753e-002
o      Gas 8.580e-002 7.651e-002 6.838e-002 6.118e-002 5.475e-002 4.897e-002
ho2    Gas 1.287e-002 1.327e-002 1.362e-002 1.393e-002 1.419e-002 1.441e-002
cho    Gas 8.897e-003 1.045e-002 1.218e-002 1.413e-002 1.633e-002 1.882e-002
formac Gas 8.790e-003 1.160e-002 1.515e-002 1.962e-002 2.528e-002 3.243e-002
h2o2   Gas 5.473e-003 6.066e-003 6.672e-003 7.294e-003 7.934e-0038.594e-003
hno    Gas 4.227e-003 4.705e-003 5.204e-003 5.731e-003 6.287e-003 6.875e-003
no2    Gas 3.335e-003 3.619e-003 3.912e-003 4.216e-003 4.532e-003 4.861e-003
nh3    Gas 2.307e-003 2.829e-003 3.432e-003 4.132e-003 4.945e-003 5.892e-003
hnco   Gas 1.964e-003 2.614e-003 3.446e-003 4.512e-003 5.882e-003 7.644e-003
hno2   Gas 1.609e-003 1.899e-003 2.222e-003 2.584e-003 2.990e-003 3.448e-003
n2o    Gas 1.580e-003 1.845e-003 2.144e-003 2.482e-003 2.866e-003 3.303e-003
nh2    Gas 1.213e-003 1.392e-003 1.584e-003 1.790e-003 2.013e-003 2.253e-003
ch2o   Gas 1.013e-003 1.280e-003 1.600e-003 1.987e-003 2.453e-003 3.017e-003
hcn    Gas 7.947e-004 9.960e-004 1.237e-003 1.525e-003 1.872e-003 2.288e-003
n      Gas 6.233e-004 6.165e-004 6.087e-004 5.999e-004 5.901e-004 5.792e-004
nh     Gas 5.882e-004 6.315e-004 6.740e-004 7.158e-004 7.572e-004 7.980e-004
nco    Gas 2.330e-004 2.944e-004 3.689e-004 4.594e-004 5.697e-004 7.042e-004
cn     Gas 3.510e-005 4.268e-005 5.148e-005 6.173e-005 7.368e-005 8.762e-005
ch3    Gas 4.368e-006 5.872e-006 7.771e-006 1.016e-005 1.318e-005 1.695e-005
ch2oh  Gas 3.926e-006 5.595e-006 7.833e-006 1.082e-005 1.480e-005 2.008e-005
ch2    Gas 1.590e-006 2.018e-006 2.526e-006 3.129e-006 3.843e-006 4.686e-006
ch4    Gas 1.105e-006 1.510e-006 2.022e-006 2.670e-006 3.484e-006 4.505e-006
ch4o   Gas 1.080e-006 1.648e-006 2.464e-006 3.628e-006 5.281e-006 7.620e-006
ketene Gas 9.537e-007 1.516e-006 2.366e-006 3.644e-006 5.559e-006 8.421e-006
c      Gas 2.648e-007 2.923e-007 3.202e-007 3.483e-007 3.768e-007 4.055e-007
c2h2   Gas 1.070e-007 1.643e-007 2.476e-007 3.681e-007 5.420e-007 7.918e-007
ch3cn  Gas 5.238e-010 1.008e-009 1.889e-009 3.470e-009 6.284e-009 1.126e-008
c2h4   Gas 2.597e-010 4.361e-010 7.100e-009 1.129e-009 1.762e-009 2.710e-009
c(s) solid 0.000e+000 0.000e+000 0.000e+000 0.000e+000 0.000e+000 0.000e+000

Total  Gas 3.603e+001 3.595e+001 3.587e+001 3.579e+001 3.572e+001 3.564e+001
Total Cond.0.000e+000 0.000e+000 0.000e+000 0.000e+000 0.000e+000 0.000e+000

