

FFI RAPPORT

TESTING OF PYROTECHNIC COMPOSITIONS IN CLOSED VESSEL

NEVSTAD Gunnar Ove

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Bjarne Haugstad
Director of Research

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NEVSTAD Gunnar Ove

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FORSVARETS FORSKNINGSINSTITUTT
Norwegian Defence Research Establishment
P O Box 25, NO-2027 Kjeller, Norway

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8) ABSTRACT <p>In MP (multipurpose) munitions the nose cap is filled with a pyrotechnic composition that, when it sees certain stimuli, ignite and start burning. This burning is important for how the munitions will function. Compositions based on aluminium, magnesium and aluminium /magnesium powders in combination with potassium perchlorate have been tested.</p> <p>Compositions with a loading density of up to 0.6 g/cm³ have been tested in a 150 cm³ Closed Vessel, and pressure- time curves have been recorded. The tested compositions have different burn rates and ignitability. In addition to the experimentally measured the pressures, we have done some theoretical calculations of the expected pressures by use of the thermochemical code Cheetah.</p>				
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TESTING OF PYROTECHNIC COMPOSITIONS IN CLOSED VESSEL

1 INTRODUCTION

The nose cap of MP (multipurpose) munitions is filled with pyrotechnic powder that will ignite and burn when it is exposed to certain stimulus. This burning reaction is important for how and when the other energetic compositions in the projectile will react. To be able to regulate or control the properties of the pyrotechnic powder it's important to know how it reacts after it has been ignited. One way to study the burning properties is by testing the pyrotechnic powder under controlled conditions in a Closed Vessel (CV).

The pyrotechnics we have tested is RS-41 and combination of its main ingredients, magnesium, aluminium and potassium perchlorate. The tests have been carried out with different loading densities and combinations of ingredients. The problem with this kind of energetic materials when they burn is that they give very high temperatures compared to energetic materials based on the elements C, H, N and O. Another difference when they burn is that, instead of giving mainly gas products as does propellants and explosives, pyrotechnics based on metal powders give solid products.

The combination of very high temperature and pressure set strong restrictions on what we can manage to test with regard to loading densities of pyrotechnic compositions without damaging the test equipment. In addition to the experimental testing, we have carried out some theoretical calculations by use of the thermochemical code Cheetah to determine what pressures we should expect to measure in the CV.

2 EXPERIMENTAL

2.1 Test performance and conditions

The different compositions have been tested in a 150 cm³ Closed Vessel. We have used three different CV that should be equal. For some tests we used a steel tube inside the vessel so the vessel should be easier to clean. This tube, when it was new, had a mass of 284.73 g.

The pressure was measured with a Kistler 6211 cell. A blue/brown squib surrounded with 2 g Black Powder (BP) in a plastic bag was used to ignite the tested compositions. Figure 2.1 gives a picture of the used ignition device. In Figure 2.2 is given a picture of the CV just before it should be fired. The green cable is the registration of the pressure, and the grey is for ignition of the squib.

For the majority of experiments the tested powder has been in a plastic bag that surround the squib/BP. For the rest the powder was loosely filled in the vessel.



Figure 2.1 Ignition part of the CV, showing the squib surrounded by a plastic bag with the Black Powder.



Figure 2.2 The CV ready for firing.

The pressure has been measured every 4 μs and the total number of points has been 65.536. Total sampling time 0.262 s.

2.2 Tested samples

Three composition types have been tested: RS-41, Mg + KClO_4 and Al + KClO_4 . All compositions were received from Nammo Raufoss mixed ready for testing. In addition to the pyrotechnic powder was some M1-propellant fired to check the pressure cell.

The Table 2.1 gives a summary of test conditions and tested compositions.

Firing No	Date	Composition	Vessel	Condition	Weight (g)	Loading Density (g/cm ³)
CV-309	3/11-00	M1	With tube	Loosely powder	24.84	0.2181
CV-310	23/11-00	50/50 Mg-atomized 134648/KClO ₄ 134302	With tube	Loosely powder	50.0156	0.4392
CV-311	23/11-00	M1-propellant	With tube	Loosely powder	25.09	0.2233
CV-312	23/11-00	P96-29-2 134685 Mg	With tube	Loosely powder	13.69	0.1202
CV-313	24/11-00	powder ≈ Mg/Al	With tube	Loosely powder	22.86	0.2008
CV-314	24/11-00	134582 in particle size, 50 Mg/50 KClO ₄	With tube	Loosely powder	45.56	0.4001
CV-315	5/12-00	P-96-28-2 133516 Al	With tube	Loosely powder	13.79	0.1211
CV-316	5/12-00	powder ≈ Mg/Al	With tube	Loosely powder	22.80	0.2002
CV-317	5/12-00	134582 in particle size, 50 Al/50 KClO ₄	With tube	Loosely powder	45.60	0.4005
CV-318	8/12-00	RS-41 "Skarp" delivered 30.4-98	I	Packed in bag	60.08	0.4005
CV-319	8/12-00		I	Packed in bag	18.03	0.1202
CV-320	8/12-00		I	Packed in bag	30.10	0.2007
CV-321	9/12-00		I	Packed in bag	30.00	0.2000
CV-322	9/12-00		I	Packed in bag	90.00	0.6000
CV-323	31/1-01		P-96-28-2 133516 Al	I	Packed in bag	30.00
CV-324	31/1-01	powder ≈ Mg/Al 134582 in particle size, 50 Al/50 KClO ₄	I	Packed in bag	18.11	0.1207
CV-325	01/02-01	P-96-28-1 133516 Al	II	Packed in bag	60.11	0.4007
CV-326	01/02-01	powder ≈ Mg/Al	II	Packed in bag	18.11	0.1207
CV-327	01/02-01	134582 in particle size, 49 Al/49 KClO ₄ /2 Res	II	Packed in bag	60.08	0.4005
CV-328	2/2-01	P96-29-1 134685 Mg	III	Packed in bag	18.08	0.1205
CV-329	2/2-01	powder ≈ Mg/Al	III	Packed in bag	30.15	0.2010
CV-330	2/2-01	134582 in particle size, 49 Al/49 KClO ₄ /2 Res	III	Packed in bag	60.00	0.4000

³Volume tube 36.0418 cm³.

Table 2.0.1 Firing conditions for performed Closed Vessel firings.

3 RESULTS

3.1 Mg and KClO₄ mixtures

We have used three different mixtures of magnesium and potassium perchlorate. Test conditions is given in Table 2.1. The results from the firings are summarised in Table 3.1.

Firing No	Composition	Weight (g)	Load density (g/cm ³)	Reaction	Maximum Pressure (bars)
CV-310	50/50 Mg-atomised 134648/ KClO ₄ 134302	50.0156	0.4392	Very fast	
CV-312	P96-29-2 134685 Mg powder ≈	13.69	0.1202	Normal	327
CV-313	Mg/Al 134582 in particle size,	22.86	0.2008	Normal	480.5
CV-314	50 Mg/50 KClO ₄	45.56	0.4001	Normal	795
CV-328	P96-29-1 134685 Mg powder ≈	18.08	0.1205	Normal	458.5
CV-329	Mg/Al 134582 in particle size	30.15	0.2010	Normal	649
CV-330	49 Al/49 KClO ₄ /2 Ca-Resinate	60.00	0.4000	Fast	1264.5

Table 3.1 Properties of the firings containing Mg.

The first shot, having a loading density of 0.44 g/cm³, did react very fast and the reaction is more like a deflagration than a burn, Figure 3.1. The pressure-time curves for all firings are given in Figure 3.1 to 3.7. For all firings with Mg-powder/KClO₄ the ignition of the mixture takes place instantaneous with no delay.

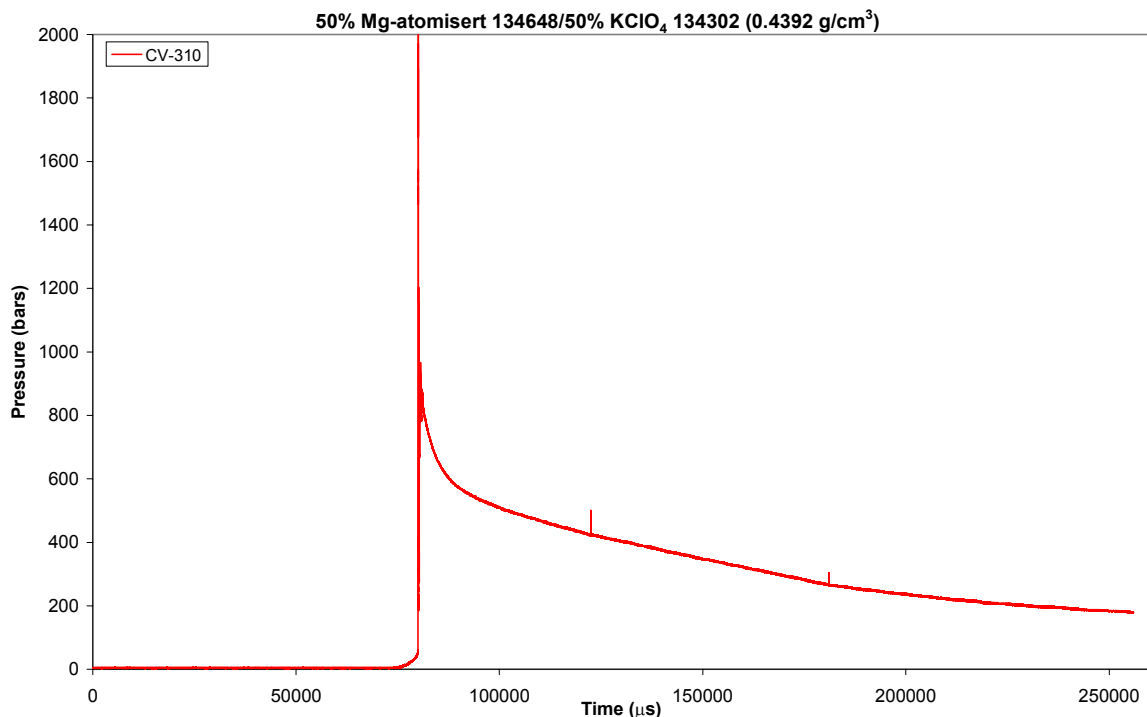


Figure 3.1 Pressure-time curve for firing CV-310, load density 0.4382 g/cm³, 50/50 atomised Mg and KClO₄.

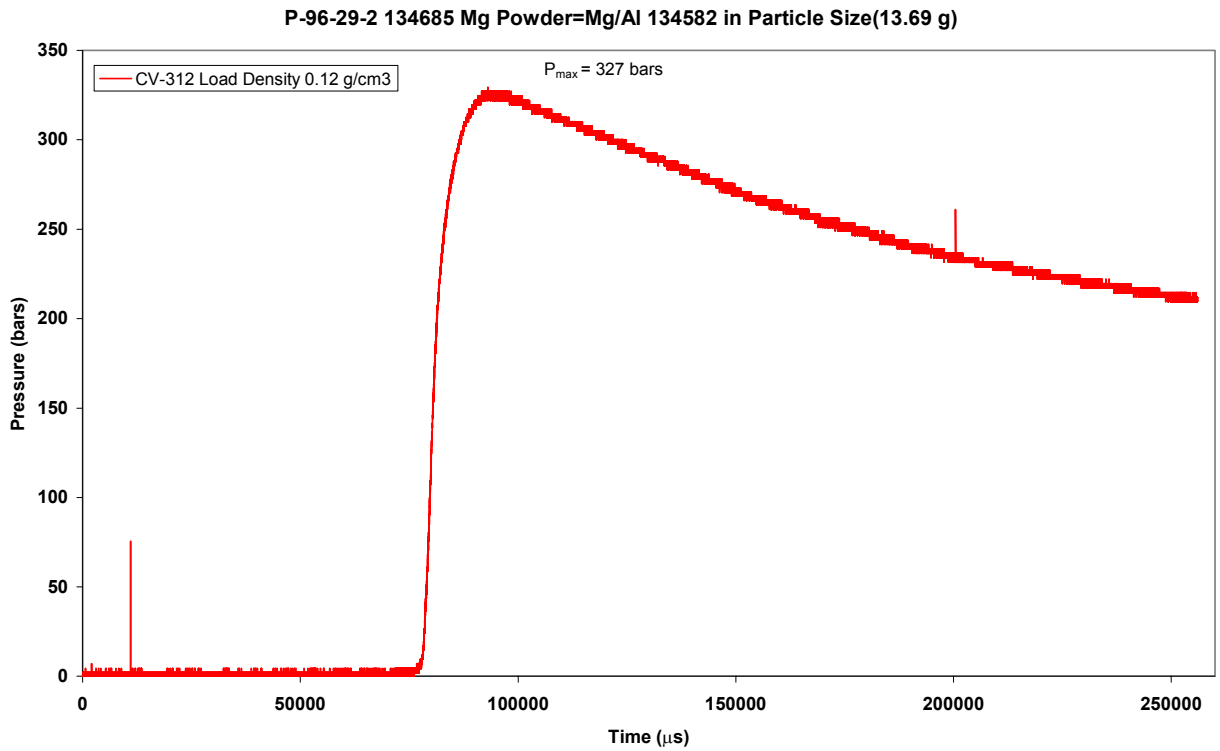


Figure 3.2 Pressure-time curve for firing CV-312, 50/50 Mg/KClO₄, load density 0.12 g/cm³.

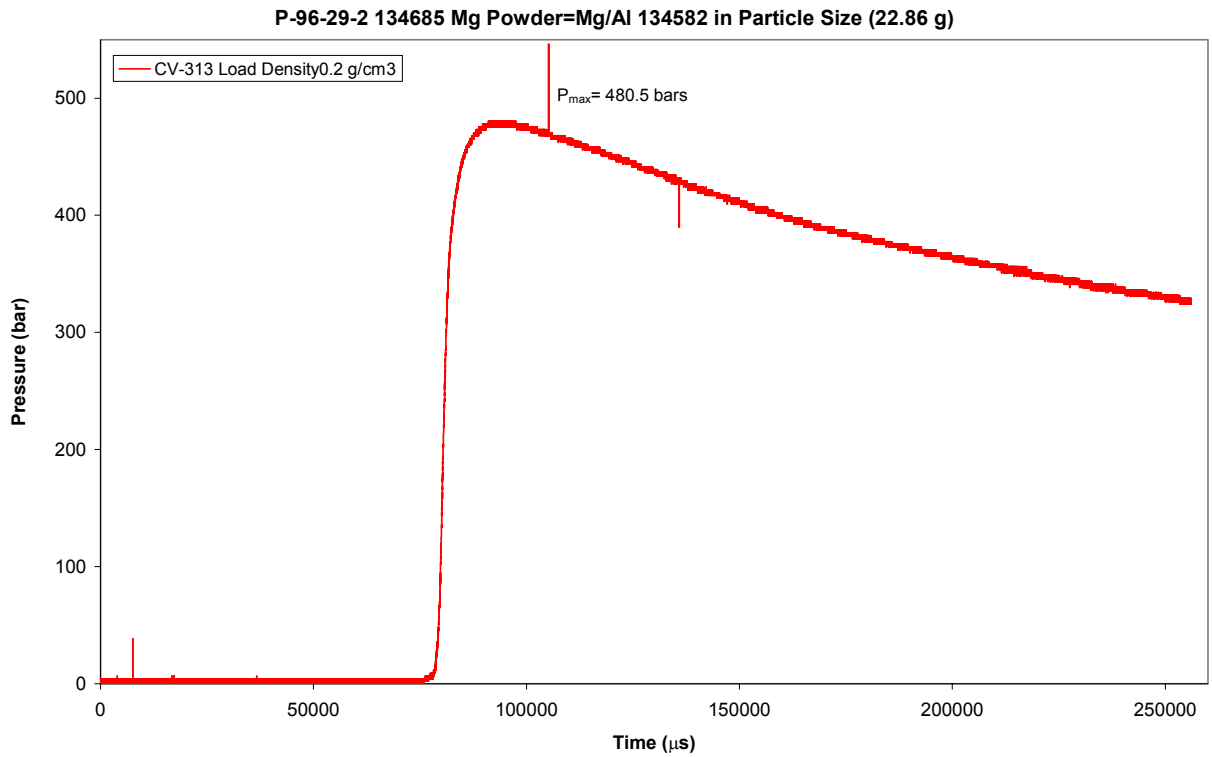


Figure 3.3 Pressure-time curve for firing CV-313, 50/50 Mg/KClO₄, load density 0.20 g/cm³.

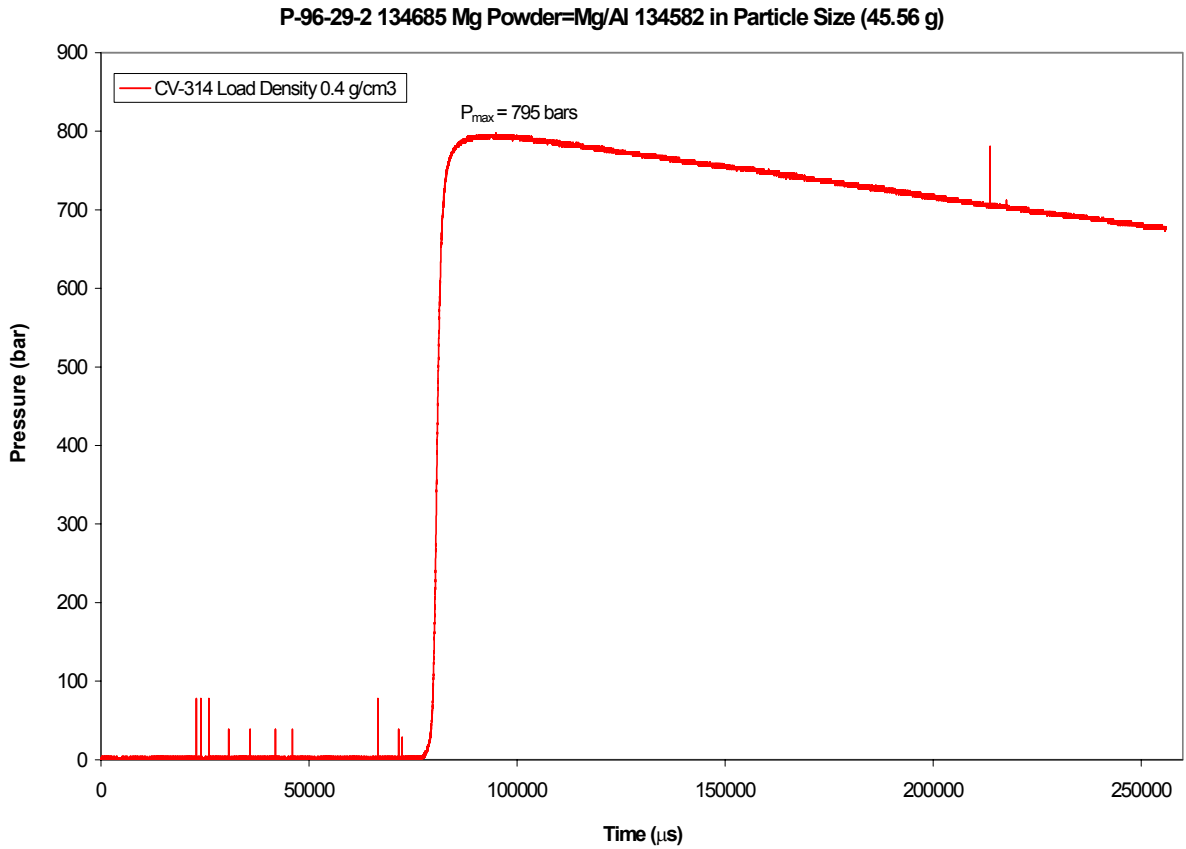


Figure 3.4 Pressure-time curve for firing CV-314, 50/50 Mg/KClO₄, load density 0.40 g/cm³.

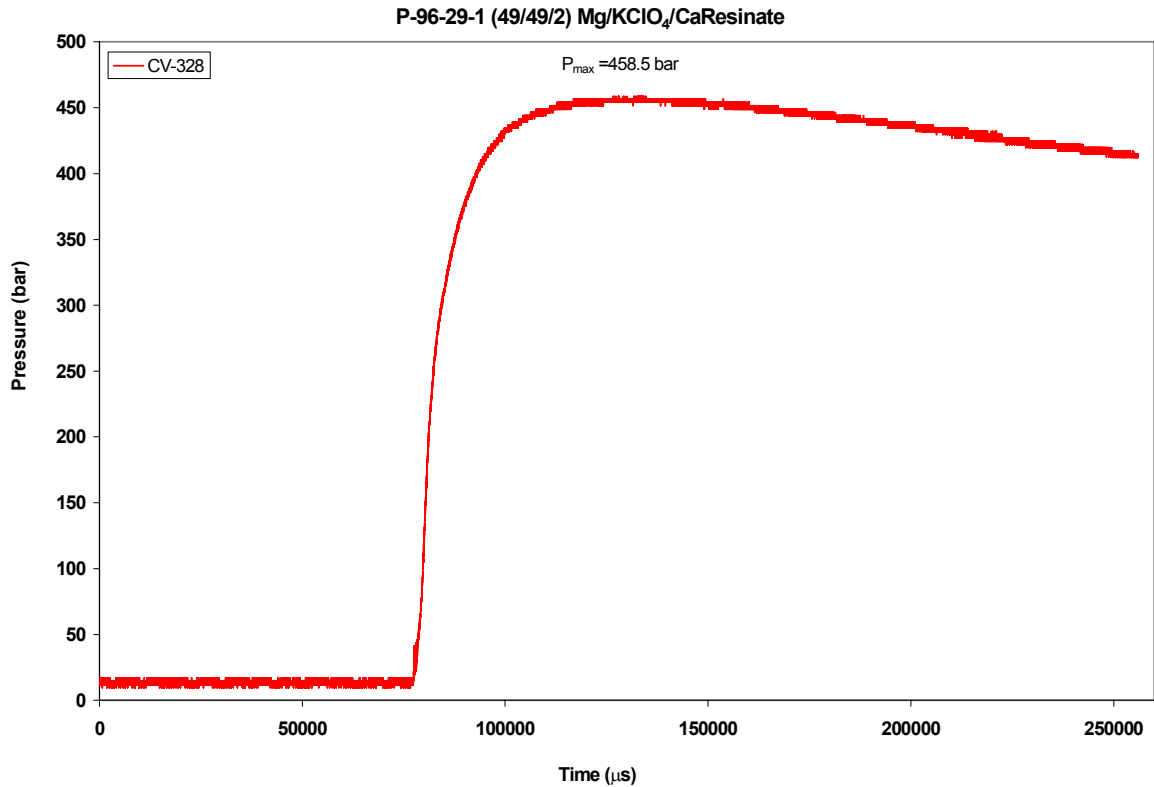


Figure 3.5 Pressure-time curve for firing CV-328, 49/49/2 Mg/KClO₄/Ca-res, load density 0.12 g/cm³.

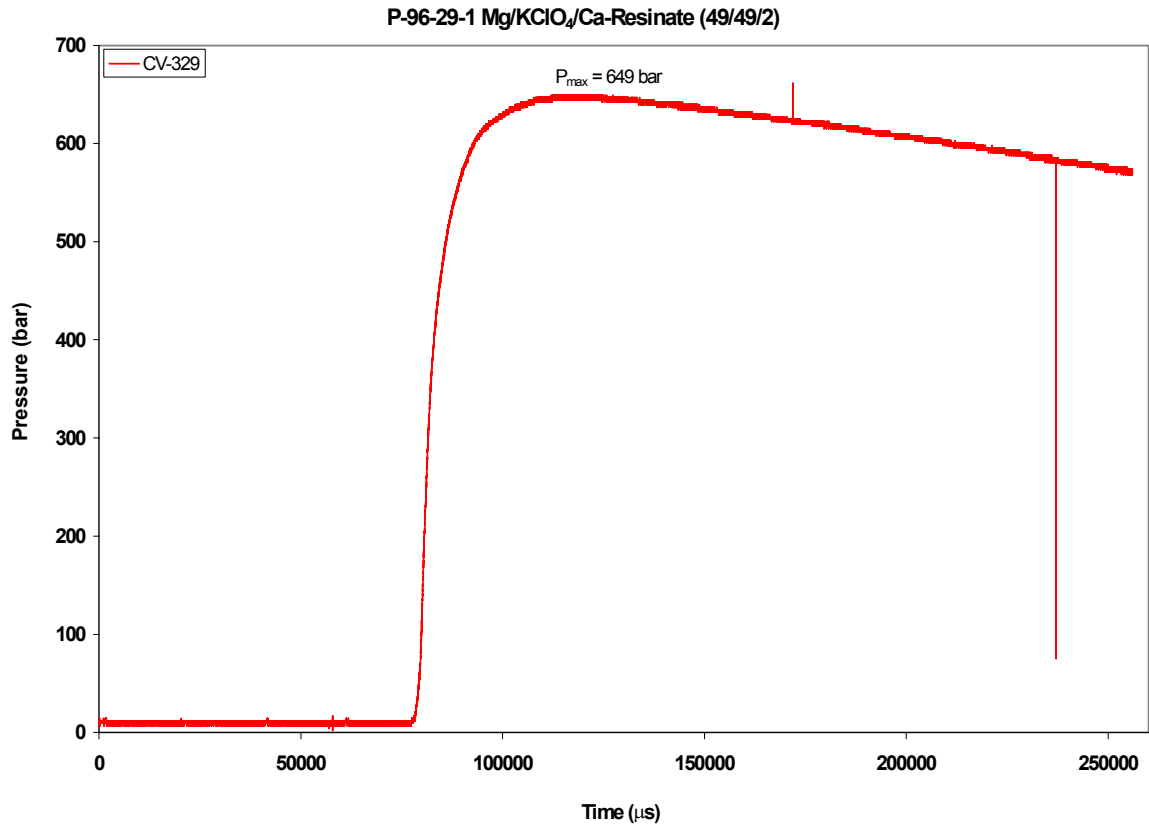


Figure 3.6 Pressure-time curve for firing CV-329, 49/49/2 Mg/KClO₄/Ca-res, load density 0.2 g/cm³.

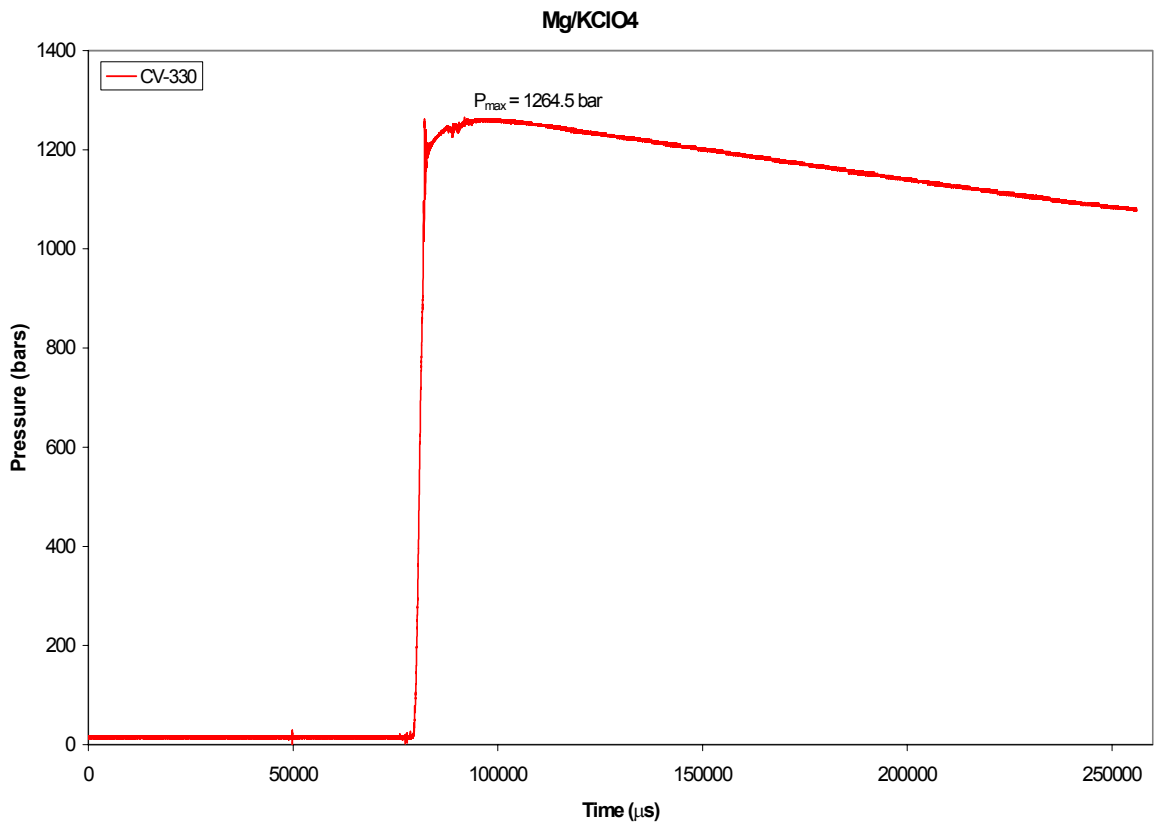


Figure 3.7 Pressure-time curve for firing CV-330, 49/49/2 Mg/KClO₄/Ca-res, load density 0.40 g/cm³.

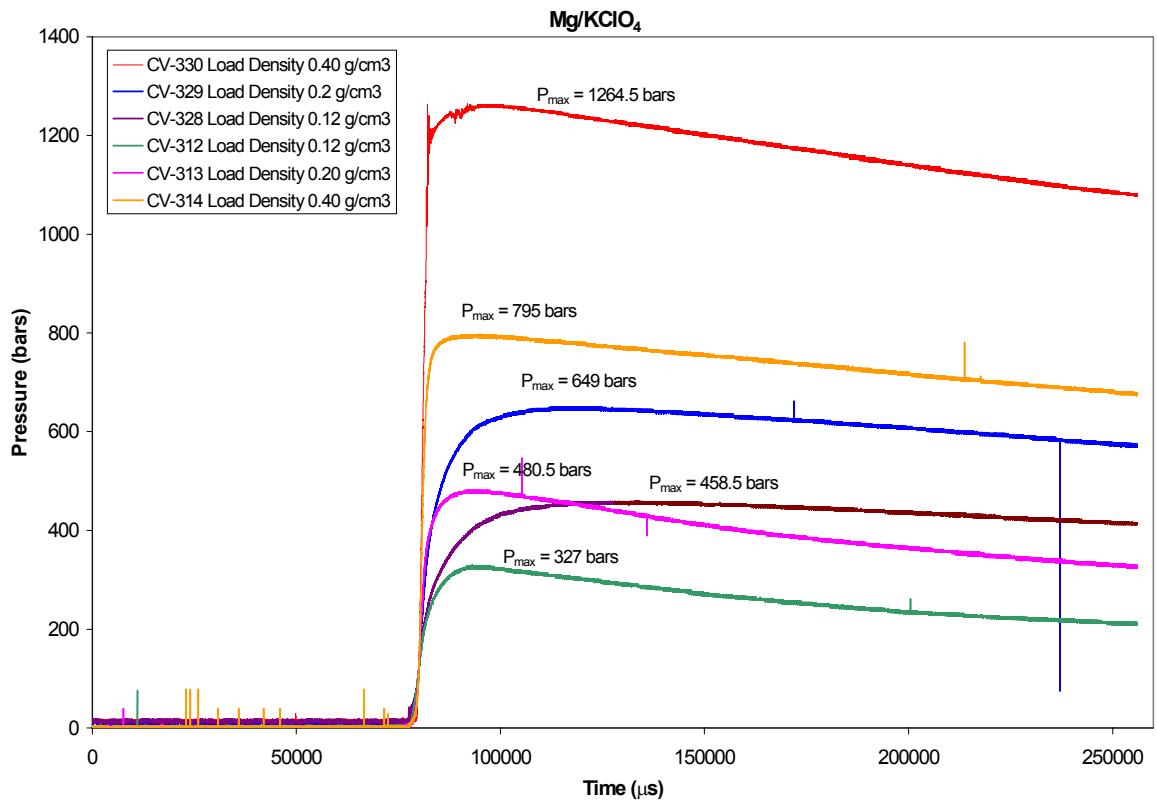


Figure 3.8 Pressure-time curves for all CV-firings containing Mg/KClO₄.

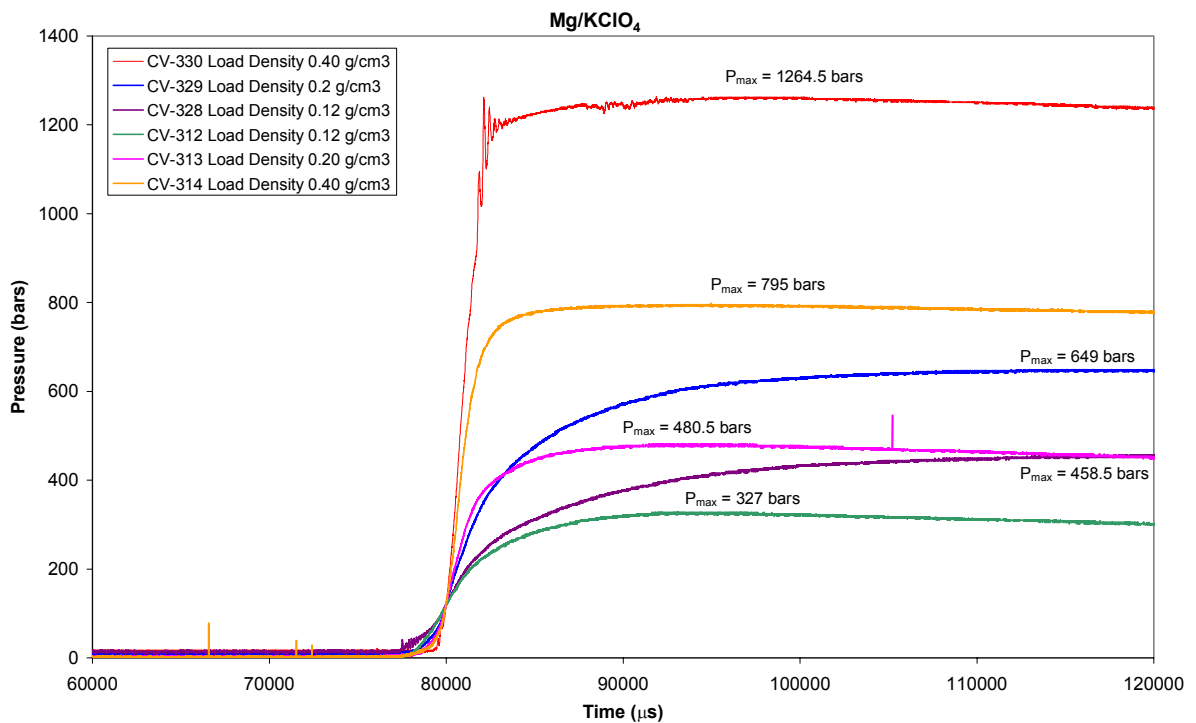


Figure 3.9 Parts of the pressure-time curves given in Figure 3.8.

For the firings (CV-312, CV-313, CV-314), where we use a steel tube inside the vessel to protect the vessel and facilitate the cleaning process, we have obtained lower maximum pressures than for the firings without the steel tube. Another difference between the results for these two series of firings is the form of the curves. The two firings with lowest loading densities have slower pressure rise with no steel tube in the vessel than the firings with steel

tube in the vessel. The exception is for the highest load density, firing CV-330, which for the first part of the reaction has a fast burning or a tendency towards a deflagration reaction, Figure 3.8. One difference between the powders used in these two series is that the one carried out with the steel tube in the vessel does not contain Ca-resinate. In Figure 3.10 we have

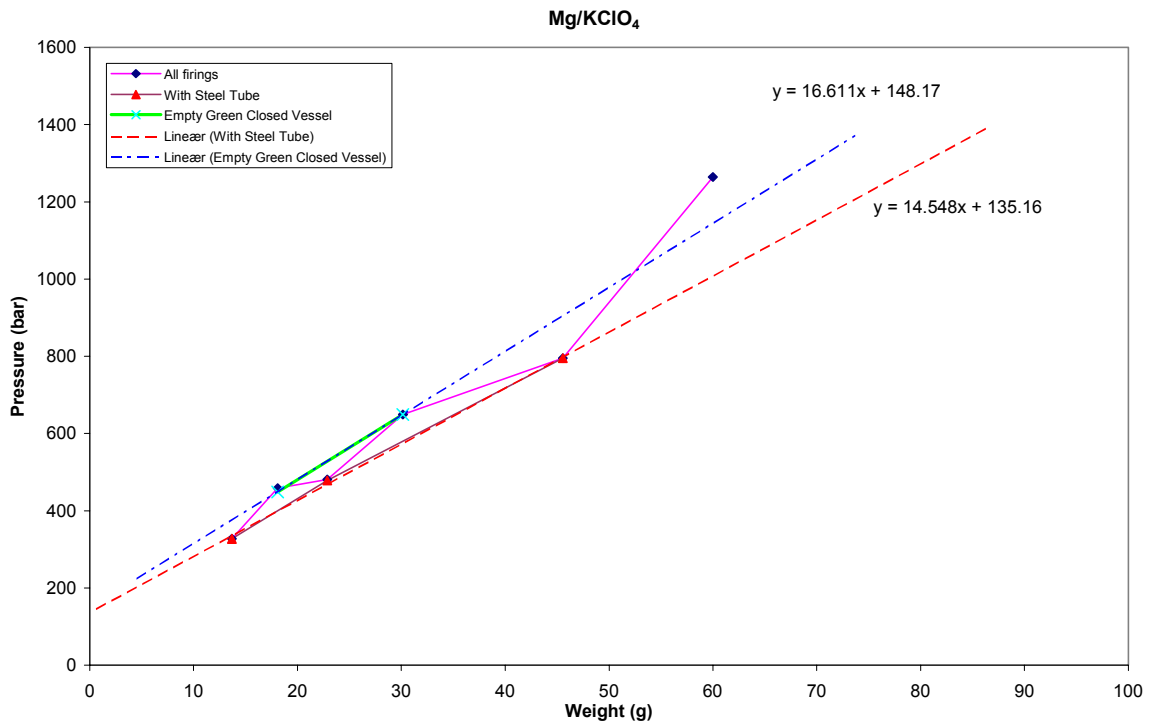


Figure 3.10 Maximum pressures as function of weights of magnesium compositions.

plotted maximum pressure as function of loaded amount of powder used in each firing. The pressures for the first series of firings (CV-312 – CV-314) lie on more or less a straight line. However, all points lie well below the second series of firings, especially if we take the chamber volume into consideration. The firings with the steel tube inside the CV have a much smaller volume available for the combustion products than the firings performed with a clean CV without the steel tube.

For the second series of firings the pressures do not lie on a straight line, the firing with load density 0.40 g/cm^3 (or 60 g) does deviate. This deviation can by looking on the pressure-time curves be explained by another reaction for CV-330 than for the other firings.

However, another strange observation for the firings of the Mg/KClO_4 compositions is, that the pressure does not increase exponentially with increasing loading density as it does for propellants and other CHNO-compositions.

3.2 Al and KClO_4 mixtures

For aluminium we have used two different mixtures, one with calcium resinate, and one mixture without Ca-resinate. Table 3.2 gives a summary of the measured pressures and other information about the firings. Figure 3.11 to 3.18 gives all pressure-time curves. Figure 3.19 and 3.20 give a summary of all curves. The trends for the firings with Al-powder are more or less the same as for the firings with Mg-powder. In general the firings with steel tube in the CV give significantly lower pressures than the firings without. Firings where the composition contains Ca-resinate, give slightly higher pressures.

Firing No	Composition	Weight (g)	Load density (g/cm^3)	Reaction	Maximum Pressure (bars)
CV-315	P-96-28-2 133516 Al powder \approx	13.79	0.1211	Normal	197.5
CV-316	Mg/Al 134582 in particle size	22.80	0.2002	Very fast	\sim 480
CV-317	50 Al/50 KClO_4	45.60	0.4005	Normal	571
CV-323	P-96-28-2 133516 Al powder \approx	30.00	0.2000	Normal	463.5
CV-324	Mg/Al 134582 in particle size 50 Al/50 KClO_4	18.11	0.1207	Normal	319
CV-325	P-96-28-1 133516 Al powder \approx	60.11	0.4007	Normal	875
CV-326	Mg/Al 134582 in particle size	18.11	0.1207	Normal	356
CV-327	49 Al/49 KClO_4 /2 Ca-Resinate	60.08	0.4005	Normal	937.5

Table 3.2 Properties of Closed Vessel firings of compositions containing aluminium.

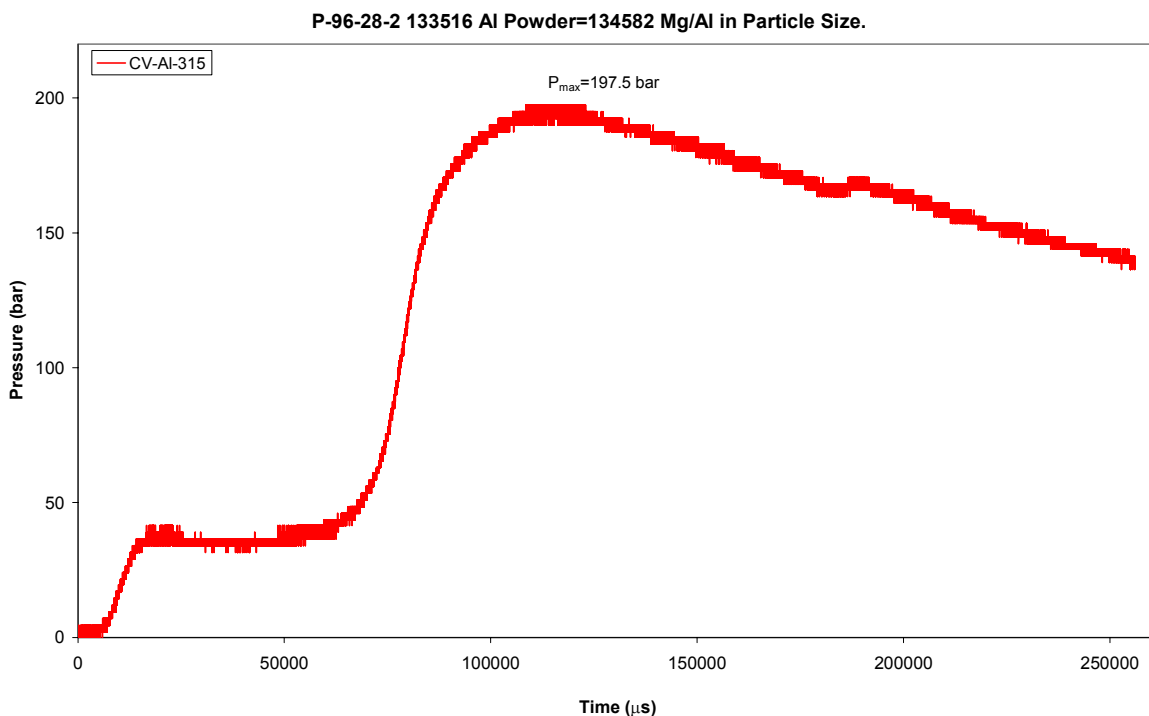


Figure 3.11 Pressure-time curve for firing CV-315, 50/50 Al/ KClO_4 , load density $0.12 \text{ g}/\text{cm}^3$.

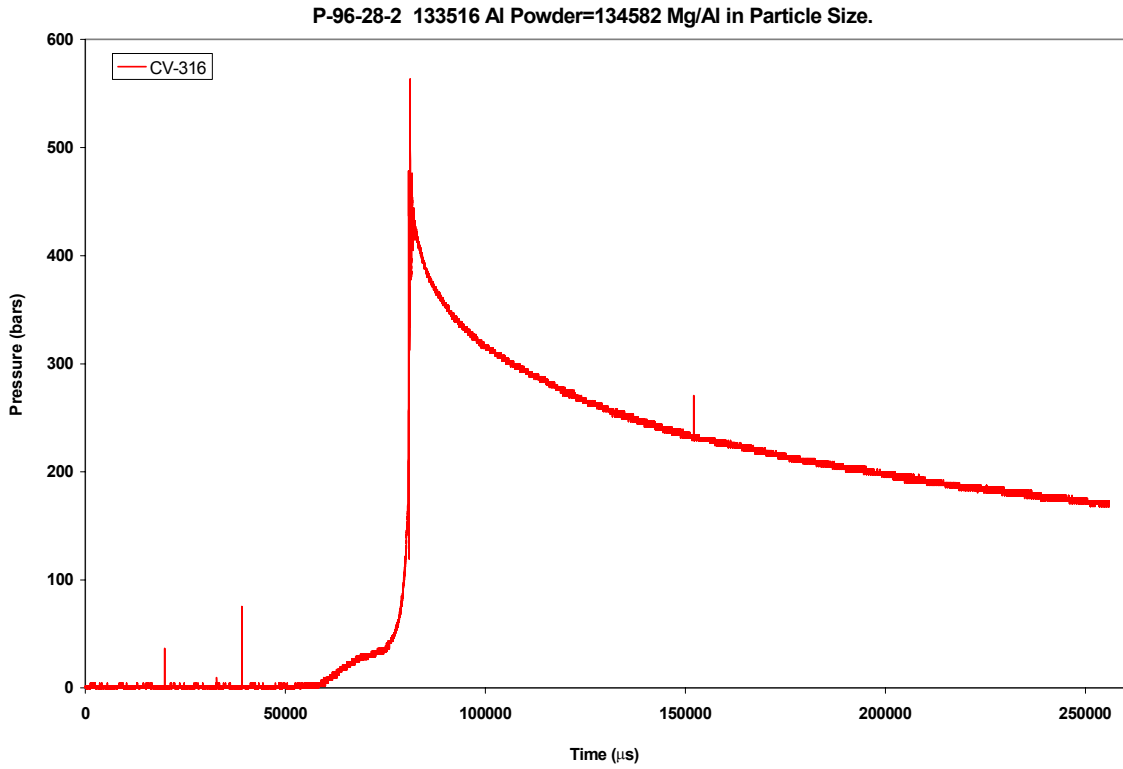


Figure 3.12 Pressure-time curve for firing CV-316, 50/50 Al/KClO₄, load density 0.20 g/cm³.