Product concentrations (mol/kg)
Name            13.)       14.)       15.)       16.)       17.)       18.)
h2o    Gas 1.144e+001 1.148e+001 1.150e+001 1.153e+001 1.154e+001 1.155e+001
co2    Gas 9.007e+000 9.052e+000 9.094e+000 9.134e+000 9.172e+000 9.208e+000
co     Gas 6.728e+000 6.665e+000 6.598e+000 6.529e+000 6.454e+000 6.372e+000
n2     Gas 6.085e+000 6.087e+000 6.088e+000 6.089e+000 6.088e+000 6.087e+000
oh     Gas 7.280e-001 6.866e-001 6.466e-001 6.081e-001 5.709e-001 5.350e-001
h2     Gas 7.140e-001 6.844e-001 6.552e-001 6.262e-001 5.972e-001 5.681e-001
no     Gas 4.346e-001 4.221e-001 4.095e-001 3.969e-001 3.842e-001 3.716e-001
o2     Gas 1.857e-001 1.677e-001 1.512e-001 1.361e-001 1.224e-001 1.100e-001
h      Gas 6.978e-002 6.271e-002 5.625e-002 5.034e-002 4.494e-002 4.000e-002
o      Gas 4.375e-002 3.903e-002 3.476e-002 3.090e-002 2.742e-002 2.428e-002
formac Gas 4.150e-002 5.300e-002 6.756e-002 8.599e-002 1.093e-001 1.385e-001
cho    Gas 2.164e-002 2.482e-002 2.840e-002 3.243e-002 3.693e-002 4.191e-002
ho2    Gas 1.460e-002 1.475e-002 1.486e-002 1.493e-002 1.498e-002 1.499e-002
hnco   Gas 9.913e-003 1.284e-002 1.660e-002 2.145e-002 2.766e-002 3.561e-002
h2o2   Gas 9.276e-003 9.981e-003 1.071e-002 1.146e-002 1.223e-002 1.303e-002
hno    Gas 7.500e-003 8.161e-003 8.863e-003 9.605e-003 1.039e-002 1.121e-002
nh3    Gas 6.994e-003 8.275e-003 9.762e-003 1.148e-002 1.346e-002 1.573e-002
no2    Gas 5.206e-003 5.567e-003 5.946e-003 6.345e-003 6.766e-003 7.213e-003
hno2   Gas 3.964e-003 4.546e-003 5.204e-003 5.946e-003 6.785e-003 7.733e-003
n2o    Gas 3.802e-003 4.373e-003 5.026e-003 5.774e-003 6.631e-003 7.613e-003
ch2o   Gas 3.698e-003 4.520e-003 5.512e-003 6.703e-003 8.128e-003 9.819e-003
hcn    Gas 2.789e-003 3.391e-003 4.112e-003 4.974e-003 5.997e-003 7.201e-003
nh2    Gas 2.513e-003 2.793e-003 3.093e-003 3.414e-003 3.755e-003 4.113e-003
nco    Gas 8.684e-004 1.069e-003 1.313e-003 1.609e-003 1.969e-003 2.402e-003
nh     Gas 8.382e-004 8.775e-004 9.155e-004 9.519e-004 9.862e-004 1.018e-003
n      Gas 5.673e-004 5.543e-004 5.403e-004 5.251e-004 5.088e-004 4.914e-004
cn     Gas 1.039e-004 1.228e-004 1.447e-004 1.700e-004 1.990e-004 2.319e-004
ch2oh  Gas 2.706e-005 3.628e-005 4.839e-005 6.422e-005 8.477e-005 1.112e-004
ch3    Gas 2.169e-005 2.759e-005 3.491e-005 4.395e-005 5.498e-005 6.830e-005
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ketene	Gas	1.269e-005	1.903e-005	2.843e-005	4.231e-005	6.265e-005	9.223e-005
ch4o	Gas	1.092e-005	1.556e-005	2.205e-005	3.110e-005	4.362e-005	6.078e-005
ch4	Gas	5.780e-006	7.365e-006	9.323e-006	1.173e-005	1.464e-005	1.813e-005
ch2	Gas	5.680e-006	6.845e-006	8.202e-006	9.772e-006	1.157e-005	1.359e-005
c2h2	Gas	1.149e-006	1.660e-006	2.384e-006	3.406e-006	4.834e-006	6.807e-006
c	Gas	4.341e-007	4.625e-007	4.901e-007	5.165e-007	5.409e-007	5.625e-007
ch3cn	Gas	2.002e-008	3.536e-008	6.209e-008	1.084e-007	1.879e-007	3.231e-007
c2h4	Gas	4.117e-009	6.187e-009	9.202e-009	1.355e-008	1.972e-008	2.836e-008
c(s)	solid	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000
Total	Gas	3.557e+001	3.550e+001	3.543e+001	3.535e+001	3.527e+001	3.518e+001
Total	Cond.	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000

Product concentrations (mol/kg)