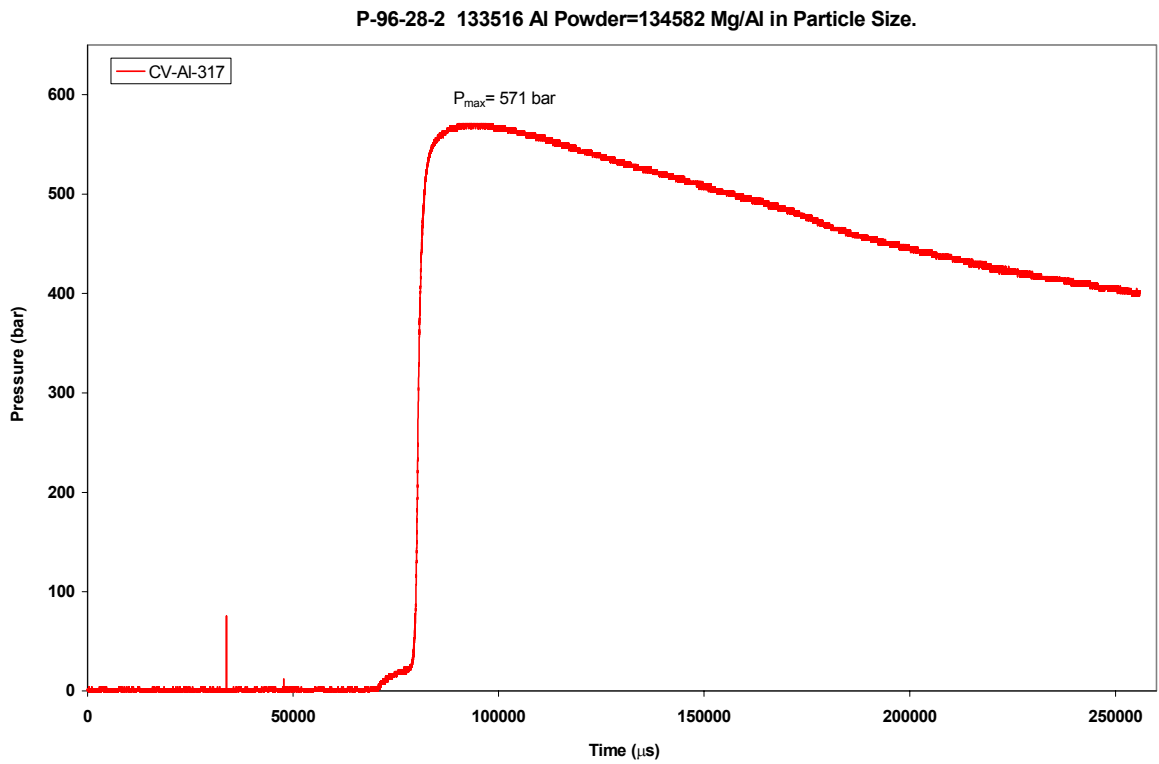


Figure 3.13 Pressure-time curve for firing CV-317, 50/50 Al/KClO₄, load density 0.40 g/cm³.

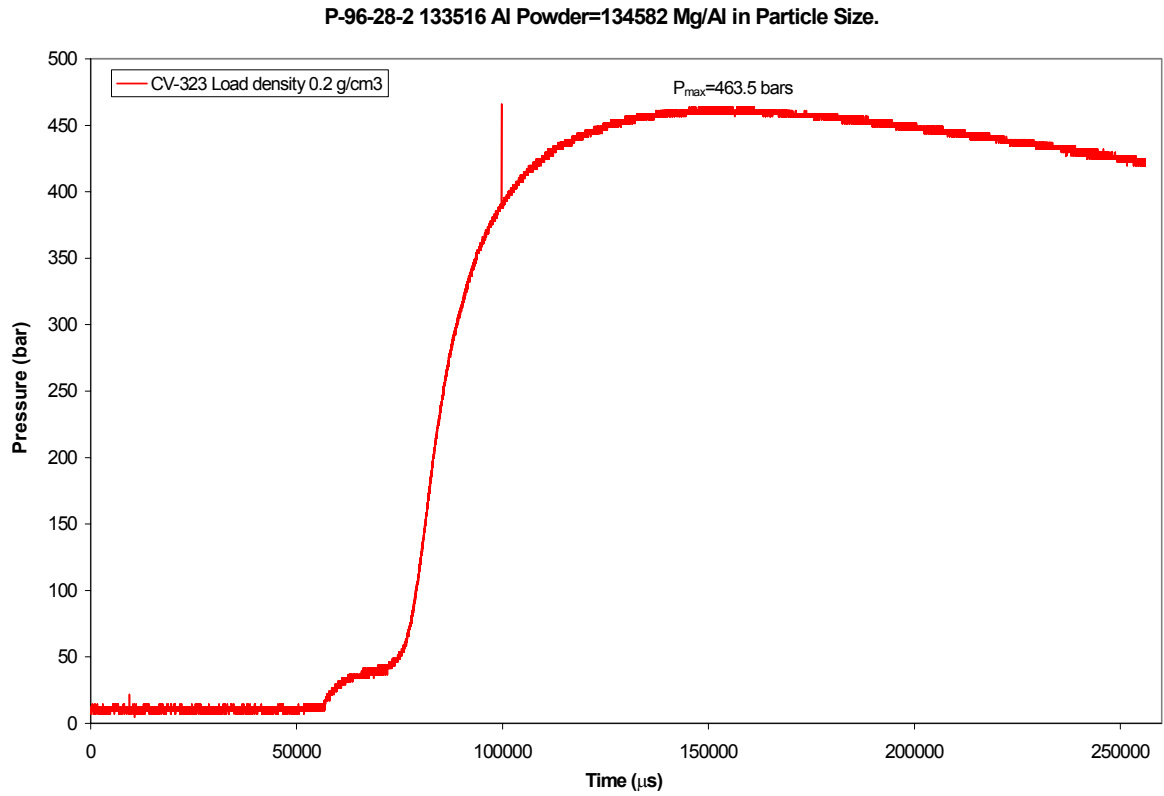


Figure 3.14 Pressure-time curve for firing CV-323, 50/50 Al/KClO₄, load density 0.20 g/cm³.

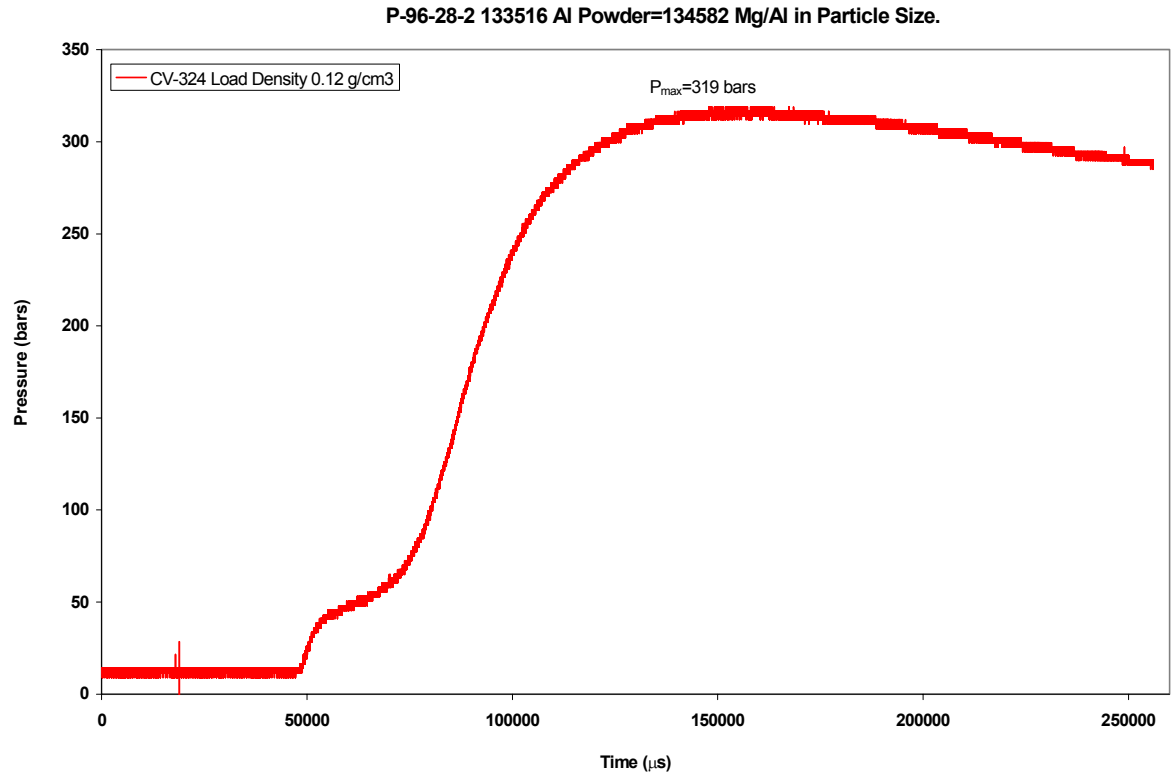


Figure 3.15 Pressure-time curve for firing CV-324, 50/50 Al/KClO₄, load density 0.12 g/cm³.

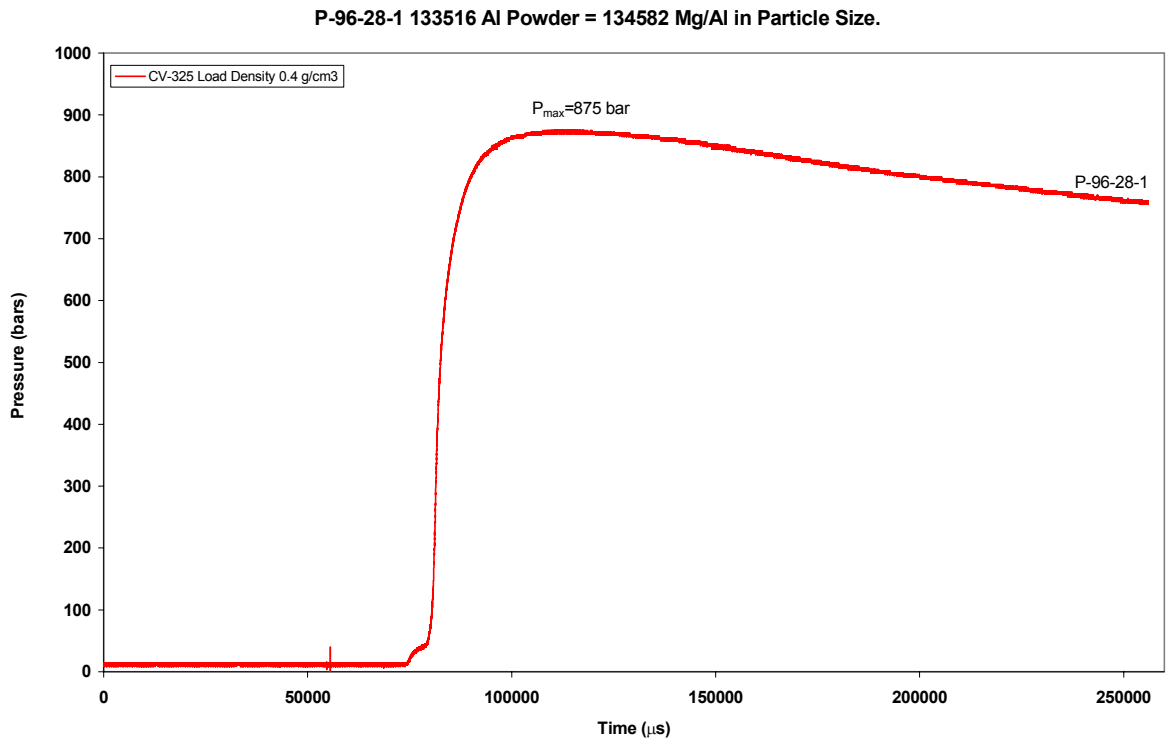


Figure 3.16 Pressure-time curve CV-325, 49/49/2 Al/KClO₄/Ca-res, load density 0.40 g/cm³

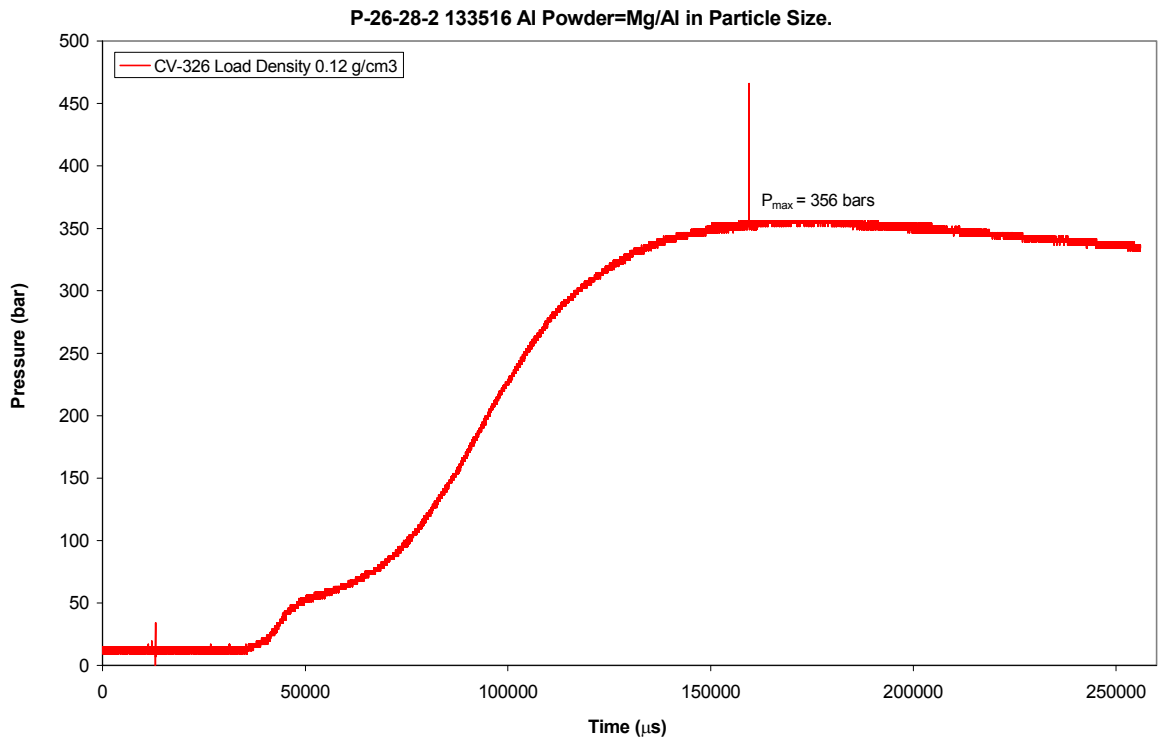


Figure 3.17 Pressure-time curve for firing CV-326, 49/49/2 Al/KClO₄/Ca-res, load density 0.12 g/cm³

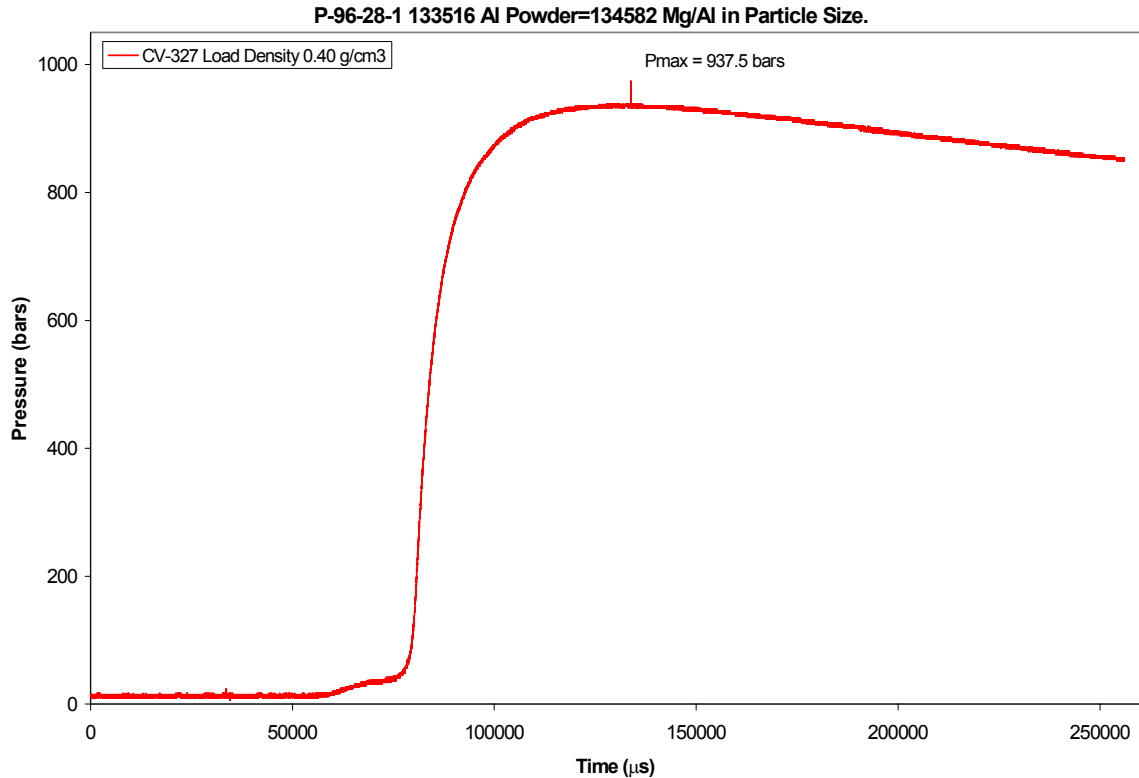


Figure 3.18 Pressure-time curve for firing CV-327, 49/49/2 Al/KClO₄/Ca-res, load density 0.40 g/cm³.

As for the Mg-powder firings, gives one of the firing with Al-powder, firing CV-316, a reaction that is faster than normal burning. This firing was carried out with a steel tube inside the CV and loosely loaded powder.

One difference between the pressure-time curves for Mg and Al is that for the Al-curves the ignition is much slower than for Mg. After the BP has been ignited there is a delay in the ignition of the composition of up to 60.000 μs for CV-315, the firing that has the lowest amount of powder. For CV-315 the powder was loosely loaded. However, since the other two firings with loosely load powder, CV-316 and CV-317, are among the firings having fastest ignition, it may not explain the observed delay.

All firings with aluminium/potassium perchlorate give significantly lower maximum pressure, burn rate or reaction rate than similar compositions containing Mg instead of Al.

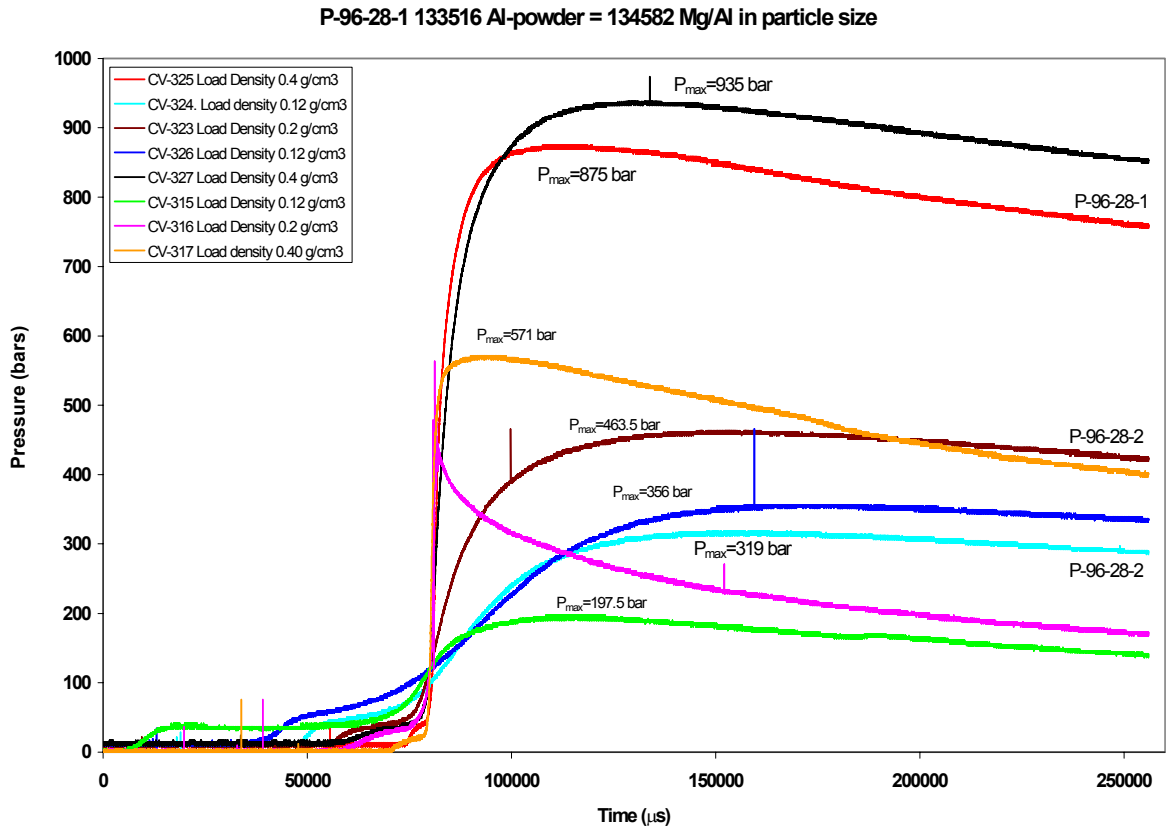


Figure 3.19 Pressure-time curves for all firings with aluminium.

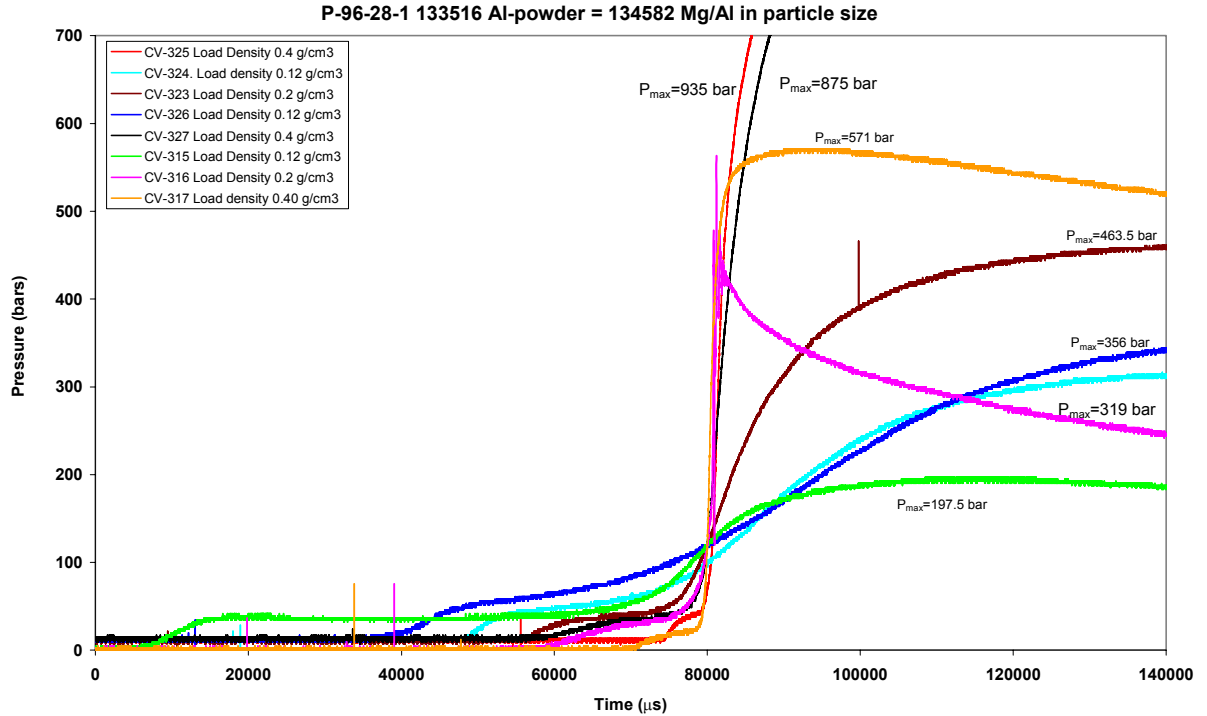


Figure 3.20 Parts of the pressure-time curves given in Figure 3.19 enlarged.

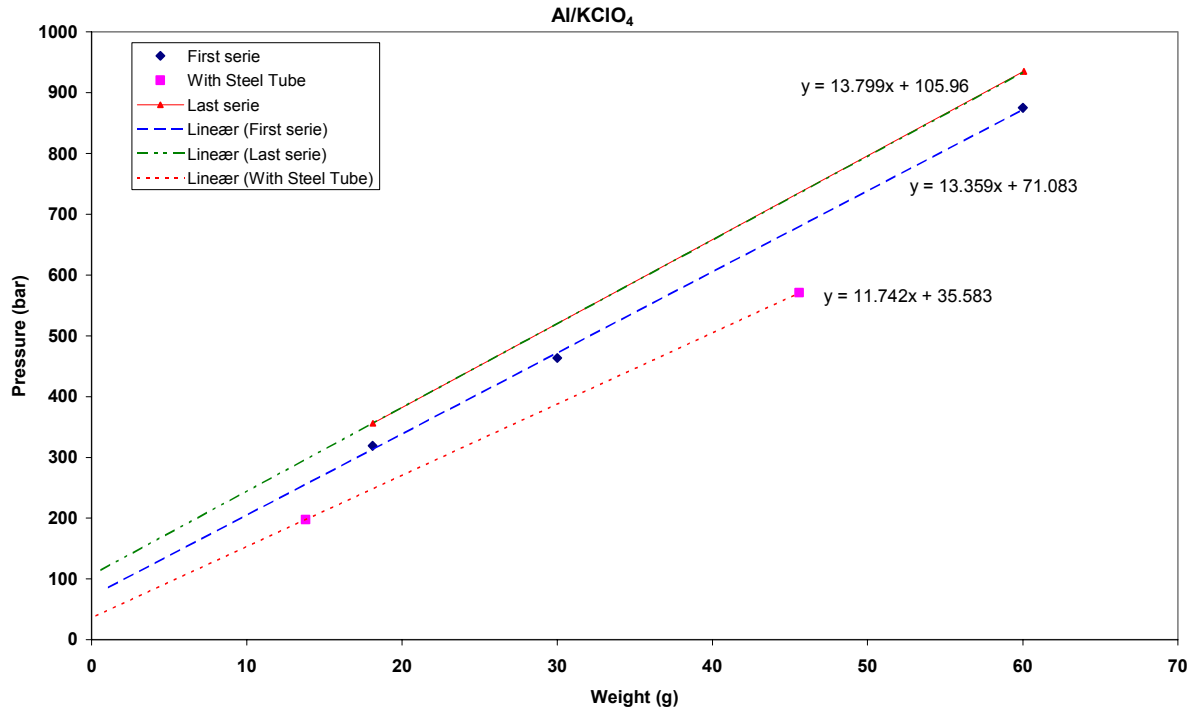


Figure 3.21 Maximum pressure as function of weight of aluminium powder for firings containing aluminium and potassium perchlorate (1/1).

In Figure 3.21 maximum pressure as function of the loaded amount of powder for most firings has been plotted. Firings under the same conditions can be connected with straight lines that are nearly parallel to each other. Why we obtain these lines is difficult to explain but one of the reasons may be that the consumption of material is not complete.

3.3 RS-41

For the composition RS-41 (24.5 wt.% Al/24.5 wt.% Mg/2 wt.% Resinate/49 wt.% KClO_4) all tests have been done in a clean vessel without any steel tube. We have performed 5 firings with RS-41. For firing CV-320 we got a leakage of the vessel. However, the part of the reaction we were able to register did follow the same pressure increase as for firing CV-321. CV-321 was a repetition of the CV-320 firing. For the other firings, CV-318 has an

Firing No	Composition	Weight (g)	Load density (g/cm^3)	Reaction	Maximum Pressure (bars)
CV-318	RS-41 "Skarp" delivered 30.4-98	60.08	0.4005	Fast	1186.5
CV-319		18.03	0.1202	Normal	317
CV-320		30.10	0.2007	Normal	444*
CV-321		30.00	0.2000	Normal	539.5
CV-322		90.00	0.6000	Normal	1604

*Leakage in the vessel

Table 3.3 Results and properties of CV-firings with RS-41 powder.

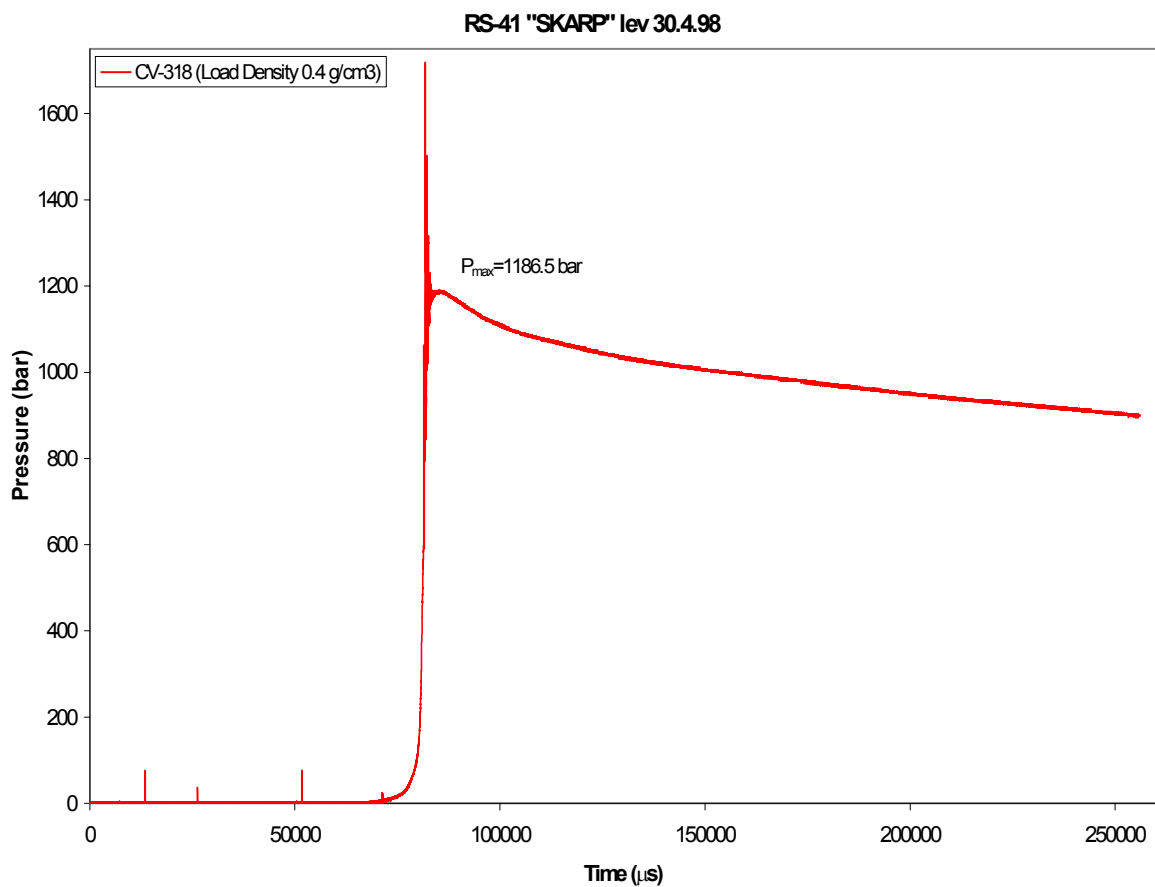


Figure 3.22 Pressure-time curve for firing CV-318, RS-41, load density $0.40 \text{ g}/\text{cm}^3$.

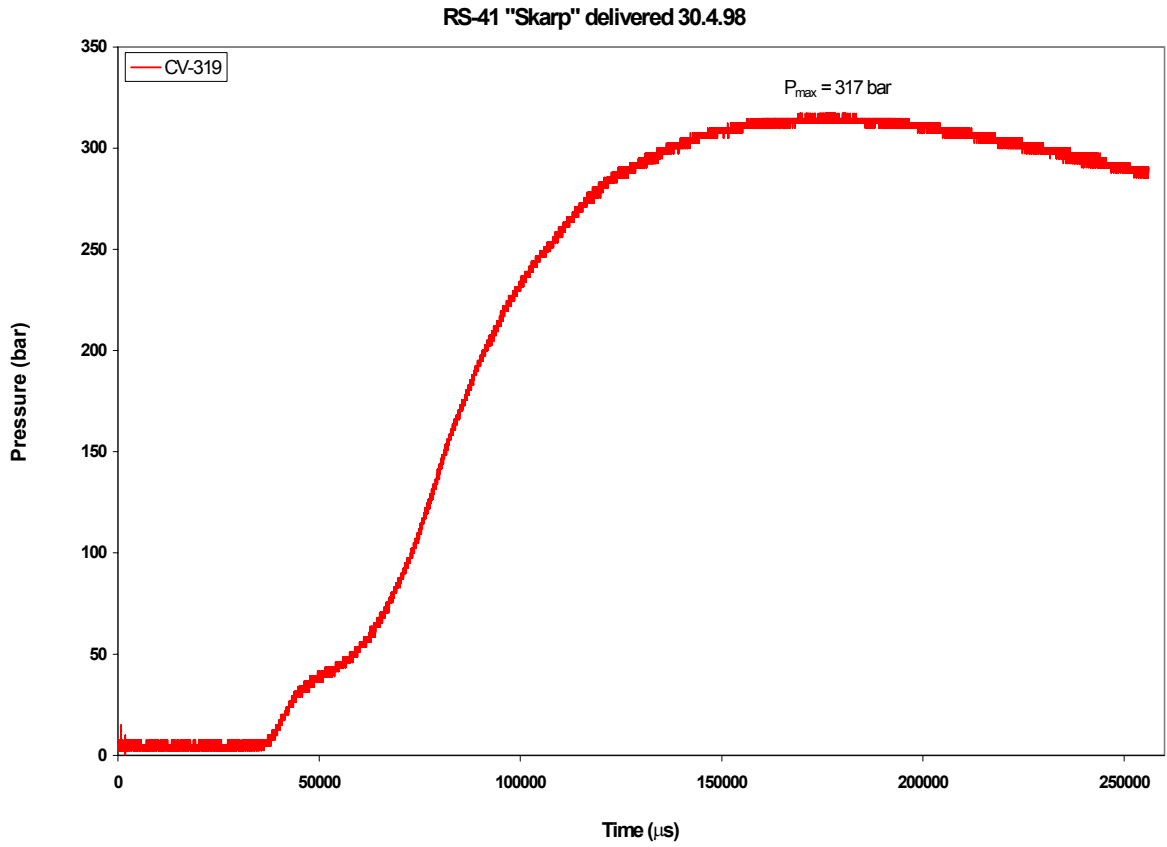


Figure 3.23 Pressure-time curve for firing CV-319, RS-41, load density 0.12 g/cm^3 .

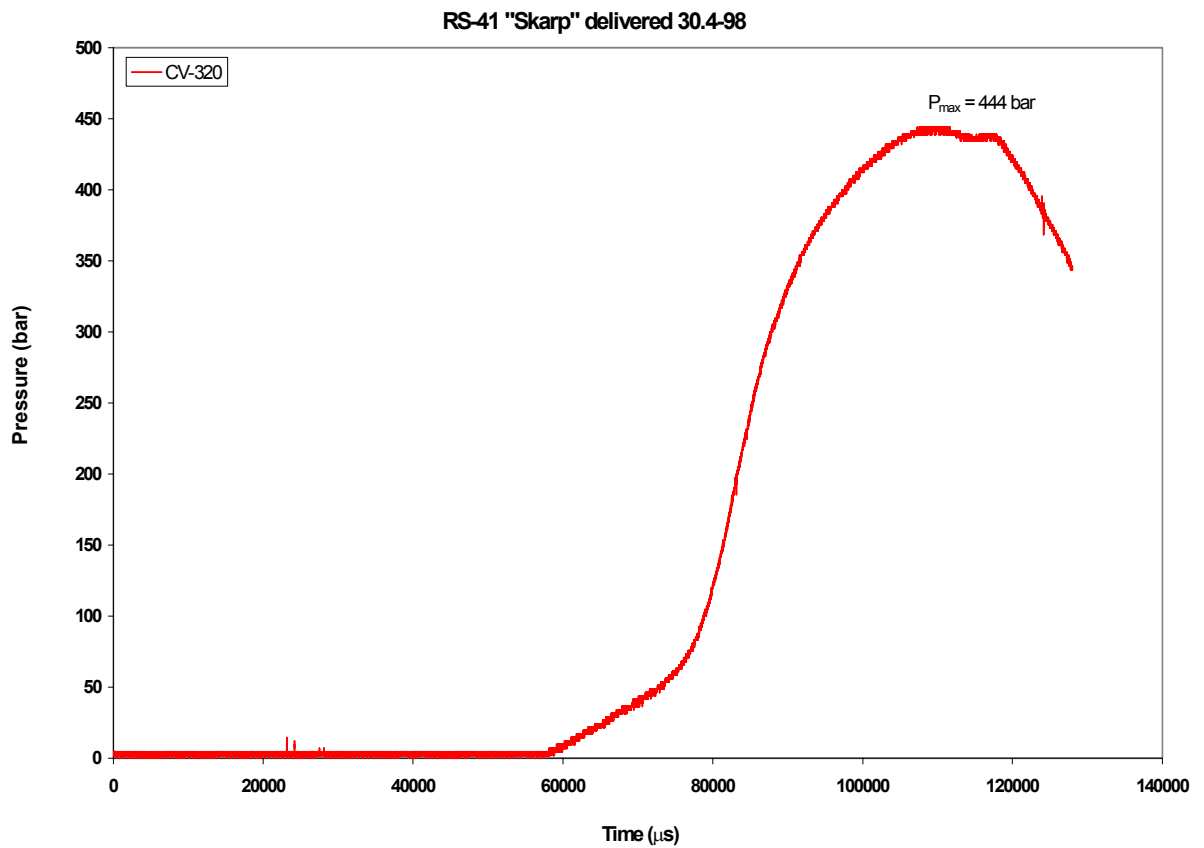


Figure 3.24 Pressure-time curve for firing CV-320, RS-41, load density 0.20 g/cm^3 .

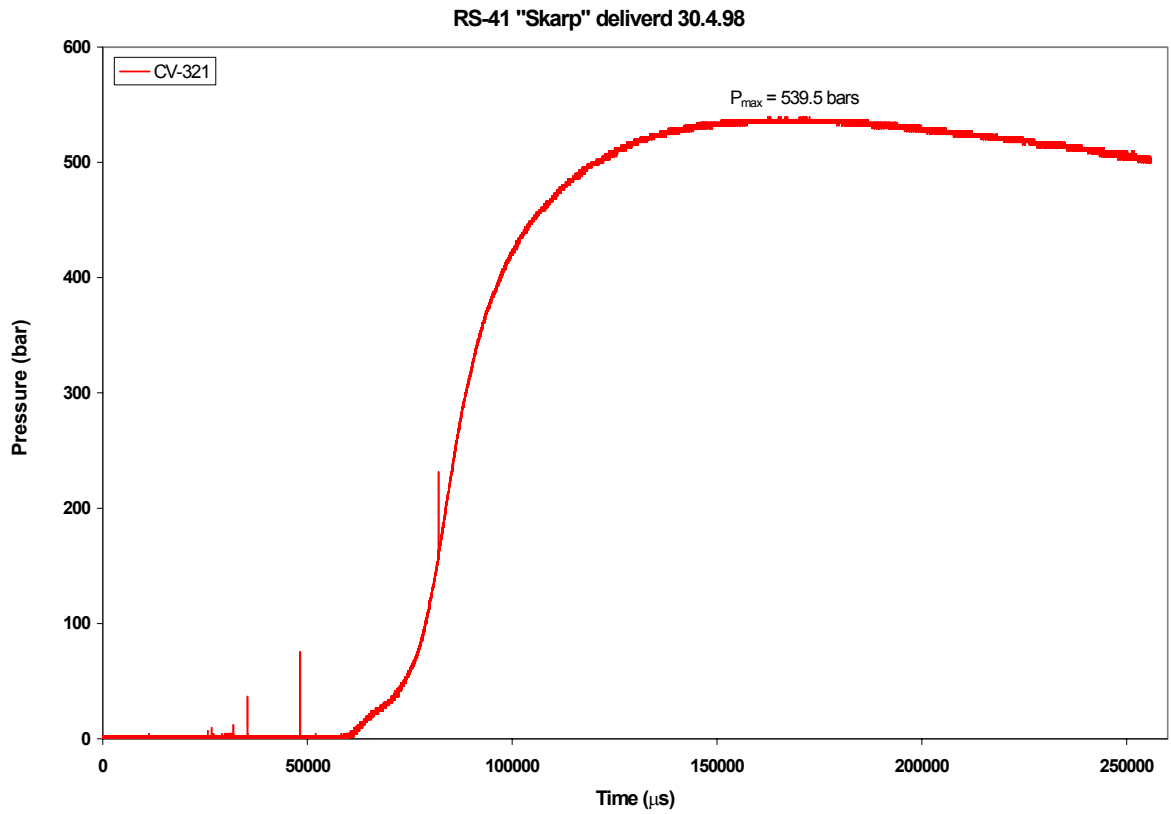


Figure 3.25 Pressure-time curve for firing CV-321, RS-41, load density 0.20 g/cm^3

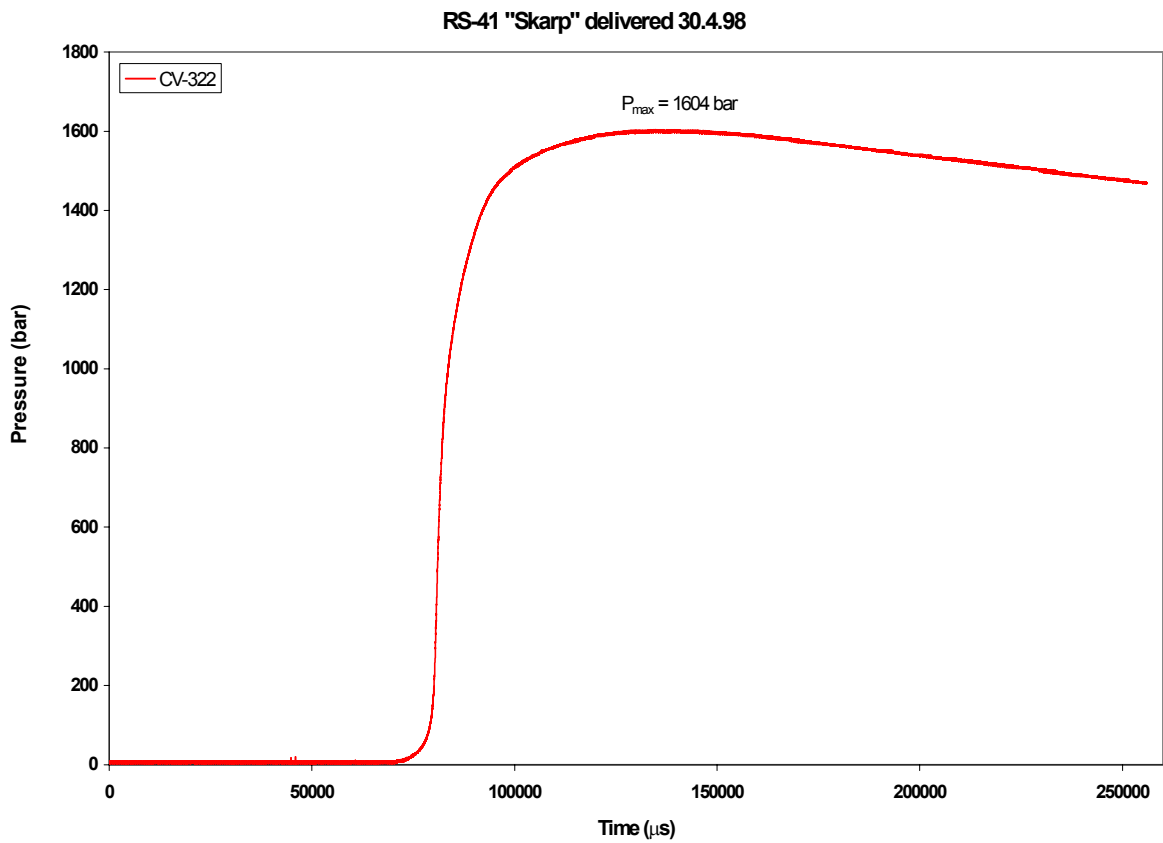


Figure 3.26 Pressure-time curve for firing CV-322, RS-41, load density 0.60 g/cm^3 .

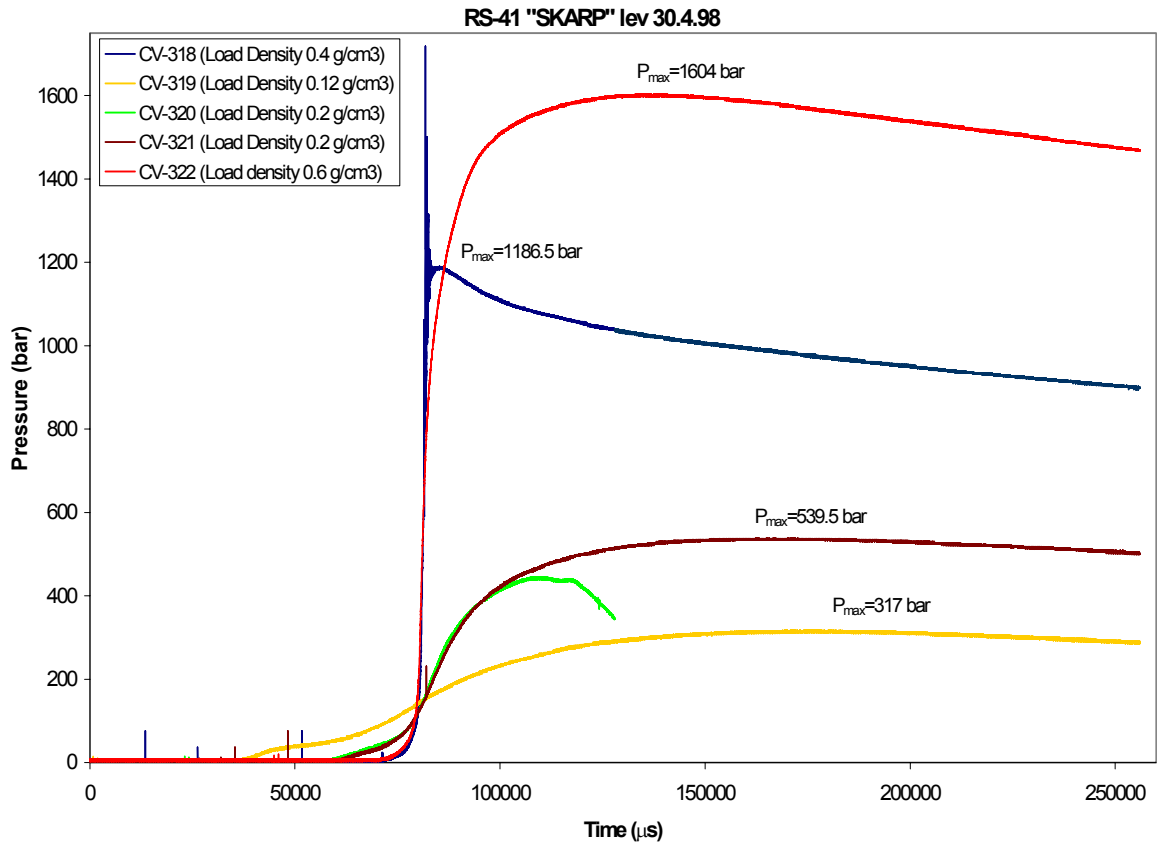


Figure 3.27 Pressure-time curves for CV-firings with RS-41.