Name		19.)	20.)	21.)	22.)	23.)	24.)
h2o	Gas	1.154e+001	1.153e+001	1.150e+001	1.145e+001	1.138e+001	1.130e+001
co2	Gas	9.243e+000	9.276e+000	9.308e+000	9.339e+000	9.368e+000	9.396e+000
co	Gas	6.281e+000	6.178e+000	6.063e+000	5.931e+000	5.783e+000	5.616e+000
n2	Gas	6.083e+000	6.077e+000	6.069e+000	6.059e+000	6.045e+000	6.028e+000
h2	Gas	5.389e-001	5.094e-001	4.797e-001	4.497e-001	4.195e-001	3.892e-001
oh	Gas	5.006e-001	4.677e-001	4.363e-001	4.066e-001	3.784e-001	3.520e-001
no	Gas	3.592e-001	3.470e-001	3.352e-001	3.238e-001	3.131e-001	3.031e-001
formac	Gas	1.752e-001	2.207e-001	2.767e-001	3.450e-001	4.270e-001	5.240e-001
o2	Gas	9.885e-002	8.886e-002	8.000e-002	7.220e-002	6.538e-002	5.949e-002
cho	Gas	4.737e-002	5.328e-002	5.956e-002	6.610e-002	7.273e-002	7.925e-002
hnco	Gas	4.570e-002	5.842e-002	7.430e-002	9.385e-002	1.175e-001	1.458e-001
h	Gas	3.549e-002	3.139e-002	2.766e-002	2.428e-002	2.124e-002	1.850e-002
o	Gas	2.146e-002	1.894e-002	1.670e-002	1.472e-002	1.298e-002	1.145e-002
nh3	Gas	1.829e-002	2.115e-002	2.430e-002	2.771e-002	3.130e-002	3.498e-002
ho2	Gas	1.498e-002	1.495e-002	1.490e-002	1.484e-002	1.478e-002	1.472e-002
h2o2	Gas	1.384e-002	1.468e-002	1.553e-002	1.639e-002	1.727e-002	1.817e-002
hno	Gas	1.207e-002	1.297e-002	1.390e-002	1.485e-002	1.583e-002	1.681e-002
ch2o	Gas	1.181e-002	1.412e-002	1.676e-002	1.972e-002	2.296e-002	2.641e-002
hno2	Gas	8.804e-003	1.001e-002	1.138e-002	1.293e-002	1.468e-002	1.666e-002
n2o	Gas	8.738e-003	1.003e-002	1.150e-002	1.318e-002	1.510e-002	1.728e-002
hcn	Gas	8.605e-003	1.022e-002	1.203e-002	1.404e-002	1.618e-002	1.841e-002
no2	Gas	7.689e-003	8.201e-003	8.754e-003	9.357e-003	1.002e-002	1.076e-002
nh2	Gas	4.484e-003	4.862e-003	5.238e-003	5.604e-003	5.946e-003	6.252e-003
nco	Gas	2.921e-003	3.537e-003	4.260e-003	5.099e-003	6.055e-003	7.128e-003
nh	Gas	1.045e-003	1.068e-003	1.086e-003	1.097e-003	1.101e-003	1.098e-003
n	Gas	4.729e-004	4.535e-004	4.332e-004	4.120e-004	3.903e-004	3.681e-004
cn	Gas	2.687e-004	3.094e-004	3.533e-004	3.995e-004	4.468e-004	4.933e-004
ch2oh	Gas	1.448e-004	1.868e-004	2.385e-004	3.006e-004	3.732e-004	4.554e-004
ketene	Gas	1.347e-004	1.949e-004	2.783e-004	3.913e-004	5.399e-004	7.287e-004
ch3	Gas	8.412e-005	1.025e-004	1.234e-004	1.463e-004	1.705e-004	1.948e-004
ch4o	Gas	8.405e-005	1.151e-004	1.559e-004	2.081e-004	2.731e-004	3.517e-004
ch4	Gas	2.225e-005	2.698e-005	3.227e-005	3.798e-005	4.387e-005	4.959e-005
ch2	Gas	1.582e-005	1.824e-005	2.076e-005	2.330e-005	2.572e-005	2.787e-005
c2h2	Gas	9.489e-006	1.306e-005	1.770e-005	2.354e-005	3.060e-005	3.875e-005
c	Gas	5.803e-007	5.931e-007	6.000e-007	5.999e-007	5.920e-007	5.760e-007
ch3cn	Gas	5.497e-007	9.224e-007	1.521e-006	2.455e-006	3.860e-006	5.890e-006
c2h4	Gas	4.019e-008	5.598e-008	7.636e-008	1.016e-007	1.315e-007	1.648e-007
c(s)	solid	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000
Total	Gas	3.509e+001	3.498e+001	3.486e+001	3.473e+001	3.458e+001	3.442e+001
Total	Cond.	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000