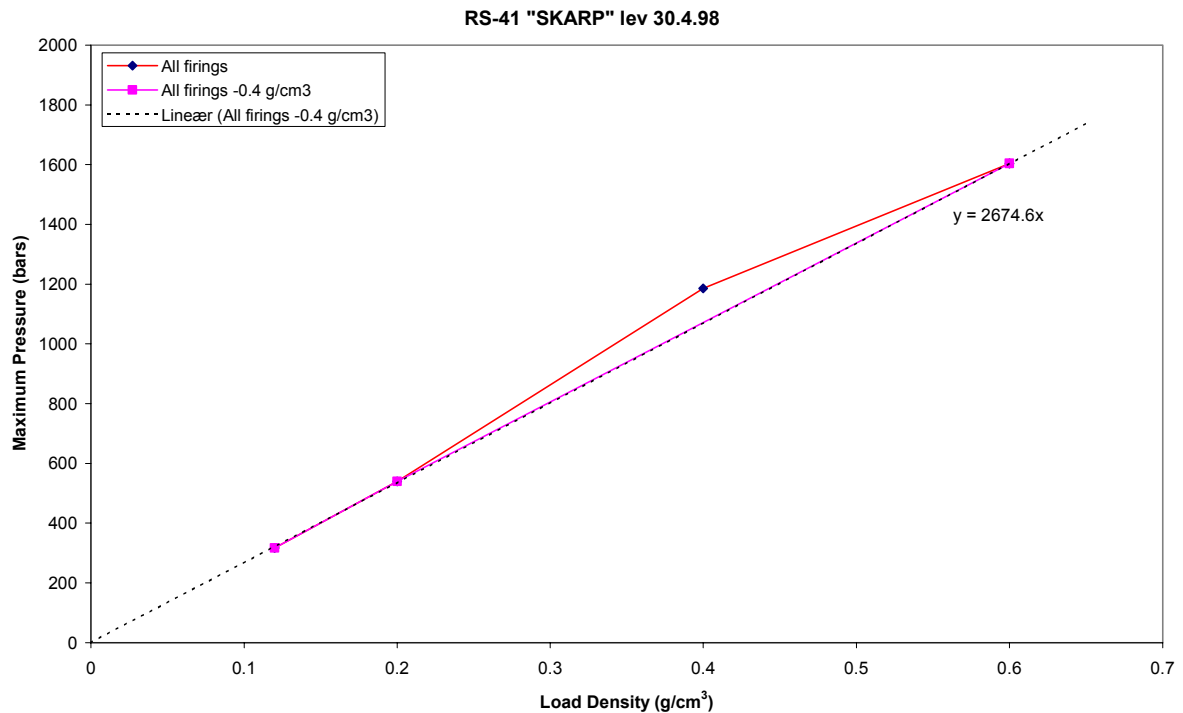


Figure 3.28 Maximum pressures as function of load density for firings with RS-41.

abnormal pressure increase which is faster than one expects for a normal burn reaction. However, the reaction did stop in the same way and does not go to detonation. If we plot the

maximum pressure as function of loading density, we get a straight line that goes through the point (0,0). The point for loading density 0.4 g/cm^3 deviates from this line. However, if we look at the pressure-time curve for CV-318, we see that after some few μs this firing will have a pressure that fit to the curve given in Figure 3.28.

With regard to burn rate have we slightly slower burn rate or pressure increase for RS-41 than for the Mg-powder firings, but faster than for the firings that contain Al-powder.

4 THEORETICAL CALCULATIONS

4.1 RS-41

In addition to the experimentally measuring pressures for given loading density of studied compositions, we have tried to calculate, by the use of Cheetah (2), what pressure one should expect to find in the closed vessel firings. Figure 4.1 gives calculated pressures for RS-41 + 2 g Black Powder and three other compositions with different ratio between Mg and Al powder.

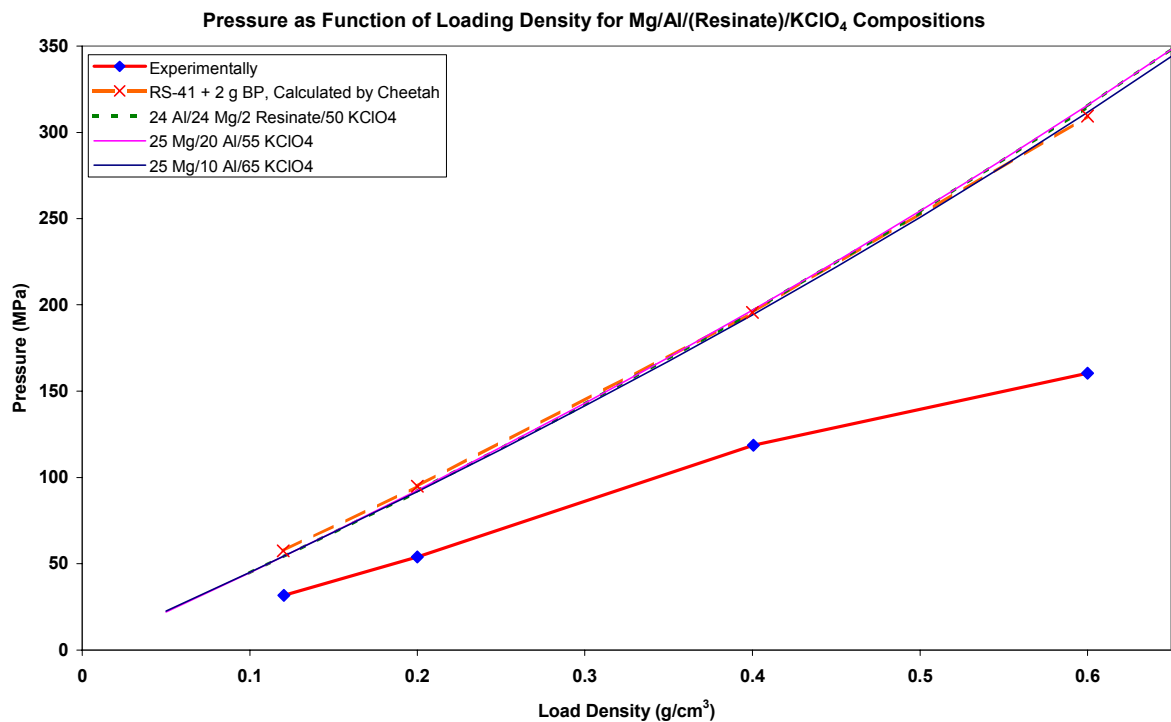


Figure 4.1 Experimentally measured and theoretically calculated pressures as function of loading density for RS-41 and similar compositions.

Appendix C gives the data used for the calculations, and the full report as it is obtained from the Cheetah program for a representative choice of the performed calculations. The Cheetah code has a problem with compositions containing too much magnesium. However for RS-41 with Black Powder there are no problems, while we for pure RS-41 get problems. The composition 24/24/2/50 (Al/Mg/Res/KClO₄) has a content very close to the nominal content in RS-41. From Figure 4.1 we see that the experimental pressures are all significantly lower than the theoretically calculated. In addition, the difference increase with increasing loading density. For RS-41 there are no significant differences in maximum pressure due to Black

Powder, Resinate or lower content of aluminium powder. Figure 4.2 gives the main products and their concentration as a function of loading density for RS-41 + 2 g BP.

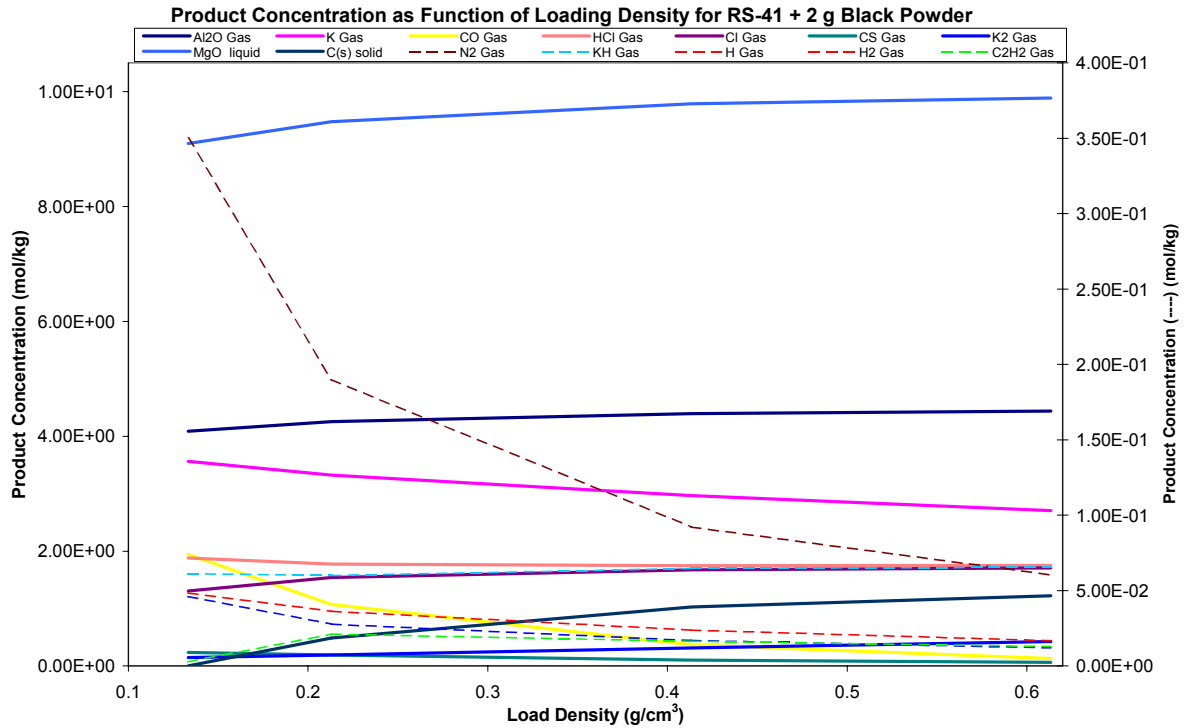


Figure 4.2 Product concentration as a function of load density for RS-41 + 2 g Black Powder.

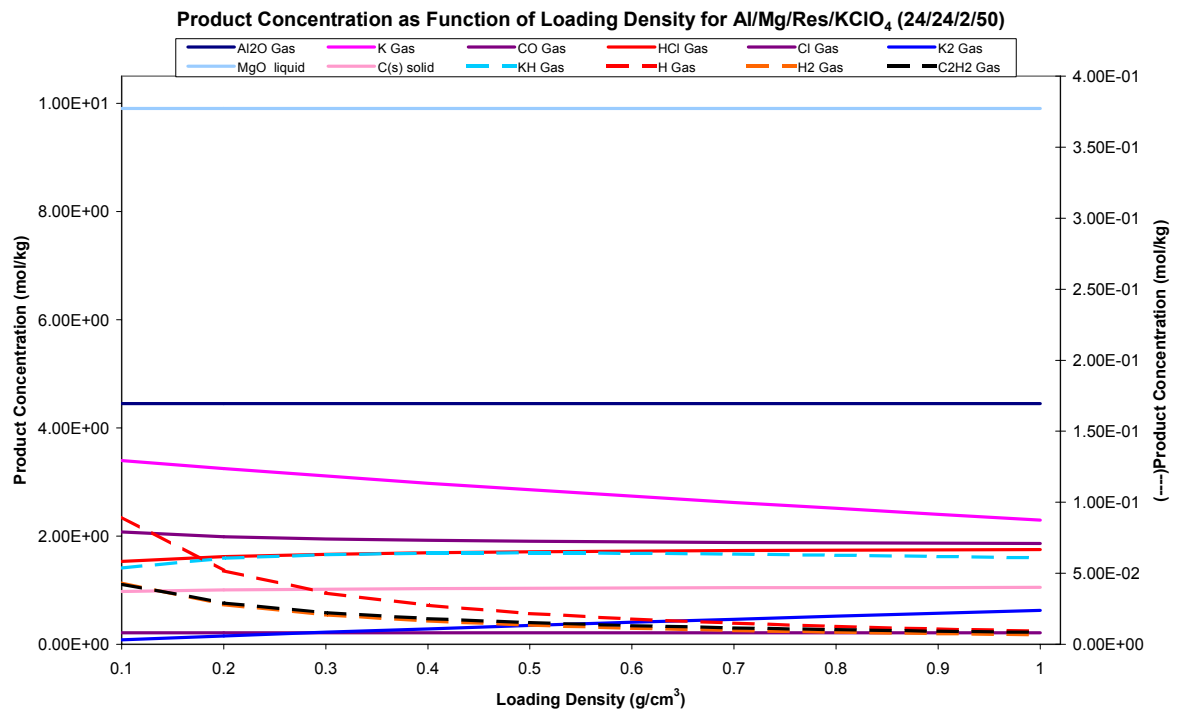


Figure 4.3 Product concentration as a function of loading density for the main products of Al/Mg/Res/KClO₄ (24/24/2/59).

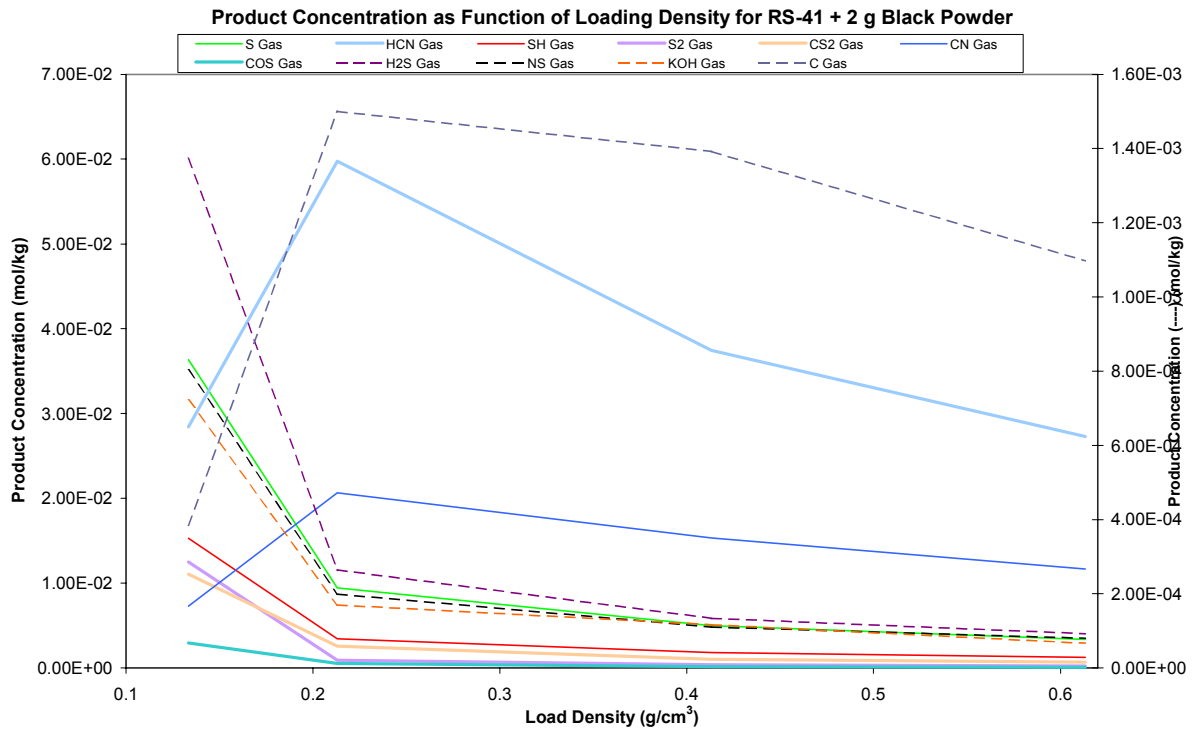


Figure 4.4 Product concentration as function of loading density for some of the minor products of RS-41 + 2 g Black Powder after combustion.

Figure 4.4 gives some of the minor products with the highest concentrations. Totally the code takes into consideration 68 products, but as can be seen in Appendix C, the majority of them exist in very low concentrations and have no significant influence on the maximum pressure. Figure 4.3 gives the main products for Al/Mg/Res/KClO₄ (24/24/2/50) with no BP, and comparing the products and their concentration with the products for RS-41 + BP give only small differences. For RS-41 + 2 g BP we get N₂ (g) and CS (g) as new products but in low concentrations.

4.2 Mg/KClO₄

For magnesium and potassium perchlorate we were not able to use the same content in the calculations as for the experimentally tested compositions due to the problem with the code to handle high concentrations of magnesium. Figure 4.5 give a summary of calculated pressures for some compositions. Appendix A gives the complete print-out from the Cheetah programme, again taken into consideration that the BP used to ignite the compositions has no significant influence on the maximum pressure. The difference between calculated and experimentally measured pressures are significant and increase with increasing loading density. The difference is of the same magnitude as for RS-41.

In Figure 4.6 the concentrations for the main products as function of loading density has been given for Mg/KClO₄ (40/60) and for loading density 0.12 g/cm³ of the Mg/KClO₄/BP (40/50/10) composition. The difference between the concentrations of the main products is small.

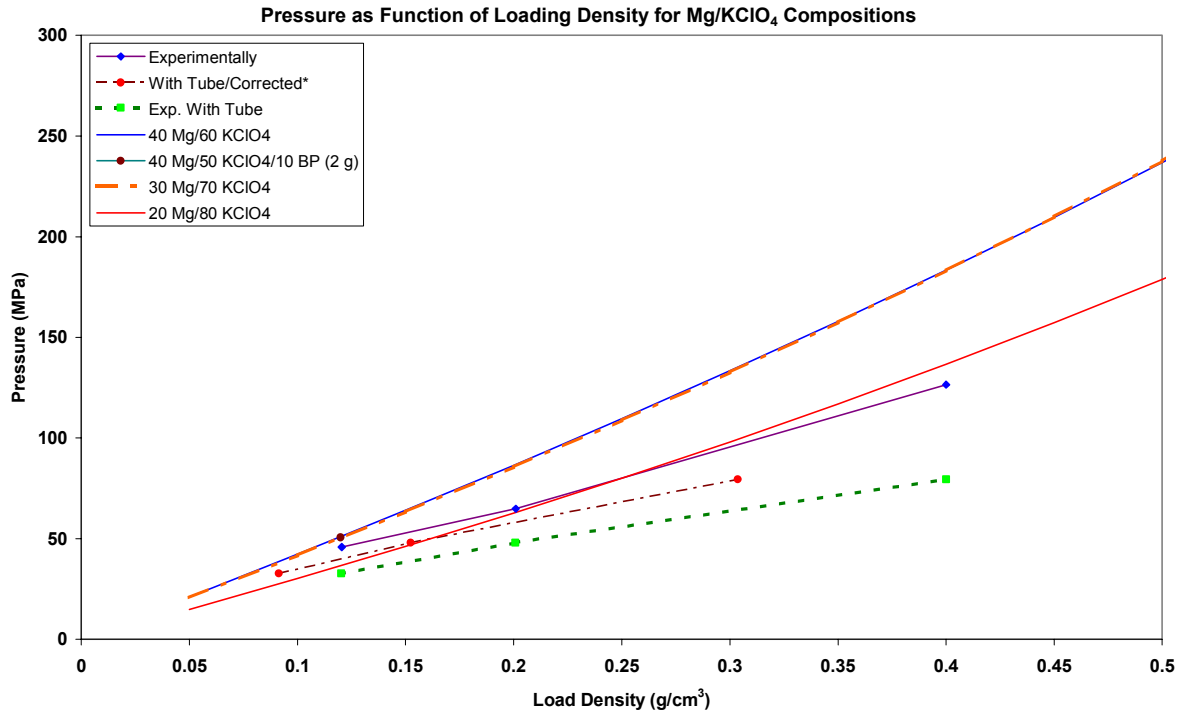


Figure 4.5 Experimentally measured and theoretically calculated pressures as function of loading density for different compositions containing Mg-powder and $KClO_4$.

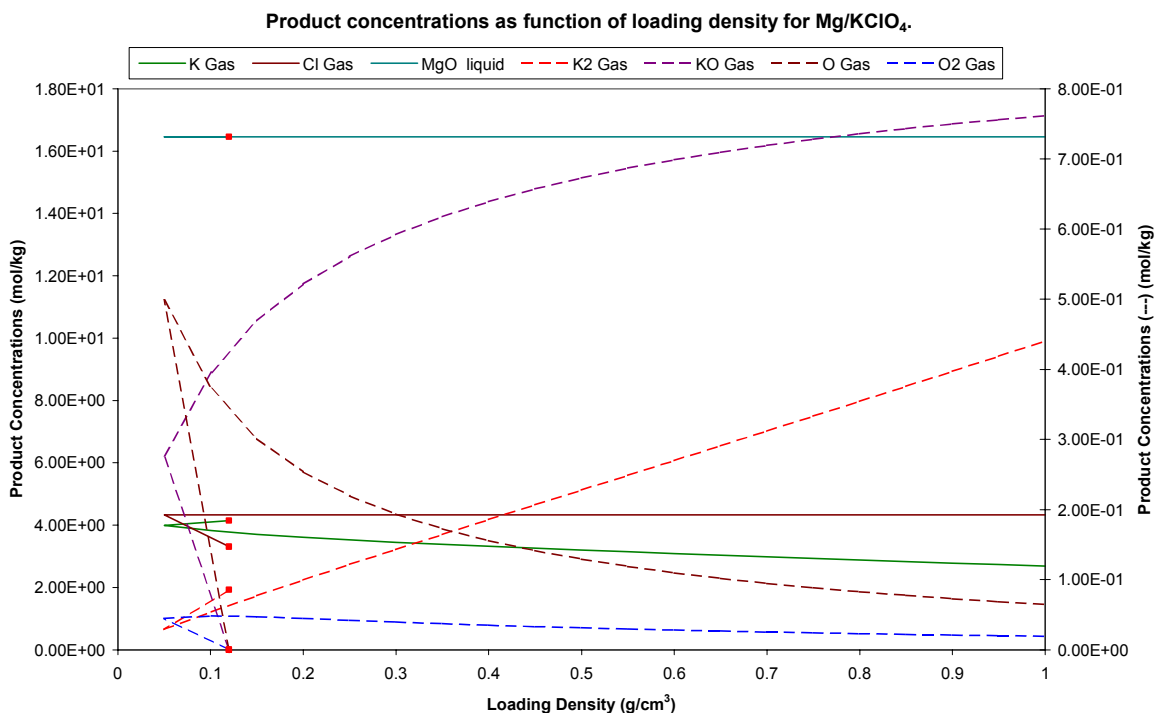


Figure 4.6 Product concentration as function of loading density for $Mg/KClO_4$ and $Mg/KClO_4 + 2 g$ Black Powder.

4.3 Al/ $KClO_4$

In Figure 4.7 the pressures for different compositions of Al-powder and potassium perchlorate are calculated by use of virial coefficients and the Blake database in Cheetah code and shown together with the experimentally measured pressures from testing in CV. For 50/50 Al/ $KClO_4$

we obtain higher pressures if we include the BP in the calculations. Beyond that the calculations show little dependence on pressure for Al contents up to 50 wt%. First at 60 wt.% Al do the calculations show significant lower pressures. The experimentally measured pressures are all significantly lower than the theoretically calculated, and the deviation increase with increasing loading density.