Product concentrations (mol/kg)

Name		25.)	26.)	27.)	28.)	29.)	30.)
h2o	Gas	1.120e+001	1.108e+001	1.094e+001	1.078e+001	1.061e+001	1.042e+001
co2	Gas	9.422e+000	9.446e+000	9.467e+000	9.485e+000	9.499e+000	9.509e+000
n2	Gas	6.008e+000	5.985e+000	5.959e+000	5.929e+000	5.898e+000	5.864e+000
co	Gas	5.430e+000	5.226e+000	5.006e+000	4.772e+000	4.526e+000	4.272e+000
formac	Gas	6.368e-001	7.657e-001	9.104e-001	1.070e+000	1.243e+000	1.427e+000
h2	Gas	3.591e-001	3.293e-001	3.002e-001	2.721e-001	2.452e-001	2.198e-001

oh	Gas	3.272e-001	3.042e-001	2.829e-001	2.632e-001	2.450e-001	2.283e-001
no	Gas	2.938e-001	2.854e-001	2.779e-001	2.714e-001	2.657e-001	2.608e-001
hnco	Gas	1.787e-001	2.164e-001	2.585e-001	3.047e-001	3.543e-001	4.065e-001
cho	Gas	8.544e-002	9.105e-002	9.587e-002	9.973e-002	1.025e-001	1.041e-001
o2	Gas	5.444e-002	5.014e-002	4.653e-002	4.351e-002	4.102e-002	3.898e-002
nh3	Gas	3.865e-002	4.218e-002	4.543e-002	4.830e-002	5.069e-002	5.255e-002
ch2o	Gas	2.998e-002	3.353e-002	3.694e-002	4.007e-002	4.279e-002	4.502e-002
hcn	Gas	2.063e-002	2.276e-002	2.468e-002	2.630e-002	2.756e-002	2.840e-002
n2o	Gas	1.977e-002	2.259e-002	2.579e-002	2.942e-002	3.355e-002	3.822e-002
h2o2	Gas	1.907e-002	1.999e-002	2.093e-002	2.188e-002	2.286e-002	2.387e-002
hno2	Gas	1.890e-002	2.144e-002	2.433e-002	2.761e-002	3.134e-002	3.560e-002
hno	Gas	1.781e-002	1.880e-002	1.978e-002	2.076e-002	2.172e-002	2.268e-002
h	Gas	1.606e-002	1.389e-002	1.198e-002	1.029e-002	8.823e-003	7.543e-003
ho2	Gas	1.468e-002	1.466e-002	1.467e-002	1.471e-002	1.478e-002	1.490e-002
no2	Gas	1.159e-002	1.253e-002	1.360e-002	1.482e-002	1.622e-002	1.784e-002
o	Gas	1.012e-002	8.957e-003	7.953e-003	7.084e-003	6.332e-003	5.680e-003
nco	Gas	8.308e-003	9.580e-003	1.092e-002	1.232e-002	1.373e-002	1.514e-002
nh2	Gas	6.511e-003	6.711e-003	6.846e-003	6.912e-003	6.908e-003	6.838e-003
nh	Gas	1.086e-003	1.066e-003	1.039e-003	1.006e-003	9.661e-004	9.221e-004
ketene	Gas	9.596e-004	1.230e-003	1.533e-003	1.855e-003	2.182e-003	2.494e-003
ch2oh	Gas	5.452e-004	6.397e-004	7.347e-004	8.259e-004	9.088e-004	9.797e-004
cn	Gas	5.371e-004	5.761e-004	6.084e-004	6.327e-004	6.478e-004	6.534e-004
ch4o	Gas	4.433e-004	5.459e-004	6.562e-004	7.696e-004	8.807e-004	9.841e-004
n	Gas	3.458e-004	3.236e-004	3.016e-004	2.802e-004	2.594e-004	2.396e-004
ch3	Gas	2.177e-004	2.376e-004	2.532e-004	2.631e-004	2.669e-004	2.644e-004
ch4	Gas	5.475e-005	5.894e-005	6.180e-005	6.311e-005	6.276e-005	6.084e-005
c2h2	Gas	4.768e-005	5.685e-005	6.560e-005	7.320e-005	7.901e-005	8.255e-005
ch2	Gas	2.960e-005	3.078e-005	3.131e-005	3.115e-005	3.032e-005	2.890e-005
ch3cn	Gas	8.687e-006	1.235e-005	1.688e-005	2.218e-005	2.800e-005	3.401e-005
c	Gas	5.521e-007	5.210e-007	4.839e-007	4.425e-007	3.984e-007	3.535e-007
c2h4	Gas	1.992e-007	2.319e-007	2.595e-007	2.790e-007	2.882e-007	2.864e-007
c(s)	solid	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000
Total	Gas	3.423e+001	3.403e+001	3.381e+001	3.358e+001	3.333e+001	3.307e+001
Total	Cond.	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+0000.000e+000	

Product concentrations (mol/kg)

Name		31.)	32.)	33.)	34.)	35.)	36.)
h2o	Gas	1.022e+001	1.002e+001	9.803e+000	9.585e+000	9.365e+000	9.143e+000
co2	Gas	9.514e+000	9.514e+000	9.509e+000	9.498e+000	9.480e+000	9.456e+000
n2	Gas	5.828e+000	5.791e+000	5.753e+000	5.714e+000	5.673e+000	5.632e+000
co	Gas	4.014e+000	3.755e+000	3.497e+000	3.244e+000	2.997e+000	2.760e+000
formac	Gas	1.622e+000	1.824e+000	2.032e+000	2.244e+000	2.459e+000	2.674e+000
hnco	Gas	4.605e-001	5.154e-001	5.705e-001	6.249e-001	6.780e-001	7.293e-001
no	Gas	2.568e-001	2.536e-001	2.510e-001	2.490e-001	2.476e-001	2.465e-001
oh	Gas	2.129e-001	1.988e-001	1.857e-001	1.737e-001	1.625e-001	1.521e-001
h2	Gas	1.960e-001	1.740e-001	1.537e-001	1.353e-001	1.186e-001	1.037e-001
cho	Gas	1.046e-001	1.040e-001	1.023e-001	9.979e-002	9.649e-002	9.256e-002
nh3	Gas	5.384e-002	5.455e-002	5.472e-002	5.438e-002	5.359e-002	5.241e-002
ch2o	Gas	4.668e-002	4.775e-002	4.823e-002	4.815e-002	4.755e-002	4.650e-002
n2o	Gas	4.354e-002	4.957e-002	5.643e-002	6.423e-002	7.310e-002	8.318e-002
hno2	Gas	4.047e-002	4.604e-002	5.242e-002	5.974e-002	6.812e-002	7.772e-002
o2	Gas	3.733e-002	3.601e-002	3.498e-002	3.419e-002	3.361e-002	3.320e-002
hcn	Gas	2.880e-002	2.876e-002	2.833e-002	2.754e-002	2.644e-002	2.511e-002
h2o2	Gas	2.491e-002	2.598e-002	2.710e-002	2.825e-002	2.945e-002	3.069e-002
hno	Gas	2.362e-002	2.455e-002	2.547e-002	2.639e-002	2.729e-002	2.818e-002
no2	Gas	1.970e-002	2.185e-002	2.432e-002	2.718e-002	3.048e-002	3.427e-002
nco	Gas	1.652e-002	1.785e-002	1.911e-002	2.028e-002	2.135e-002	2.231e-002
ho2	Gas	1.506e-002	1.526e-002	1.550e-002	1.578e-002	1.610e-002	1.645e-002
nh2	Gas	6.707e-003	6.523e-003	6.295e-003	6.030e-003	5.739e-003	5.427e-003
h	Gas	6.434e-003	5.476e-003	4.652e-003	3.943e-003	3.337e-003	2.818e-003
o	Gas	5.113e-003	4.619e-003	4.185e-003	3.803e-003	3.464e-003	3.162e-003
ketene	Gas	2.774e-003	3.008e-003	3.184e-003	3.296e-003	3.343e-003	3.327e-003
ch4o	Gas	1.075e-003	1.150e-003	1.205e-003	1.240e-003	1.255e-003	1.251e-003