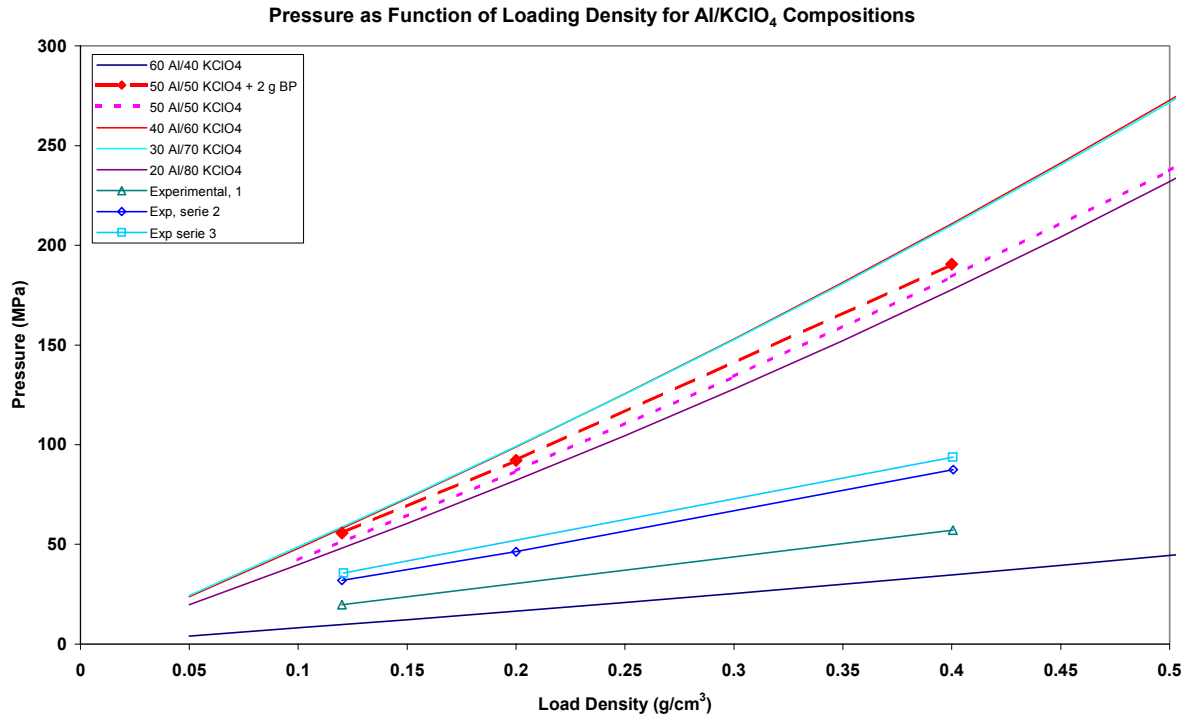


Figure 4.7 Experimentally measured and theoretically calculated pressures as function of loading density for different compositions containing Al-powder and KClO₄.

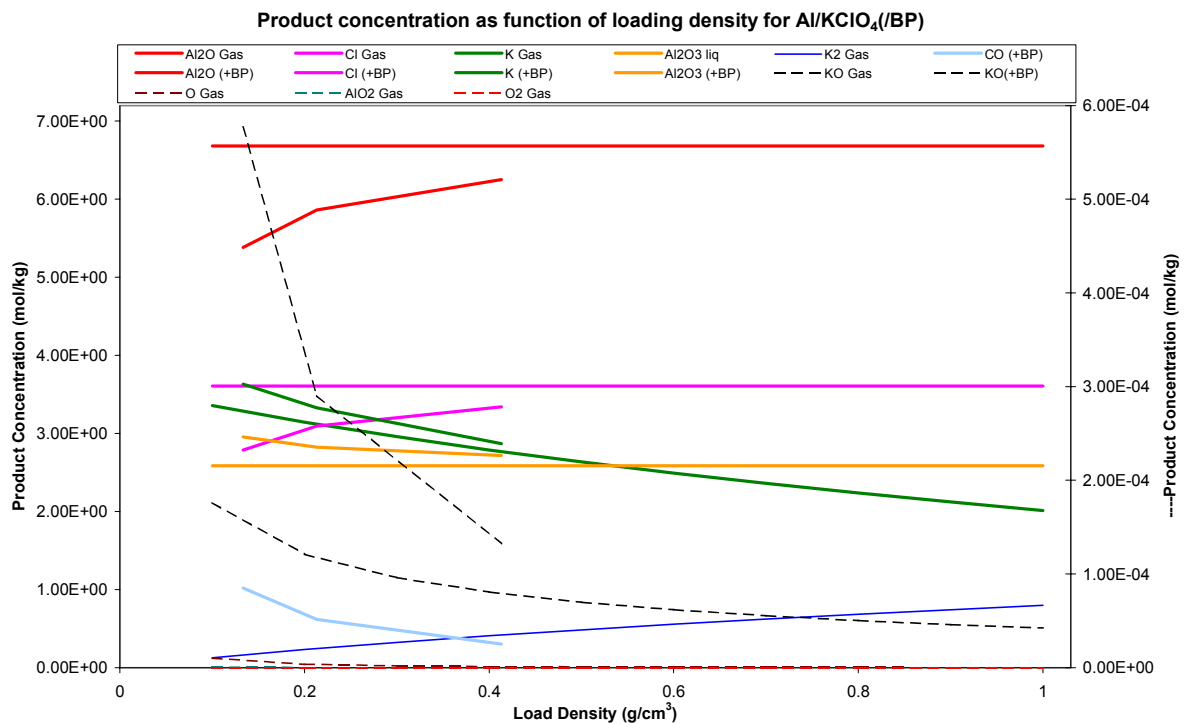


Figure 4.8 Product concentrations as function of loading density for Al/KClO₄ and Al/KClO₄ + 2 g Black Powder.

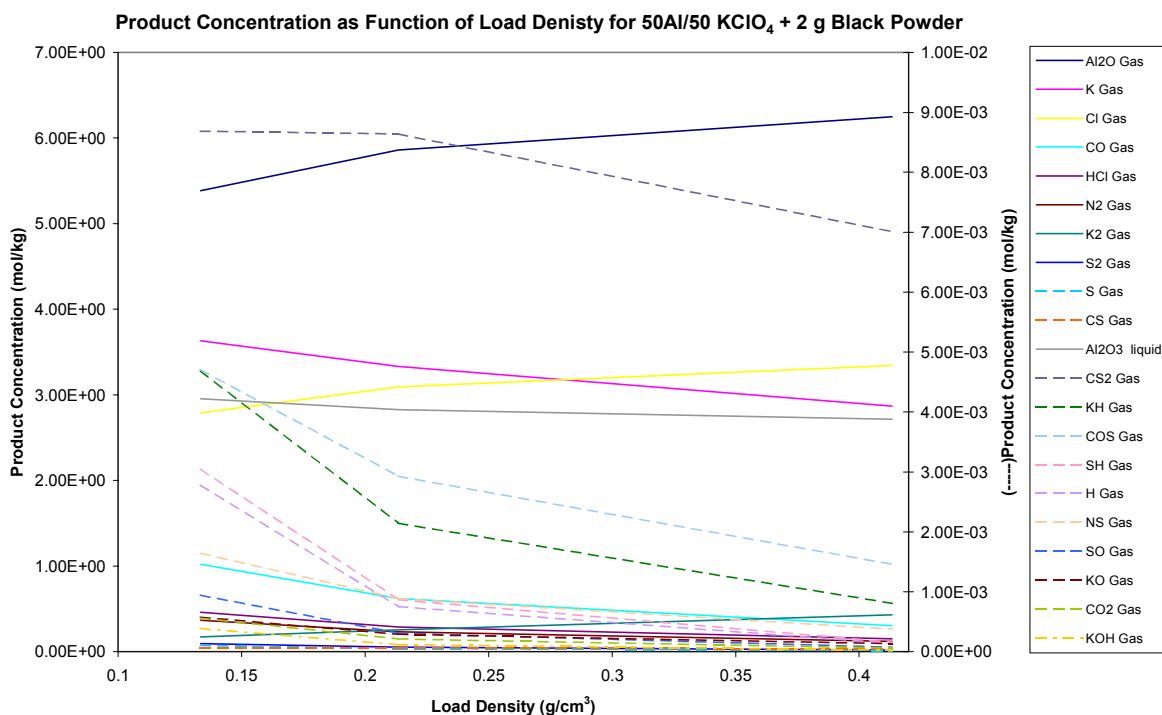


Figure 4.9 Product concentrations as function of loading density for Al/KClO₄ + 2 g BP.

Figure 4.8 shows the product concentrations for the main products for both 50/50 Al/KClO₄ and 50/50 Al/KClO₄ + 2 g BP. There are differences in the concentrations, and as shown in Figure 4.7, these differences have influence on the maximum pressure. However, these difference decrease as the loading density increase. Figure 4.9 gives some of the minor products for Al/KClO₄ + 2 g BP, while Appendix B gives the complete list.

5 SUMMARY

Pyrotechnic powders of different mixtures have been tested under different conditions in CV. Measured pressure-time curves give indication of several reaction mechanism for tested compositions. For the three main combinations (Al/KClO₄, Mg/KClO₄, RS-41) all give one firing with fast or very fast reaction rate. The burn rate or gas evolution rate is much higher than what one normally connects with burning. The observed phenomenon is observed when the powder was loosely packed as in the case of Al/KClO₄ or the loading density was high as in the case of RS-41 and Mg/KClO₄.

Measured maximum pressures are in general significantly lower than the theoretical calculations by use of Cheetah gives. In (1) we explained some of this deviation with incomplete reactions of the metal powders. Another effect must be the loss of heat to the CV.

APPENDIX

A THEORETICAL CALCULATION FOR Mg/KClO₄ COMPOSITIONSA.1 Loading density 0.12 g/cm³ 40Mg/50 KClO₄ + 2 g Black Powder

Product library title: the blake product library

Executing library command: gas eos, virial

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

Input>composition, sulfur, 1.07, susqkull, 1.499, potass nit, 7.417, ash, 0.014, potass per, 50, magnesium, 40, weight

The Composition							
Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. Formula wt.
sulfur	1.07	1.58	1.08	0	15.49	0.000	32.06 s1
susqkull	1.50	0.00	2.09	-4489962	12194.95	0.000	18292.43 c1321h573n4o100s6
potass nit	7.42	3.47	7.37	-118069	48.03	0.000	101.10 n1o3k1
ash	0.01	0.00	0.02	-271989	106.31	0.000	138.20 c1o3k2
potass per	50.00	17.07	41.36	-103250	54.81	0.000	138.55 o4c11k1
magnesium	40.00	77.87	48.08	0	13.97	0.000	24.31 mg1

Heat of formation = -463.180 cal/gm
 Standard volume = 0.478 cc/gm
 Standard entropy = 0.000 cal/k/gm
 Standard energy = -463.192 cal/gm

The elements and percent by mole

s	0.774
c	2.476
h	1.073
n	1.684
o	38.210
k	9.928
cl	8.247
mg	37.608

The average mol. wt. = 47.314 g/mol

Input>gun, 0.120000, 0.013300, 0.150000

GUN calculation:

	Rho g/cc	Temp K	Pressure MPa	Impetus J/g	Mol Wt. Gas	Covol cc/g	Frozen Cp/Cv	Phi
1.)	0.1200	5242.5	50.6	402.93	108.182	0.171	1.057	1.021
2.)	0.1333	5246.8	56.4	402.43	108.406	0.171	1.057	1.023
3.)	0.1466	5250.7	62.2	401.96	108.614	0.171	1.056	1.026

Product concentrations (mol/kg)

Name		1.)	2.)	3.)
k	Gas	4.146e+000	4.127e+000	4.109e+000
cl	Gas	3.311e+000	3.307e+000	3.303e+000
cs	Gas	3.130e-001	3.143e-001	3.153e-001
hcl	Gas	2.979e-001	3.022e-001	3.058e-001
cn	Gas	2.958e-001	2.983e-001	3.006e-001
co	Gas	2.633e-001	2.633e-001	2.633e-001
n2	Gas	1.967e-001	1.951e-001	1.935e-001
c	Gas	1.492e-001	1.434e-001	1.383e-001
k2	Gas	8.549e-002	9.457e-002	1.036e-001
h	Gas	7.253e-002	6.643e-002	6.124e-002
hcn	Gas	4.377e-002	4.477e-002	4.565e-002
kh	Gas	2.779e-002	2.826e-002	2.865e-002
s	Gas	2.272e-002	2.149e-002	2.042e-002
c2h2	Gas	8.849e-003	9.335e-003	9.775e-003
h2	Gas	4.200e-003	3.913e-003	3.659e-003
n	Gas	3.443e-003	3.273e-003	3.125e-003
sh	Gas	1.036e-003	9.973e-004	9.624e-004
cs2	Gas	4.872e-004	5.139e-004	5.394e-004
ns	Gas	3.367e-004	3.357e-004	3.349e-004
s2	Gas	2.330e-004	2.315e-004	2.301e-004
ch2	Gas	1.381e-004	1.375e-004	1.366e-004
nh	Gas	5.862e-005	5.679e-005	5.511e-005
cos	Gas	3.506e-005	3.699e-005	3.886e-005
cho	Gas	2.193e-005	2.250e-005	2.300e-005
ko	Gas	2.016e-005	2.123e-005	2.226e-005
o	Gas	1.172e-005	1.114e-005	1.064e-005
h2s	Gas	9.567e-006	9.362e-006	9.156e-006

koh	Gas	3.989e-006	4.267e-006	4.532e-006
ch3	Gas	3.237e-006	3.277e-006	3.301e-006
nco	Gas	2.901e-006	3.082e-006	3.258e-006
no	Gas	2.294e-006	2.290e-006	2.286e-006
nh2	Gas	1.376e-006	1.356e-006	1.336e-006
oh	Gas	1.261e-006	1.219e-006	1.180e-006
so	Gas	9.880e-007	9.844e-007	9.813e-007
co2	Gas	5.492e-007	5.782e-007	6.061e-007
hnco	Gas	1.759e-007	1.899e-007	2.034e-007
ch3cl	Gas	1.435e-007	1.614e-007	1.790e-007
ketene	Gas	1.040e-007	1.155e-007	1.268e-007
h2o	Gas	8.155e-008	8.005e-008	7.855e-008
ch3cn	Gas	5.026e-008	5.696e-008	6.360e-008
ch2o	Gas	3.485e-008	3.640e-008	3.780e-008
nh3	Gas	2.127e-008	2.131e-008	2.128e-008
c2h4	Gas	1.302e-008	1.423e-008	1.534e-008
ch4	Gas	1.029e-008	1.057e-008	1.078e-008
hno	Gas	5.783e-010	5.901e-010	6.005e-010
n2o	Gas	5.040e-010	5.312e-010	5.576e-010
s2o	Gas	4.379e-010	4.590e-010	4.792e-010
o2	Gas	8.521e-011	8.524e-011	8.531e-011
ch2oh	Gas	8.077e-012	8.633e-012	9.141e-012
so2	Gas	6.038e-012	6.334e-012	6.621e-012
formac	Gas	5.364e-013	5.908e-013	6.439e-013
ho2	Gas	1.023e-013	1.047e-013	1.068e-013
no2	Gas	6.644e-014	7.023e-014	7.391e-014
ch4o	Gas	2.689e-014	2.925e-014	3.143e-014
k2h2o2	Gas	1.080e-015	1.380e-015	1.721e-015
hno2	Gas	6.173e-016	6.651e-016	7.114e-016
h2o2	Gas	5.808e-016	6.048e-016	6.264e-016
mgo2h2	Gas	1.786e-018	1.767e-018	1.746e-018
mgo	liquid	1.646e+001	1.646e+001	1.646e+001
*koh	liquid	0.000e+000	0.000e+000	0.000e+000
mgo	solid	0.000e+000	0.000e+000	0.000e+000
c(s)	solid	0.000e+000	0.000e+000	1.827e-018
Total Gas		9.244e+000	9.225e+000	9.207e+000
Total Cond.		1.646e+001	1.646e+001	1.646e+001

A.2 40 Mg/60 KClO₄

Input>composition, mg, 40, potass per, 60, weight

Name	% wt.	% mol	% vol.	The Composition		Standard entropy (cal/K/mol)	Mol. wt.	Formula
				Heat of formation (cal/mol)	Standard volume (cc/mol)			
mg	40.00	79.17	49.20	0	13.97	0.000	24.31	mg1
potass per	60.00	20.83	50.80	-103250	54.81	0.000	138.55	o4cl1k1

Heat of formation = -447.130 cal/gm
Standard volume = 0.467 cc/gm
Standard entropy = 0.000 cal/k/gm
Standard energy = -447.141 cal/gm

The elements and percent by mole

mg	38.778
o	40.815
cl	10.204
k	10.204

The average mol. wt. = 48.105 g/mol
Input>gun, 0.050000, 0.050000, 1.050000
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	5408.5	21.0	412.61	108.988	0.158	1.056	1.008
2.)	0.1000	5434.5	42.3	407.94	110.767	0.157	1.055	1.016
3.)	0.1500	5450.1	64.1	404.77	111.956	0.157	1.054	1.024
4.)	0.2000	5461.1	86.5	402.31	112.868	0.157	1.054	1.032
5.)	0.2500	5469.6	109.6	400.26	113.622	0.157	1.053	1.041
6.)	0.3000	5476.6	133.4	398.48	114.275	0.157	1.053	1.050
7.)	0.3500	5482.5	157.9	396.88	114.859	0.158	1.053	1.058
8.)	0.4000	5487.7	183.3	395.41	115.394	0.158	1.052	1.068
9.)	0.4500	5492.3	209.6	394.04	115.893	0.159	1.052	1.077
10.)	0.5000	5496.5	236.7	392.75	116.364	0.159	1.052	1.087
11.)	0.5500	5500.4	264.9	391.52	116.813	0.160	1.052	1.096
12.)	0.6000	5504.1	294.0	390.33	117.246	0.160	1.051	1.107
13.)	0.6500	5507.5	324.2	389.18	117.666	0.161	1.051	1.117
14.)	0.7000	5510.8	355.5	388.06	118.076	0.162	1.051	1.128
15.)	0.7500	5513.9	388.0	386.96	118.477	0.163	1.051	1.139
16.)	0.8000	5516.9	421.7	385.89	118.873	0.163	1.051	1.150
17.)	0.8500	5519.8	456.8	384.83	119.263	0.164	1.050	1.162
18.)	0.9000	5522.7	493.2	383.78	119.650	0.165	1.050	1.174

19.) 0.9500 5525.5 531.1 382.75 120.034 0.165 1.050 1.187
 20.) 1.0000 5528.2 570.5 381.72 120.417 0.166 1.050 1.199

Product concentrations (mol/kg)

Name	1.)	2.)	3.)	4.)	5.)	6.)
cl Gas	4.331e+000	4.331e+000	4.331e+000	4.331e+000	4.331e+000	4.331e+000
k Gas	3.996e+000	3.827e+000	3.707e+000	3.610e+000	3.526e+000	3.452e+000
o Gas	4.986e-001	3.724e-001	3.012e-001	2.538e-001	2.196e-001	1.934e-001
ko Gas	2.768e-001	3.955e-001	4.693e-001	5.215e-001	5.610e-001	5.922e-001
o2 Gas	4.460e-002	4.837e-002	4.708e-002	4.466e-002	4.204e-002	3.951e-002
k2 Gas	2.904e-002	5.391e-002	7.721e-002	9.965e-002	1.216e-001	1.431e-001
mgo liqui	1.646e+001	1.646e+001	1.646e+001	1.646e+001	1.646e+001	1.646e+001
mgo solid	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000
Total Gas	9.175e+000	9.028e+000	8.932e+000	8.860e+000	8.801e+000	8.751e+000
Total Con	1.646e+001	1.646e+001	1.646e+001	1.646e+001	1.646e+001	1.646e+001

Product concentrations (mol/kg)

Name	7.)	8.)	9.)	10.)	11.)	12.)
cl Gas	4.331e+000	4.331e+000	4.331e+000	4.331e+000	4.331e+000	4.331e+000
k Gas	3.384e+000	3.320e+000	3.260e+000	3.202e+000	3.146e+000	3.092e+000
ko Gas	6.178e-001	6.391e-001	6.573e-001	6.730e-001	6.867e-001	6.988e-001
o Gas	1.725e-001	1.555e-001	1.413e-001	1.293e-001	1.189e-001	1.098e-001
k2 Gas	1.645e-001	1.857e-001	2.068e-001	2.278e-001	2.488e-001	2.698e-001
o2 Gas	3.716e-002	3.499e-002	3.301e-002	3.120e-002	2.954e-002	2.802e-002
mgo liqui	1.646e+001	1.646e+001	1.646e+001	1.646e+001	1.646e+001	1.646e+001
mgo solid	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000
Total Gas	8.706e+000	8.666e+000	8.629e+000	8.594e+000	8.561e+000	8.529e+000
Total Con	1.646e+001	1.646e+001	1.646e+001	1.646e+001	1.646e+001	1.646e+001

Product concentrations (mol/kg)

Name	13.)	14.)	15.)	16.)	17.)	18.)
cl Gas	4.331e+000	4.331e+000	4.331e+000	4.331e+000	4.331e+000	4.331e+000
k Gas	3.039e+000	2.987e+000	2.936e+000	2.886e+000	2.836e+000	2.786e+000
ko Gas	7.096e-001	7.192e-001	7.280e-001	7.359e-001	7.432e-001	7.499e-001
k2 Gas	2.909e-001	3.120e-001	3.331e-001	3.544e-001	3.757e-001	3.971e-001
o Gas	1.018e-001	9.474e-002	8.840e-002	8.268e-002	7.750e-002	7.278e-002
o2 Gas	2.661e-002	2.532e-002	2.412e-002	2.300e-002	2.196e-002	2.099e-002
mgo liqui	1.646e+001	1.646e+001	1.646e+001	1.646e+001	1.646e+001	1.646e+001
mgo solid	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000
Total Gas	8.499e+000	8.469e+000	8.440e+000	8.412e+000	8.385e+000	8.358e+000
Total Con	1.646e+001	1.646e+001	1.646e+001	1.646e+001	1.646e+001	1.646e+001

Product concentrations (mol/kg)

Name	19.)	20.)
cl Gas	4.331e+000	4.331e+000
k Gas	2.737e+000	2.688e+000
ko Gas	7.560e-001	7.617e-001
k2 Gas	4.187e-001	4.403e-001
o Gas	6.846e-002	6.450e-002
o2 Gas	2.008e-002	1.923e-002
mgo liquid	1.646e+001	1.646e+001
mgo solid	0.000e+000	0.000e+000
Total Gas	8.331e+000	8.304e+000
Total Cond.	1.646e+001	1.646e+001

B THEORETICAL CALCULATION FOR Al/KClO₄ COMPOSITIONS

B.1 0.12 Al/KClO₄ + 2 g Black Powder

Product library title: the blake product library

Executing library command: gas eos, virial

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

Input > composition, al, 45, potass per, 45, potass nit, 7.417, sulfur, 1.07, susqkull, 1.499, ash, 0.014, weight

The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
al	45.00	79.44	42.18	0	9.99	0.000	26.98	al1
potass per	45.00	15.47	45.04	-103250	54.81	0.000	138.55	o4cl1k1
potass nit	7.42	3.49	8.92	-118069	48.03	0.000	101.10	n1o3k1
sulfur	1.07	1.59	1.31	0	15.49	0.000	32.06	s1
susqkull	1.50	0.00	2.53	-4489962	12194.95	0.000	18292.43	c1321h573n4o100s6
ash	0.01	0.00	0.03	-271989	106.31	0.000	138.20	c1o3k2

Heat of formation = -425.919 cal/gm

Standard volume = 0.395 cc/gm

Standard entropy = 0.000 cal/k/gm
 Standard energy = -425.929 cal/gm

The elements and percent by mole

al	39.884
o	36.536
cl	7.767
k	9.527
n	1.762
s	0.810
c	2.591
h	1.123

The average mol. wt. = 47.631 g/mol

Input>gun, 0.120000, 0.013300, 0.146600
 GUN calculation:

	Rho	Temp	Pressure	Impetus	Mol Wt.	Covol	Frozen	Phi
	g/cc	K	MPa	J/g	Gas	cc/g	Cp/Cv	
1.)	0.1200	3782.2	55.7	443.19	70.958	0.273	1.114	1.034
2.)	0.1333	3786.0	62.1	442.86	71.081	0.273	1.114	1.038
3.)	0.1466	3789.5	68.6	442.53	71.201	0.272	1.113	1.042

Product concentrations (mol/kg)

Name		1.)	2.)	3.)
al2o	Gas	5.386e+000	5.383e+000	5.381e+000
k	Gas	3.663e+000	3.632e+000	3.601e+000
cl	Gas	2.791e+000	2.790e+000	2.790e+000
co	Gas	1.025e+000	1.020e+000	1.014e+000
hcl	Gas	4.573e-001	4.578e-001	4.582e-001
n2	Gas	3.673e-001	3.673e-001	3.672e-001
k2	Gas	1.575e-001	1.731e-001	1.884e-001
s2	Gas	9.589e-002	9.472e-002	9.336e-002
s	Gas	7.636e-002	7.216e-002	6.844e-002
cs	Gas	4.485e-002	4.922e-002	5.345e-002
cs2	Gas	7.569e-003	8.685e-003	9.805e-003
kh	Gas	4.682e-003	4.692e-003	4.701e-003
cos	Gas	4.500e-003	4.712e-003	4.906e-003
sh	Gas	3.211e-003	3.050e-003	2.906e-003
h	Gas	3.072e-003	2.786e-003	2.550e-003
ns	Gas	1.642e-003	1.645e-003	1.645e-003
so	Gas	1.046e-003	9.466e-004	8.637e-004
ko	Gas	6.028e-004	5.771e-004	5.548e-004
co2	Gas	5.873e-004	5.588e-004	5.341e-004
koh	Gas	4.034e-004	3.864e-004	3.716e-004
cn	Gas	3.520e-004	3.921e-004	4.325e-004
h2	Gas	3.351e-004	3.049e-004	2.799e-004
hcn	Gas	1.748e-004	1.945e-004	2.144e-004
n	Gas	7.424e-005	7.129e-005	6.875e-005
no	Gas	4.413e-005	4.036e-005	3.724e-005
o	Gas	4.291e-005	3.727e-005	3.282e-005
h2s	Gas	2.948e-005	2.806e-005	2.678e-005
s2o	Gas	2.652e-005	2.516e-005	2.393e-005
c	Gas	1.238e-005	1.312e-005	1.383e-005
oh	Gas	8.220e-006	7.159e-006	6.320e-006
alho2	Gas	7.599e-006	6.797e-006	6.148e-006
cho	Gas	5.249e-006	5.312e-006	5.371e-006
alo2	Gas	2.888e-006	2.589e-006	2.347e-006
so2	Gas	2.481e-006	2.149e-006	1.885e-006
h2o	Gas	1.642e-006	1.432e-006	1.266e-006
halo	Gas	1.353e-006	1.273e-006	1.204e-006
nco	Gas	1.001e-006	1.069e-006	1.135e-006
nh	Gas	7.925e-007	7.659e-007	7.431e-007
hnco	Gas	1.556e-007	1.664e-007	1.768e-007
c2h2	Gas	1.045e-007	1.293e-007	1.568e-007
o2	Gas	7.968e-008	6.621e-008	5.602e-008
nh2	Gas	2.380e-008	2.309e-008	2.248e-008
ch2	Gas	1.411e-008	1.508e-008	1.603e-008
n2o	Gas	1.042e-008	1.013e-008	9.884e-009
ch2o	Gas	7.821e-009	7.953e-009	8.080e-009
hno	Gas	2.540e-009	2.351e-009	2.195e-009
nh3	Gas	7.174e-010	6.980e-010	6.814e-010
ch3	Gas	6.568e-010	7.038e-010	7.496e-010
ketene	Gas	4.226e-010	5.006e-010	5.839e-010
ch3cl	Gas	3.917e-010	4.655e-010	5.447e-010
no2	Gas	5.626e-011	4.973e-011	4.453e-011
k2h2o2	Gas	3.700e-011	3.785e-011	3.866e-011
formac	Gas	2.672e-011	2.606e-011	2.550e-011
ho2	Gas	2.094e-011	1.762e-011	1.508e-011
ch4	Gas	3.349e-012	3.587e-012	3.819e-012
ch3cn	Gas	5.726e-013	7.552e-013	9.715e-013
hno2	Gas	3.006e-013	2.675e-013	2.410e-013
ch2oh	Gas	1.829e-013	1.884e-013	1.937e-013
h2o2	Gas	1.174e-013	9.919e-014	8.528e-014
c2h4	Gas	4.440e-014	5.539e-014	6.767e-014

```

ch4o Gas 7.112e-016 7.356e-016 7.594e-016
al2o3 liquid 2.953e+000 2.955e+000 2.958e+000
*koh liquid 0.000e+000 0.000e+000 0.000e+000
c(s) solid 0.000e+000 0.000e+000 0.000e+000
al2o3 solid 0.000e+000 0.000e+000 0.000e+000

Total Gas 1.409e+001 1.407e+001 1.404e+001
Total Cond. 2.953e+000 2.955e+000 2.958e+000

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B.2 Load Density 0.2 g/cm³ Al/KClO₄ + 2 g Black Powder

Al svart krutt

Product library title: the blake product library

Executing library command: gas eos, virial

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

Input>composition, al, 75, potass per, 75, potass nit, 7.417, sulfur, 1.07,
susqkull, 1.499, ash, 0.014, weight

The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
al	46.88	81.09	44.45	0	9.99	0.000	26.98	al1
potass per	46.88	15.79	47.47	-103250	54.81	0.000	138.55	o4cl1k1
potass nit	4.64	2.14	5.64	-118069	48.03	0.000	101.10	n1o3k1
sulfur	0.67	0.97	0.83	0	15.49	0.000	32.06	s1
susqkull	0.94	0.00	1.60	-4489962	12194.95	0.000	18292.43	c1321h573n4o100s6
ash	0.01	0.00	0.02	-271989	106.31	0.000	138.20	c1o3k2

Heat of formation = -405.928 cal/gm
Standard volume = 0.391 cc/gm
Standard entropy = 0.000 cal/k/gm
Standard energy = -405.937 cal/gm

The elements and percent by mole

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al 42.163
o 36.312
cl 8.211
k 9.327
n 1.118
s 0.514
c 1.644
h 0.712

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The average mol. wt. = 46.676 g/mol

Input>gun, 0.20000, 0.013300, 0.226600

GUN calculation:

	Rho g/cc	Temp K	Pressure MPa	Impetus J/g	Mol Wt. Gas	Covol cc/g	Frozen Cp/Cv	Phi
1.)	0.2000	3719.1	92.1	428.30	72.200	0.260	1.115	1.055
2.)	0.2133	3721.3	98.7	428.00	72.293	0.260	1.115	1.059

Product concentrations (mol/kg)

Name	1.)	2.)
al2o	Gas 5.862e+000	5.861e+000
k	Gas 3.358e+000	3.331e+000
cl	Gas 3.094e+000	3.094e+000
co	Gas 6.229e-001	6.198e-001
hcl	Gas 2.893e-001	2.894e-001
k2	Gas 2.412e-001	2.549e-001
n2	Gas 2.296e-001	2.296e-001
s2	Gas 5.441e-002	5.341e-002
cs	Gas 4.285e-002	4.518e-002
s	Gas 3.895e-002	3.735e-002
cs2	Gas 8.004e-003	8.639e-003
cos	Gas 2.859e-003	2.928e-003
kh	Gas 2.146e-003	2.143e-003
sh	Gas 9.031e-004	8.689e-004
ns	Gas 8.872e-004	8.838e-004
h	Gas 8.020e-004	7.531e-004
so	Gas 3.320e-004	3.100e-004
cn	Gas 3.146e-004	3.368e-004
ko	Gas 2.994e-004	2.906e-004
co2	Gas 2.189e-004	2.119e-004
koh	Gas 1.197e-004	1.163e-004
hcn	Gas 9.253e-005	9.897e-005
h2	Gas 5.064e-005	4.766e-005
n	Gas 3.478e-005	3.389e-005
no	Gas 1.354e-005	1.279e-005
o	Gas 1.162e-005	1.062e-005
c	Gas 9.064e-006	9.390e-006
s2o	Gas 8.929e-006	8.549e-006
h2s	Gas 4.533e-006	4.363e-006

cho	Gas	1.517e-006	1.528e-006
alho2	Gas	1.483e-006	1.382e-006
oh	Gas	1.278e-006	1.170e-006
alo2	Gas	9.014e-007	8.415e-007
nco	Gas	5.538e-007	5.775e-007
so2	Gas	4.962e-007	4.510e-007
halo	Gas	3.776e-007	3.630e-007
nh	Gas	2.001e-007	1.958e-007
h2o	Gas	1.524e-007	1.397e-007
hnco	Gas	5.057e-008	5.278e-008
c2h2	Gas	4.772e-008	5.452e-008
o2	Gas	1.312e-008	1.166e-008
nh2	Gas	3.388e-009	3.323e-009
n2o	Gas	3.371e-009	3.317e-009
ch2	Gas	3.217e-009	3.351e-009
ch2o	Gas	1.251e-009	1.263e-009
hno	Gas	3.996e-010	3.807e-010
ketene	Gas	1.205e-010	1.341e-010
ch3cl	Gas	1.192e-010	1.330e-010
ch3	Gas	8.671e-011	9.047e-011
nh3	Gas	5.916e-011	5.814e-011
no2	Gas	9.638e-012	8.924e-012
k2h2o2	Gas	6.170e-012	6.239e-012
formac	Gas	2.606e-012	2.565e-012
ho2	Gas	1.764e-012	1.580e-012
ch4	Gas	2.483e-013	2.587e-013
ch3cn	Gas	1.501e-013	1.788e-013
hno2	Gas	2.767e-014	2.572e-014
ch2oh	Gas	1.411e-014	1.437e-014
c2h4	Gas	5.610e-015	6.429e-015
h2o2	Gas	5.470e-015	4.917e-015
ch4o	Gas	3.078e-017	3.143e-017
al2o3	liquid	2.824e+000	2.826e+000
*koh	liquid	0.000e+000	0.000e+000
c(s)	solid	0.000e+000	0.000e+000
al2o3	solid	0.000e+000	0.000e+000
Total Gas		1.385e+001	1.383e+001
Total Cond.		2.824e+000	2.826e+000

B.3 Load Density 0.4 g/cm³ Al/KClO₄ + 2 g Black Powder

Product library title: the blake product library

Executing library command: gas eos, virial

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

Input>composition, al, 150, potass per, 150, potass nit, 7.417, sulfur, 1.07, susqkull, 1.499, ash, 0.014, weight

The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
al	48.39	82.37	46.32	0	9.99	0.000	26.98	al1
potass per	48.39	16.04	49.47	-103250	54.81	0.000	138.55	o4cl1k1
potass nit	2.39	1.09	2.94	-118069	48.03	0.000	101.10	n1o3k1
sulfur	0.35	0.49	0.43	0	15.49	0.000	32.06	s1
susqkull	0.48	0.00	0.83	-4489962	12194.95	0.000	18292.43	c1321h573n4o100s6
ash	0.00	0.00	0.01	-271989	106.31	0.000	138.20	c1o3k2

Heat of formation = -389.805 cal/gm

Standard volume = 0.387 cc/gm

Standard entropy = 0.000 cal/k/gm

Standard energy = -389.815 cal/gm

The elements and percent by mole

al	44.051
o	36.126
cl	8.579
k	9.162
n	0.584
s	0.268
c	0.859
h	0.372

The average mol. wt. = 45.934 g/mol

Input>gun, 0.40000, 0.013300, 0.426600

GUN calculation:

	Rho g/cc	Temp K	Pressure MPa	Impetus J/g	Mol Wt. Gas	Covol cc/g	Frozen Cp/Cv	Phi
1.)	0.4000	3668.0	190.6	413.53	73.751	0.248	1.115	1.110
2.)	0.4133	3669.2	197.8	413.29	73.819	0.248	1.115	1.114
3.)	0.4266	3670.4	205.0	413.05	73.885	0.247	1.115	1.118

Product concentrations (mol/kg)

Name		1.)	2.)	3.)
al2o	Gas	6.250e+000	6.250e+000	6.249e+000
cl	Gas	3.342e+000	3.342e+000	3.342e+000
k	Gas	2.891e+000	2.869e+000	2.847e+000
k2	Gas	4.191e-001	4.300e-001	4.407e-001
co	Gas	3.061e-001	3.050e-001	3.040e-001
hcl	Gas	1.503e-001	1.503e-001	1.503e-001
n2	Gas	1.185e-001	1.185e-001	1.185e-001
cs	Gas	3.479e-002	3.564e-002	3.648e-002
s2	Gas	2.192e-002	2.148e-002	2.104e-002
s	Gas	1.497e-002	1.455e-002	1.414e-002
cs2	Gas	6.783e-003	7.009e-003	7.230e-003
cos	Gas	1.442e-003	1.456e-003	1.469e-003
kh	Gas	8.070e-004	8.043e-004	8.016e-004
ns	Gas	3.796e-004	3.772e-004	3.748e-004
cn	Gas	2.674e-004	2.779e-004	2.885e-004
sh	Gas	1.645e-004	1.602e-004	1.561e-004
h	Gas	1.432e-004	1.382e-004	1.335e-004
ko	Gas	1.349e-004	1.324e-004	1.301e-004
so	Gas	7.500e-005	7.190e-005	6.899e-005
co2	Gas	6.154e-005	6.041e-005	5.933e-005
hcn	Gas	3.901e-005	4.052e-005	4.205e-005
koh	Gas	2.735e-005	2.688e-005	2.643e-005
n	Gas	1.378e-005	1.359e-005	1.340e-005
c	Gas	6.147e-006	6.263e-006	6.379e-006
h2	Gas	4.497e-006	4.350e-006	4.212e-006
no	Gas	3.221e-006	3.123e-006	3.031e-006
o	Gas	2.397e-006	2.281e-006	2.174e-006
s2o	Gas	2.031e-006	1.966e-006	1.903e-006
h2s	Gas	3.780e-007	3.679e-007	3.582e-007
cho	Gas	3.221e-007	3.238e-007	3.254e-007
nco	Gas	2.753e-007	2.823e-007	2.894e-007
alo2	Gas	2.327e-007	2.243e-007	2.165e-007
alho2	Gas	2.014e-007	1.941e-007	1.874e-007
oh	Gas	1.292e-007	1.232e-007	1.176e-007
halo	Gas	7.918e-008	7.752e-008	7.595e-008
so2	Gas	6.658e-008	6.297e-008	5.963e-008
nh	Gas	3.687e-008	3.646e-008	3.606e-008
c2h2	Gas	1.657e-008	1.786e-008	1.921e-008
hnco	Gas	1.256e-008	1.290e-008	1.324e-008
h2o	Gas	7.875e-009	7.519e-009	7.189e-009
o2	Gas	1.531e-009	1.435e-009	1.347e-009
n2o	Gas	9.086e-010	9.033e-010	8.984e-010
ch2	Gas	5.000e-010	5.117e-010	5.233e-010
nh2	Gas	3.015e-010	2.987e-010	2.960e-010
ch2o	Gas	1.263e-010	1.272e-010	1.281e-010
hno	Gas	4.332e-011	4.226e-011	4.127e-011
ch3cl	Gas	2.589e-011	2.757e-011	2.930e-011
ketene	Gas	2.468e-011	2.624e-011	2.786e-011
ch3	Gas	6.656e-012	6.821e-012	6.986e-012
nh3	Gas	2.612e-012	2.593e-012	2.575e-012
no2	Gas	1.257e-012	1.208e-012	1.163e-012
k2h2o2	Gas	7.801e-013	7.840e-013	7.880e-013
formac	Gas	1.521e-013	1.512e-013	1.504e-013
ho2	Gas	9.340e-014	8.807e-014	8.319e-014
ch3cn	Gas	2.710e-014	2.994e-014	3.301e-014
ch4	Gas	8.856e-015	9.057e-015	9.257e-015
hno2	Gas	1.675e-015	1.614e-015	1.558e-015
ch2oh	Gas	6.040e-016	6.115e-016	6.190e-016
c2h4	Gas	3.809e-016	4.102e-016	4.410e-016
h2o2	Gas	1.377e-016	1.302e-016	1.233e-016
ch4o	Gas	6.339e-019	6.430e-019	6.522e-019
al2o3	liquid	2.716e+000	2.717e+000	2.717e+000
*koh	liquid	0.000e+000	0.000e+000	0.000e+000
c(s)	solid	0.000e+000	0.000e+000	0.000e+000
al2o3	solid	0.000e+000	0.000e+000	0.000e+000
Total Gas		1.356e+001	1.355e+001	1.353e+001
Total Cond.		2.716e+000	2.717e+000	2.717e+000

B.4 50 Al/50 KClO₄

Product library title: the blake product library

Executing library command: gas eos, virial

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

The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
al	50.00	83.70	48.36	0	9.99	0.000	26.98	al1
potass per	50.00	16.30	51.64	-103250	54.81	0.000	138.55	o4cl1k1

Heat of formation = -372.608 cal/gm
 Standard volume = 0.383 cc/gm
 Standard entropy = 0.000 cal/k/gm
 Standard energy = -372.617 cal/gm

The elements and percent by mole

al 46.116
 o 35.923
 cl 8.981
 k 8.981

The average mol. wt. = 45.168 g/mol

Input>composition, al, 50, potass per, 50, weight
 The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
al	50.00	83.70	48.36	0	9.99	0.000	26.98	al1
potass per	50.00	16.30	51.64	-103250	54.81	0.000	138.55	o4cl1k1

Heat of formation = -372.608 cal/gm
 Standard volume = 0.383 cc/gm
 Standard entropy = 0.000 cal/k/gm
 Standard energy = -372.617 cal/gm

The elements and percent by mole

al 46.116
 o 35.923
 cl 8.981
 k 8.981

The average mol. wt. = 45.168 g/mol

Input>gun, 0.100000, 0.100000, 1.050000

GUN calculation:

	Rho g/cc	Temp K	Pressure MPa	Impetus J/g	Mol Wt. Gas	Covol cc/g	Frozen Cp/Cv	Phi
1.)	0.1000	3564.6	42.2	408.22	72.605	0.245	1.120	1.025
2.)	0.2000	3572.0	86.8	405.90	73.172	0.243	1.119	1.051
3.)	0.3000	3578.4	134.1	403.84	73.678	0.241	1.118	1.078
4.)	0.4000	3584.2	184.3	401.97	74.138	0.239	1.117	1.106
5.)	0.5000	3589.3	237.5	400.26	74.562	0.238	1.117	1.135
6.)	0.6000	3594.1	294.1	398.67	74.958	0.236	1.116	1.165
7.)	0.7000	3598.4	354.3	397.18	75.330	0.234	1.116	1.196
8.)	0.8000	3602.5	418.3	395.78	75.682	0.233	1.116	1.229
9.)	0.9000	3606.2	486.5	394.45	76.017	0.231	1.116	1.262
10.)	1.0000	3609.8	559.2	393.18	76.338	0.229	1.116	1.298

Product concentrations (mol/kg)

Name		1.)	2.)	3.)	4.)	5.)	6.)
al2o	Gas	6.681e+000	6.681e+000	6.681e+000	6.681e+000	6.681e+000	6.681e+000
cl	Gas	3.609e+000	3.609e+000	3.609e+000	3.609e+000	3.609e+000	3.609e+000
k	Gas	3.359e+000	3.145e+000	2.958e+000	2.789e+000	2.636e+000	2.494e+000
k2	Gas	1.250e-001	2.318e-001	3.256e-001	4.098e-001	4.865e-001	5.573e-001
ko	Gas	1.763e-004	1.211e-004	9.594e-005	8.059e-005	6.990e-005	6.186e-005
o	Gas	1.032e-005	3.624e-006	1.943e-006	1.235e-006	8.595e-007	6.333e-007
alo2	Gas	6.245e-007	2.693e-007	1.650e-007	1.165e-007	8.870e-008	7.086e-008
o2	Gas	9.685e-009	2.421e-009	1.063e-009	5.855e-010	3.642e-010	2.444e-010
al2o3	liq	2.585e+000	2.585e+000	2.585e+000	2.585e+000	2.585e+000	2.585e+000
al2o3	sol	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000

Total Gas 1.377e+001 1.367e+001 1.357e+001 1.349e+001 1.341e+001 1.334e+001
 Total Con 2.585e+000 2.585e+000 2.585e+000 2.585e+000 2.585e+000 2.585e+000

Product concentrations (mol/kg)

Name		7.)	8.)	9.)	10.)
al2o	Gas	6.681e+000	6.681e+000	6.681e+000	6.681e+000
cl	Gas	3.609e+000	3.609e+000	3.609e+000	3.609e+000
k	Gas	2.362e+000	2.239e+000	2.122e+000	2.012e+000
k2	Gas	6.232e-001	6.850e-001	7.433e-001	7.985e-001
ko	Gas	5.551e-005	5.032e-005	4.598e-005	4.227e-005
o	Gas	4.848e-007	3.815e-007	3.064e-007	2.500e-007
alo2	Gas	5.847e-008	4.941e-008	4.252e-008	3.711e-008
o2	Gas	1.727e-010	1.266e-010	9.540e-011	7.348e-011
al2o3	liquid	2.585e+000	2.585e+000	2.585e+000	2.585e+000
al2o3	solid	0.000e+000	0.000e+000	0.000e+000	0.000e+000
Total Gas		1.327e+001	1.321e+001	1.315e+001	1.310e+001
Total Cond.		2.585e+000	2.585e+000	2.585e+000	2.585e+000

C THEORETICAL CALCULATIONS FOR Mg/ Al/KClO₄ COMPOSITIONS

C.1 0.12 g/cm³ RS-41 + 2 g Black Powder

Input>composition, magnesium, 22.05, al, 22.05, potass per, 44.1, potass nit, 7.417, resinat, 1.8, sulfur, 1.07, susqkull, 1.499, ash, 0.014, weight
The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
magnesium	22.05	42.15	28.16	0	13.97	0.000	24.31	mg1
al	22.05	37.97	18.15	0	9.99	0.000	26.98	al1
potass per	44.10	14.79	38.77	-103250	54.81	0.000	138.55	o4cl1k1
potass nit	7.42	3.41	7.83	-118069	48.03	0.000	101.10	n1o3k1
resinat	1.80	0.13	3.70	-23901	580.75	0.000	627.20	c40h58o4mg1
sulfur	1.07	1.55	1.15	0	15.49	0.000	32.06	s1
susqkull	1.50	0.00	2.22	-4489962	12194.95	0.000	18292.43	c1321h573n4o100s6
ash	0.01	0.00	0.02	-271989	106.31	0.000	138.20	cl03k2

Heat of formation = -419.898 cal/gm
Standard volume = 0.450 cc/gm
Standard entropy = 0.000 cal/k/gm
Standard energy = -419.909 cal/gm