ch2oh	Gas	1.035e-003	1.074e-003	1.096e-003	1.099e-003	1.087e-003	1.061e-003
nh	Gas	8.746e-004	8.249e-004	7.739e-004	7.224e-004	6.711e-004	6.208e-004
cn	Gas	6.497e-004	6.374e-004	6.174e-004	5.910e-004	5.595e-004	5.243e-004
ch3	Gas	2.560e-004	2.427e-004	2.255e-004	2.058e-004	1.845e-004	1.629e-004
n	Gas	2.206e-004	2.027e-004	1.859e-004	1.700e-004	1.552e-004	1.414e-004
c2h2	Gas	8.361e-005	8.222e-005	7.865e-005	7.333e-005	6.677e-005	5.950e-005
ch4	Gas	5.755e-005	5.320e-005	4.813e-005	4.267e-005	3.715e-005	3.180e-005
ch3cn	Gas	3.981e-005	4.499e-005	4.920e-005	5.220e-005	5.386e-005	5.418e-005
ch2	Gas	2.700e-005	2.475e-005	2.228e-005	1.974e-005	1.721e-005	1.480e-005
c	Gas	3.094e-007	2.672e-007	2.279e-007	1.920e-007	1.601e-007	1.320e-007
c2h4	Gas	2.743e-007	2.536e-007	2.268e-007	1.968e-007	1.660e-007	1.365e-007
c(s)	solid	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000
Total	Gas	3.281e+001	3.254e+001	3.227e+001	3.199e+001	3.172e+001	3.146e+001
Total	Cond.	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000

Product concentrations (mol/kg)

Name		37.)	38.)	39.)	40.)	41.)	42.)
co2	Gas	9.426e+000	9.389e+000	9.345e+000	9.294e+000	9.236e+000	9.171e+000
h2o	Gas	8.922e+000	8.701e+000	8.482e+000	8.265e+000	8.051e+000	7.840e+000
n2	Gas	5.590e+000	5.546e+000	5.501e+000	5.455e+000	5.407e+000	5.357e+000
formac	Gas	2.890e+000	3.104e+000	3.316e+000	3.525e+000	3.731e+000	3.933e+000
co	Gas	2.532e+000	2.317e+000	2.114e+000	1.924e+000	1.747e+000	1.584e+000
hnco	Gas	7.783e-001	8.248e-001	8.685e-001	9.093e-001	9.471e-001	9.822e-001
no	Gas	2.458e-001	2.453e-001	2.449e-001	2.444e-001	2.439e-001	2.430e-001
oh	Gas	1.424e-001	1.333e-001	1.248e-001	1.168e-001	1.091e-001	1.019e-001
n2o	Gas	9.461e-002	1.075e-001	1.221e-001	1.385e-001	1.568e-001	1.772e-001
h2	Gas	9.032e-002	7.847e-002	6.802e-002	5.883e-002	5.080e-002	4.380e-002
hno2	Gas	8.868e-002	1.012e-001	1.154e-001	1.314e-001	1.493e-001	1.693e-001
cho	Gas	8.814e-002	8.337e-002	7.838e-002	7.328e-002	6.817e-002	6.313e-002
nh3	Gas	5.090e-002	4.914e-002	4.718e-002	4.509e-002	4.291e-002	4.070e-002
ch2o	Gas	4.507e-002	4.332e-002	4.135e-002	3.921e-002	3.698e-002	3.471e-002
no2	Gas	3.863e-002	4.360e-002	4.925e-002	5.564e-002	6.280e-002	7.078e-002
o2	Gas	3.293e-002	3.276e-002	3.267e-002	3.263e-002	3.260e-002	3.256e-002
h2o2	Gas	3.197e-002	3.327e-002	3.458e-002	3.590e-002	3.719e-002	3.844e-002
hno	Gas	2.905e-002	2.990e-002	3.071e-002	3.147e-002	3.218e-002	3.281e-002
hcn	Gas	2.361e-002	2.200e-002	2.033e-002	1.866e-002	1.702e-002	1.544e-002
nco	Gas	2.315e-002	2.387e-002	2.446e-002	2.492e-002	2.526e-002	2.548e-002
ho2	Gas	1.683e-002	1.722e-002	1.762e-002	1.802e-002	1.841e-002	1.876e-002
nh2	Gas	5.104e-003	4.774e-003	4.444e-003	4.118e-003	3.800e-003	3.493e-003
ketene	Gas	3.255e-003	3.137e-003	2.982e-003	2.800e-003	2.603e-003	2.399e-003
o	Gas	2.889e-003	2.643e-003	2.418e-003	2.212e-003	2.022e-003	1.846e-003
h	Gas	2.376e-003	1.999e-003	1.679e-003	1.408e-003	1.179e-003	9.852e-004
ch4o	Gas	1.230e-003	1.194e-003	1.146e-003	1.090e-003	1.028e-003	9.621e-004
ch2oh	Gas	1.022e-003	9.741e-004	9.189e-004	8.589e-004	7.964e-004	7.332e-004
nh	Gas	5.717e-004	5.244e-004	4.790e-004	4.359e-004	3.951e-004	3.567e-004
cn	Gas	4.867e-004	4.478e-004	4.087e-004	3.703e-004	3.332e-004	2.980e-004
ch3	Gas	1.418e-004	1.219e-004	1.036e-004	8.715e-005	7.268e-005	6.018e-005
n	Gas	1.285e-004	1.165e-004	1.053e-004	9.499e-005	8.540e-005	7.655e-005
ch3cn	Gas	5.328e-005	5.132e-005	4.854e-005	4.519e-005	4.151e-005	3.768e-005
c2h2	Gas	5.198e-005	4.461e-005	3.769e-005	3.141e-005	2.586e-005	2.108e-005
ch4	Gas	2.682e-005	2.231e-005	1.834e-005	1.492e-005	1.203e-005	9.628e-006
ch2	Gas	1.256e-005	1.054e-005	8.739e-006	7.179e-006	5.846e-006	4.724e-006
c2h4	Gas	1.096e-007	8.611e-008	6.642e-008	5.039e-008	3.769e-008	2.786e-008
c	Gas	1.078e-007	8.722e-008	6.992e-008	5.559e-008	4.385e-008	3.434e-008
c(s)	solid	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000
Total	Gas	3.120e+001	3.094e+001	3.069e+001	3.045e+001	3.022e+001	2.999e+001
Total	Cond.	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000

Product concentrations (mol/kg)

Name		43.)	44.)	45.)	46.)	47.)	48.)
co2	Gas	9.100e+000	9.022e+000	8.938e+000	8.848e+000	8.753e+000	8.653e+000
h2o	Gas	7.632e+000	7.427e+000	7.226e+000	7.028e+000	6.833e+000	6.641e+000
n2	Gas	5.305e+000	5.251e+000	5.195e+000	5.137e+000	5.076e+000	5.013e+000

formac	Gas	4.131e+000	4.326e+000	4.515e+000	4.701e+000	4.882e+000	5.060e+000
co	Gas	1.434e+000	1.297e+000	1.172e+000	1.059e+000	9.563e-001	8.639e-001
hnco	Gas	1.015e+000	1.044e+000	1.072e+000	1.097e+000	1.121e+000	1.143e+000
no	Gas	2.419e-001	2.403e-001	2.382e-001	2.355e-001	2.323e-001	2.285e-001
n2o	Gas	1.996e-001	2.243e-001	2.512e-001	2.804e-001	3.117e-001	3.453e-001
hno2	Gas	1.914e-001	2.157e-001	2.420e-001	2.703e-001	3.004e-001	3.324e-001
oh	Gas	9.502e-002	8.848e-002	8.225e-002	7.632e-002	7.070e-002	6.538e-002
no2	Gas	7.957e-002	8.917e-002	9.955e-002	1.107e-001	1.224e-001	1.348e-001
cho	Gas	5.824e-002	5.354e-002	4.908e-002	4.488e-002	4.096e-002	3.731e-002
h2o2	Gas	3.962e-002	4.071e-002	4.169e-002	4.254e-002	4.324e-002	4.377e-002
nh3	Gas	3.848e-002	3.630e-002	3.418e-002	3.212e-002	3.015e-002	2.827e-002
h2	Gas	3.773e-002	3.249e-002	2.796e-002	2.406e-002	2.071e-002	1.783e-002
hno	Gas	3.337e-002	3.383e-002	3.418e-002	3.442e-002	3.455e-002	3.455e-002
o2	Gas	3.248e-002	3.234e-002	3.212e-002	3.182e-002	3.141e-002	3.089e-002
ch2o	Gas	3.244e-002	3.022e-002	2.808e-002	2.603e-002	2.409e-002	2.226e-002
nco	Gas	2.557e-002	2.556e-002	2.544e-002	2.523e-002	2.493e-002	2.457e-002
ho2	Gas	1.908e-002	1.933e-002	1.952e-002	1.964e-002	1.967e-002	1.962e-002
hcn	Gas	1.395e-002	1.256e-002	1.127e-002	1.010e-002	9.039e-003	8.082e-003
nh2	Gas	3.200e-003	2.921e-003	2.660e-003	2.415e-003	2.188e-003	1.978e-003
ketene	Gas	2.194e-003	1.995e-003	1.806e-003	1.629e-003	1.465e-003	1.316e-003
o	Gas	1.682e-003	1.530e-003	1.388e-003	1.256e-003	1.134e-003	1.021e-003
ch4o	Gas	8.950e-004	8.282e-004	7.632e-004	7.009e-004	6.419e-004	5.866e-004
h	Gas	8.222e-004	6.854e-004	5.707e-004	4.748e-004	3.947e-004	3.280e-004
ch2oh	Gas	6.708e-004	6.104e-004	5.529e-004	4.988e-004	4.486e-004	4.023e-004
nh	Gas	3.209e-004	2.877e-004	2.571e-004	2.290e-004	2.033e-004	1.801e-004
cn	Gas	2.651e-004	2.348e-004	2.070e-004	1.820e-004	1.595e-004	1.395e-004
n	Gas	6.840e-005	6.093e-005	5.411e-005	4.790e-005	4.228e-005	3.721e-005
ch3	Gas	4.952e-005	4.055e-005	3.308e-005	2.691e-005	2.185e-005	1.772e-005
ch3cn	Gas	3.389e-005	3.025e-005	2.684e-005	2.371e-005	2.088e-005	1.835e-005
c2h2	Gas	1.705e-005	1.370e-005	1.095e-005	8.729e-006	6.941e-006	5.514e-006
ch4	Gas	7.663e-006	6.071e-006	4.794e-006	3.778e-006	2.973e-006	2.339e-006
ch2	Gas	3.792e-006	3.027e-006	2.405e-006	1.904e-006	1.503e-006	1.183e-006
c	Gas	2.672e-008	2.066e-008	1.590e-008	1.218e-008	9.289e-009	7.065e-009
c2h4	Gas	2.039e-008	1.481e-008	1.069e-008	7.687e-009	5.511e-009	3.946e-009
c(s)	solid	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000
Total	Gas	2.977e+001	2.955e+001	2.934e+001	2.914e+001	2.894e+001	2.875e+001
Total	Cond.	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000

Product concentrations (mol/kg)

Name		49.)	50.)
co2	Gas	8.550e+000	8.442e+000
h2o	Gas	6.453e+000	6.268e+000
formac	Gas	5.233e+000	5.402e+000
n2	Gas	4.948e+000	4.880e+000
hnco	Gas	1.164e+000	1.183e+000
co	Gas	7.808e-001	7.060e-001
n2o	Gas	3.809e-001	4.186e-001
hno2	Gas	3.658e-001	4.006e-001
no	Gas	2.242e-001	2.194e-001
no2	Gas	1.477e-001	1.609e-001
oh	Gas	6.035e-002	5.562e-002
h2o2	Gas	4.414e-002	4.433e-002
hno	Gas	3.444e-002	3.422e-002
cho	Gas	3.395e-002	3.086e-002
o2	Gas	3.028e-002	2.956e-002
nh3	Gas	2.649e-002	2.480e-002
nco	Gas	2.414e-002	2.366e-002
ch2o	Gas	2.056e-002	1.897e-002
ho2	Gas	1.948e-002	1.926e-002
h2	Gas	1.537e-002	1.325e-002
hcn	Gas	7.224e-003	6.456e-003
nh2	Gas	1.784e-003	1.607e-003
ketene	Gas	1.181e-003	1.059e-003
o	Gas	9.166e-004	8.209e-004

ch4o	Gas	5.351e-004	4.876e-004
ch2oh	Gas	3.600e-004	3.215e-004
h	Gas	2.725e-004	2.263e-004
nh	Gas	1.591e-004	1.402e-004
cn	Gas	1.217e-004	1.061e-004
n	Gas	3.267e-005	2.861e-005
ch3cn	Gas	1.611e-005	1.414e-005
ch3	Gas	1.436e-005	1.164e-005
c2h2	Gas	4.379e-006	3.480e-006
ch4	Gas	1.841e-006	1.449e-006
ch2	Gas	9.306e-007	7.310e-007
c	Gas	5.359e-009	4.057e-009
c2h4	Gas	2.823e-009	2.021e-009
c(s)	solid	0.000e+000	0.000e+000
Total	Gas	2.857e+001	2.839e+001
Total	Cond.	0.000e+000	0.000e+000

References

(1) Laurence E Fried, W Michael Howard, P Clark Souers (1998): Cheetah 2.0 User's Manual, UCRL-MA-117541 Rev.5, Lawrence Livermore National Laboratory.

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