The elements and percent by mole

mg	20.248
al	18.181
o	33.666
cl	7.081
k	8.718
n	1.639
c	4.965
h	4.748
s	0.753

The average mol. wt. = 46.457 g/mol
Input>gun, 0.120000, 0.013300, 0.13330000
GUN calculation:

	Rho g/cc	Temp K	Pressure MPa	Impetus J/g	Mol Wt. Gas	Covol cc/g	Frozen Cp/Cv	Phi
1.)	0.1200	3983.6	57.6	457.19	72.448	0.290	1.108	1.036
2.)	0.1333	3987.9	64.3	456.94	72.566	0.289	1.108	1.040

Product concentrations (mol/kg)

Name		1.)	2.)
al2o	Gas	4.086e+000	4.086e+000
k	Gas	3.590e+000	3.562e+000
co	Gas	1.941e+000	1.941e+000
hcl	Gas	1.869e+000	1.879e+000
cl	Gas	1.314e+000	1.304e+000
n2	Gas	3.501e-001	3.501e-001
cs	Gas	2.352e-001	2.346e-001
k2	Gas	1.337e-001	1.472e-001
kh	Gas	6.035e-002	6.127e-002
h	Gas	5.275e-002	4.842e-002
h2	Gas	4.958e-002	4.621e-002
s	Gas	3.771e-002	3.636e-002
hcn	Gas	2.832e-002	2.842e-002
sh	Gas	1.559e-002	1.529e-002
s2	Gas	1.217e-002	1.252e-002
cs2	Gas	1.037e-002	1.104e-002
cn	Gas	7.344e-003	7.288e-003
cos	Gas	2.766e-003	2.973e-003
c2h2	Gas	2.703e-003	2.717e-003
h2s	Gas	1.380e-003	1.373e-003
ns	Gas	7.851e-004	8.027e-004
koh	Gas	6.589e-004	7.220e-004
c	Gas	4.070e-004	3.842e-004
co2	Gas	1.615e-004	1.745e-004
cho	Gas	1.593e-004	1.641e-004
n	Gas	1.538e-004	1.477e-004
ko	Gas	1.272e-004	1.377e-004
so	Gas	7.362e-005	7.680e-005
ch2	Gas	4.177e-005	4.075e-005
h2o	Gas	3.610e-005	3.643e-005
oh	Gas	2.295e-005	2.285e-005
nh	Gas	1.728e-005	1.691e-005
ch3	Gas	1.655e-005	1.637e-005
o	Gas	1.374e-005	1.348e-005
no	Gas	1.081e-005	1.117e-005
halo	Gas	8.089e-006	8.185e-006
nh2	Gas	4.782e-006	4.753e-006

alho2	Gas	4.575e-006	4.973e-006
hnco	Gas	3.834e-006	4.173e-006
nco	Gas	3.031e-006	3.254e-006
ch3cl	Gas	2.794e-006	3.043e-006
ch2o	Gas	2.313e-006	2.424e-006
ketene	Gas	1.539e-006	1.673e-006
nh3	Gas	1.236e-006	1.247e-006
ch4	Gas	7.435e-007	7.444e-007
s2o	Gas	5.529e-007	6.170e-007
alo2	Gas	2.569e-007	2.765e-007
ch3cn	Gas	1.486e-007	1.613e-007
c2h4	Gas	1.339e-007	1.391e-007
so2	Gas	2.398e-008	2.704e-008
hno	Gas	7.868e-009	8.327e-009
o2	Gas	3.770e-009	3.996e-009
n2o	Gas	2.593e-009	2.848e-009
formac	Gas	1.198e-009	1.359e-009
ch2oh	Gas	7.920e-010	8.509e-010
k2h2o2	Gas	7.849e-011	1.051e-010
ch4o	Gas	2.881e-011	3.146e-011
ho2	Gas	1.262e-011	1.370e-011
no2	Gas	2.810e-012	3.169e-012
h2o2	Gas	6.871e-013	7.589e-013
hno2	Gas	1.597e-013	1.835e-013
mgo2h2	Gas	4.892e-017	5.012e-017
mgo	liquid	9.101e+000	9.101e+000
c(s)	solid	0.000e+000	0.000e+000
mgo	solid	0.000e+000	0.000e+000
*koh	liquid	0.000e+000	0.000e+000
al2o3	solid	0.000e+000	0.000e+000
al2o3	liquid	0.000e+000	0.000e+000
Total Gas		1.380e+001	1.378e+001
Total Cond.		9.101e+000	9.101e+000

C.2 0.40 g/cm³ RS-41, + 2 g Black Powder

Input>composition, potass per, 47.42, al, 23.71, magnesium, 23.71, resinat, 1.9355, potass nit, 2.39, sulfur, 0.345, susqkull, 0.4835, weight

The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
potass per	47.42	15.32	42.07	-103250	54.81	0.000	138.55	o ₄ cl ₁ k ₁
al	23.71	39.33	19.70	0	9.99	0.000	26.98	al ₁
magnesium	23.71	43.67	30.56	0	13.97	0.000	24.31	mg ₁
resinat	1.94	0.14	4.02	-23901	580.75	0.000	627.20	c ₄₀ h ₅₈ o ₄ mg ₁
potass nit	2.39	1.06	2.55	-118069	48.03	0.000	101.10	n ₁ o ₃ k ₁
sulfur	0.35	0.48	0.37	0	15.49	0.000	32.06	s ₁
susqkull	0.48	0.00	0.72	-4489962	12194.95	0.000	18292.43	c ₁₃₂₁ h ₅₇₃ n ₄ o ₁₀₀ s ₆

Heat of formation = -383.240 cal/gm
 Standard volume = 0.446 cc/gm
 Standard entropy = 0.000 cal/k/gm
 Standard energy = -383.251 cal/gm

The elements and percent by mole

o	33.010
cl	7.765
k	8.302
al	19.937
mg	22.203
c	3.593
h	4.404
n	0.539
s	0.248

The average mol. wt. = 44.760 g/mol
 Input>gun, 0.400000, 0.01330000, 0.440000
 GUN calculation:

	Rho g/cc	Temp K	Pressure MPa	Impetus J/g	Mol Wt. Gas	Covol cc/g	Frozen Cp/Cv	Phi
1.)	0.4000	4281.3	195.6	422.01	84.355	0.231	1.090	1.102
2.)	0.4133	4282.9	203.0	421.78	84.431	0.231	1.090	1.106
3.)	0.4266	4284.4	210.5	421.55	84.507	0.231	1.090	1.109
4.)	0.4399	4285.9	218.1	421.32	84.583	0.231	1.090	1.113

Product concentrations (mol/kg)

Name	1.)	2.)	3.)	4.)
al2o	Gas	4.394e+000	4.394e+000	4.394e+000
k	Gas	2.987e+000	2.969e+000	2.951e+000
hcl	Gas	1.744e+000	1.746e+000	1.749e+000

c1	Gas	1.679e+000	1.676e+000	1.674e+000	1.671e+000
co	Gas	3.692e-001	3.692e-001	3.692e-001	3.692e-001
k2	Gas	3.039e-001	3.127e-001	3.214e-001	3.301e-001
cs	Gas	9.920e-002	9.911e-002	9.901e-002	9.890e-002
n2	Gas	9.199e-002	9.224e-002	9.251e-002	9.277e-002
kh	Gas	6.457e-002	6.464e-002	6.471e-002	6.477e-002
hcn	Gas	3.776e-002	3.743e-002	3.707e-002	3.673e-002
h	Gas	2.457e-002	2.378e-002	2.304e-002	2.234e-002
h2	Gas	1.737e-002	1.691e-002	1.646e-002	1.604e-002
c2h2	Gas	1.674e-002	1.639e-002	1.602e-002	1.566e-002
cn	Gas	1.549e-002	1.532e-002	1.514e-002	1.496e-002
s	Gas	5.026e-003	5.012e-003	5.003e-003	4.994e-003
sh	Gas	1.831e-003	1.835e-003	1.842e-003	1.848e-003
c	Gas	1.438e-003	1.392e-003	1.348e-003	1.306e-003
cs2	Gas	9.997e-004	1.034e-003	1.069e-003	1.105e-003
s2	Gas	3.616e-004	3.732e-004	3.856e-004	3.981e-004
cos	Gas	1.680e-004	1.746e-004	1.815e-004	1.885e-004
h2s	Gas	1.331e-004	1.338e-004	1.346e-004	1.354e-004
koh	Gas	1.121e-004	1.168e-004	1.217e-004	1.267e-004
n	Gas	1.095e-004	1.081e-004	1.068e-004	1.055e-004
ns	Gas	1.081e-004	1.103e-004	1.127e-004	1.151e-004
ch2	Gas	1.047e-004	1.024e-004	1.001e-004	9.795e-005
cho	Gas	5.331e-005	5.391e-005	5.451e-005	5.510e-005
ko	Gas	3.349e-005	3.476e-005	3.609e-005	3.744e-005
ch3	Gas	3.035e-005	2.981e-005	2.928e-005	2.876e-005
ch3cl	Gas	1.326e-005	1.351e-005	1.375e-005	1.398e-005
nh	Gas	1.187e-005	1.178e-005	1.171e-005	1.163e-005
co2	Gas	5.698e-006	5.927e-006	6.167e-006	6.410e-006
halo	Gas	3.591e-006	3.623e-006	3.658e-006	3.691e-006
nh2	Gas	2.666e-006	2.660e-006	2.655e-006	2.650e-006
h2o	Gas	2.473e-006	2.507e-006	2.545e-006	2.582e-006
oh	Gas	2.350e-006	2.371e-006	2.395e-006	2.419e-006
o	Gas	1.867e-006	1.875e-006	1.886e-006	1.897e-006
so	Gas	1.818e-006	1.889e-006	1.964e-006	2.041e-006
ketene	Gas	1.735e-006	1.768e-006	1.800e-006	1.832e-006
nco	Gas	1.210e-006	1.246e-006	1.283e-006	1.320e-006
no	Gas	1.077e-006	1.104e-006	1.132e-006	1.161e-006
hnco	Gas	1.056e-006	1.093e-006	1.129e-006	1.167e-006
ch4	Gas	9.863e-007	9.703e-007	9.541e-007	9.383e-007
ch3cn	Gas	9.013e-007	9.083e-007	9.136e-007	9.188e-007
c2h4	Gas	7.474e-007	7.361e-007	7.238e-007	7.118e-007
ch2o	Gas	6.764e-007	6.875e-007	6.988e-007	7.100e-007
nh3	Gas	5.119e-007	5.132e-007	5.147e-007	5.161e-007
alho2	Gas	2.392e-007	2.508e-007	2.632e-007	2.759e-007
alo2	Gas	2.478e-008	2.591e-008	2.711e-008	2.834e-008
s2o	Gas	3.655e-009	3.933e-009	4.237e-009	4.557e-009
hno	Gas	9.953e-010	1.029e-009	1.065e-009	1.101e-009
ch2oh	Gas	3.440e-010	3.524e-010	3.609e-010	3.695e-010
n2o	Gas	2.956e-010	3.109e-010	3.272e-010	3.439e-010
so2	Gas	1.045e-010	1.130e-010	1.224e-010	1.323e-010
o2	Gas	9.626e-011	1.006e-010	1.052e-010	1.099e-010
formac	Gas	7.037e-011	7.454e-011	7.896e-011	8.353e-011
ch4o	Gas	1.037e-011	1.068e-011	1.099e-011	1.131e-011
k2h2o2	Gas	6.641e-012	7.505e-012	8.475e-012	9.541e-012
ho2	Gas	4.122e-013	4.344e-013	4.584e-013	4.831e-013
no2	Gas	8.575e-014	9.194e-014	9.866e-014	1.057e-013
h2o2	Gas	1.947e-014	2.063e-014	2.188e-014	2.317e-014
hno2	Gas	4.778e-015	5.153e-015	5.561e-015	5.992e-015
mgo2h2	Gas	8.205e-018	8.367e-018	8.541e-018	8.715e-018
mgo	liquid	9.787e+000	9.787e+000	9.787e+000	9.787e+000
c(s)	solid	1.026e+000	1.027e+000	1.028e+000	1.030e+000
mgo	solid	0.000e+000	0.000e+000	0.000e+000	0.000e+000
*koh	liquid	0.000e+000	0.000e+000	0.000e+000	0.000e+000
al2o3	solid	0.000e+000	0.000e+000	0.000e+000	0.000e+000
al2o3	liquid	0.000e+000	0.000e+000	0.000e+000	0.000e+000
Total	Gas	1.185e+001	1.184e+001	1.183e+001	1.182e+001
Total	Cond.	1.081e+001	1.081e+001	1.082e+001	1.082e+001

C.3 0.60 g/cm³ RS-41, + 2 g Black Powder

Input>composition, potass per, 47.93, al, 23.96, magnesium, 23.96, resinat, 1.957, potass nit, 1.612, sulfur, 0.233, susqkull, 0.326 weight
The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
potass per	47.94	15.40	42.59	-103250	54.81	0.000	138.55	o4c11k1
al	23.97	39.54	19.94	0	9.99	0.000	26.98	al1
magnesium	23.97	43.89	30.94	0	13.97	0.000	24.31	mg1
resinat	1.96	0.14	4.07	-23901	580.75	0.000	627.20	c40h58o4mg1
potass nit	1.61	0.71	1.72	-118069	48.03	0.000	101.10	n1o3k1

sulfur 0.23 0.32 0.25 0 15.49 0.000 32.06 s1
 susqkull 0.33 0.00 0.49-4489962 12194.95 0.00018292.43 c₁₃₂₁h₅₇₃n₄o₁₀₀s₆

Heat of formation = -377.636 cal/gm
 Standard volume = 0.445 cc/gm
 Standard entropy = 0.000 cal/k/gm
 Standard energy = -377.647 cal/gm

The elements and percent by mole

o 32.909
 cl 7.874
 k 8.237
 al 20.212
 mg 22.509
 c 3.377
 h 4.351
 n 0.365
 s 0.168

The average mol. wt. = 44.512 g/mol
 Input>gun, 0.600000, 0.01330000, 0.640000
 GUN calculation:

	Rho g/cc	Temp K	Pressure MPa	Impetus J/g	Mol Wt. Gas	Covol cc/g	Frozen Cp/Cv	Phi
1.)	0.6000	4343.2	309.4	413.55	87.324	0.222	1.087	1.154
2.)	0.6133	4344.4	317.8	413.33	87.392	0.222	1.087	1.157
3.)	0.6266	4345.5	326.2	413.12	87.460	0.222	1.087	1.161
4.)	0.6399	4346.6	334.7	412.90	87.527	0.222	1.087	1.165

Product concentrations (mol/kg)

Name		1.)	2.)	3.)	4.)
al2o	Gas	4.441e+000	4.441e+000	4.441e+000	4.441e+000
k	Gas	2.725e+000	2.709e+000	2.693e+000	2.678e+000
hcl	Gas	1.749e+000	1.751e+000	1.752e+000	1.754e+000
cl	Gas	1.711e+000	1.709e+000	1.708e+000	1.706e+000
k2	Gas	4.147e-001	4.226e-001	4.304e-001	4.382e-001
co	Gas	1.291e-001	1.291e-001	1.290e-001	1.290e-001
cs	Gas	6.706e-002	6.701e-002	6.696e-002	6.691e-002
kh	Gas	6.552e-002	6.548e-002	6.543e-002	6.538e-002
n2	Gas	6.036e-002	6.051e-002	6.065e-002	6.079e-002
hcn	Gas	2.751e-002	2.731e-002	2.713e-002	2.694e-002
h	Gas	1.719e-002	1.677e-002	1.637e-002	1.598e-002
c2h2	Gas	1.323e-002	1.300e-002	1.278e-002	1.256e-002
h2	Gas	1.231e-002	1.206e-002	1.182e-002	1.158e-002
cn	Gas	1.179e-002	1.169e-002	1.159e-002	1.150e-002
s	Gas	3.385e-003	3.380e-003	3.375e-003	3.369e-003
sh	Gas	1.277e-003	1.280e-003	1.283e-003	1.285e-003
c	Gas	1.125e-003	1.097e-003	1.070e-003	1.045e-003
cs2	Gas	6.615e-004	6.789e-004	6.963e-004	7.139e-004
s2	Gas	2.372e-004	2.432e-004	2.492e-004	2.552e-004
h2s	Gas	9.217e-005	9.248e-005	9.276e-005	9.303e-005
ch2	Gas	8.633e-005	8.481e-005	8.336e-005	8.195e-005
n	Gas	8.402e-005	8.326e-005	8.252e-005	8.179e-005
ns	Gas	7.854e-005	7.988e-005	8.121e-005	8.254e-005
koh	Gas	6.445e-005	6.649e-005	6.853e-005	7.061e-005
cos	Gas	6.319e-005	6.515e-005	6.714e-005	6.916e-005
ch3	Gas	2.502e-005	2.466e-005	2.431e-005	2.398e-005
cho	Gas	2.271e-005	2.292e-005	2.313e-005	2.333e-005
ko	Gas	1.973e-005	2.030e-005	2.086e-005	2.144e-005
ch3cl	Gas	1.671e-005	1.693e-005	1.716e-005	1.739e-005
nh	Gas	9.593e-006	9.545e-006	9.499e-006	9.453e-006
halo	Gas	2.553e-006	2.572e-006	2.590e-006	2.608e-006
nh2	Gas	2.198e-006	2.195e-006	2.192e-006	2.189e-006
co2	Gas	1.144e-006	1.179e-006	1.215e-006	1.252e-006
h2o	Gas	1.033e-006	1.046e-006	1.058e-006	1.070e-006
oh	Gas	9.910e-007	9.992e-007	1.007e-006	1.015e-006
ch3cn	Gas	8.074e-007	8.113e-007	8.154e-007	8.195e-007
ketene	Gas	7.972e-007	8.086e-007	8.203e-007	8.321e-007
o	Gas	7.833e-007	7.872e-007	7.908e-007	7.945e-007
ch4	Gas	7.824e-007	7.711e-007	7.601e-007	7.494e-007
so	Gas	7.147e-007	7.370e-007	7.594e-007	7.821e-007
c2h4	Gas	6.119e-007	6.025e-007	5.936e-007	5.849e-007
nco	Gas	5.393e-007	5.522e-007	5.653e-007	5.785e-007
hnco	Gas	4.654e-007	4.780e-007	4.908e-007	5.038e-007
no	Gas	4.470e-007	4.561e-007	4.652e-007	4.743e-007
nh3	Gas	4.248e-007	4.258e-007	4.267e-007	4.277e-007
ch2o	Gas	2.981e-007	3.019e-007	3.058e-007	3.097e-007
alho2	Gas	9.105e-008	9.456e-008	9.813e-008	1.018e-007
alo2	Gas	9.993e-009	1.036e-008	1.072e-008	1.110e-008
s2o	Gas	1.448e-009	1.535e-009	1.624e-009	1.717e-009
hno	Gas	4.689e-010	4.818e-010	4.948e-010	5.080e-010
ch2oh	Gas	1.734e-010	1.767e-010	1.799e-010	1.832e-010
n2o	Gas	1.381e-010	1.438e-010	1.497e-010	1.558e-010
so2	Gas	2.374e-011	2.528e-011	2.687e-011	2.855e-011
o2	Gas	2.317e-011	2.400e-011	2.484e-011	2.570e-011

formac	Gas	1.838e-011	1.924e-011	2.011e-011	2.102e-011
ch4o	Gas	5.354e-012	5.474e-012	5.595e-012	5.718e-012
k2h2o2	Gas	3.536e-012	3.877e-012	4.243e-012	4.638e-012
ho2	Gas	1.126e-013	1.174e-013	1.224e-013	1.275e-013
no2	Gas	2.337e-014	2.471e-014	2.611e-014	2.756e-014
h2o2	Gas	5.489e-015	5.747e-015	6.012e-015	6.285e-015
hno2	Gas	1.377e-015	1.462e-015	1.551e-015	1.644e-015
mgo2h2	Gas	4.131e-018	4.200e-018	4.269e-018	4.339e-018
mgo	liquid	9.891e+000	9.891e+000	9.891e+000	9.891e+000
c(s)	solid	1.220e+000	1.221e+000	1.222e+000	1.222e+000
mgo	solid	0.000e+000	0.000e+000	0.000e+000	0.000e+000
*koh	liquid	0.000e+000	0.000e+000	0.000e+000	0.000e+000
al2o3	solid	0.000e+000	0.000e+000	0.000e+000	0.000e+000
al2o3	liquid	0.000e+000	0.000e+000	0.000e+000	0.000e+000
Total Gas		1.145e+001	1.144e+001	1.143e+001	1.143e+001
Total Cond.		1.111e+001	1.111e+001	1.111e+001	1.111e+001

C.4 The Composition 24 Al/24 Mg/2 Res/50 KClO₄

Product library title: the blake product library

Executing library command: gas eos, virial

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

Input>composition, potass per, 50, al, 24, resinat, 2, magnesium, 24, weight
The Composition

Name	% wt.	% mol	% vol.	Heat of formation (cal/mol)	Standard volume (cc/mol)	Standard entropy (cal/K/mol)	Mol. wt.	Formula
potass per	50.00	16.10	44.63	-103250	54.81	0.000	138.55	o4cl1k1
al	24.00	39.69	20.06	0	9.99	0.000	26.98	al1
resinat	2.00	0.14	4.18	-23901	580.75	0.000	627.20	c40h58o4mg1
magnesium	24.00	44.06	31.13	0	13.97	0.000	24.31	mg1

Heat of formation = -373.370 cal/gm
Standard volume = 0.443 cc/gm
Standard entropy = 0.000 cal/k/gm
Standard energy = -373.381 cal/gm

The elements and percent by mole

o	33.319
cl	8.257
k	8.257
al	20.351
c	2.918
h	4.232
mg	22.666

The average mol. wt. = 44.623 g/mol

Input>gun, 0.100000, 0.100000, 1.000000

GUN calculation:

	Rho g/cc	Temp K	Pressure MPa	Impetus J/g	Mol Wt. Gas	Covol cc/g	Frozen Cp/Cv	Phi
1.)	0.1000	4314.3	44.5	429.65	83.491	0.225	1.091	1.023
2.)	0.2000	4348.8	91.9	427.95	84.493	0.224	1.090	1.047
3.)	0.3000	4367.2	142.3	426.17	85.204	0.223	1.089	1.072
4.)	0.4000	4380.0	196.1	424.42	85.807	0.223	1.088	1.098
5.)	0.5000	4390.0	253.6	422.71	86.352	0.223	1.088	1.125
6.)	0.6000	4398.5	315.0	421.04	86.863	0.222	1.088	1.154
7.)	0.7000	4406.0	380.7	419.41	87.348	0.222	1.087	1.184
8.)	0.8000	4412.8	451.1	417.82	87.816	0.222	1.087	1.216
9.)	0.9000	4419.1	526.6	416.26	88.270	0.221	1.087	1.249
10.)	1.0000	4425.0	607.7	414.74	88.712	0.221	1.087	1.283

Product concentrations (mol/kg)

Name	1.)	2.)	3.)	4.)	5.)	6.)
al2o	Gas 4.447e+000	4.447e+000	4.447e+000	4.447e+000	4.447e+000	4.447e+000
k	Gas 3.395e+000	3.245e+000	3.107e+000	2.977e+000	2.854e+000	2.735e+000
cl	Gas 2.075e+000	1.986e+000	1.945e+000	1.920e+000	1.903e+000	1.890e+000
hcl	Gas 1.534e+000	1.623e+000	1.664e+000	1.689e+000	1.706e+000	1.719e+000
co	Gas 2.088e-001	2.088e-001	2.088e-001	2.087e-001	2.087e-001	2.087e-001
h	Gas 8.970e-002	5.181e-002	3.611e-002	2.734e-002	2.169e-002	1.773e-002
k2	Gas 8.000e-002	1.518e-001	2.194e-001	2.837e-001	3.454e-001	4.049e-001
kh	Gas 5.369e-002	6.054e-002	6.313e-002	6.410e-002	6.429e-002	6.401e-002
h2	Gas 4.324e-002	2.795e-002	2.068e-002	1.633e-002	1.341e-002	1.129e-002
c2h2	Gas 4.244e-002	2.901e-002	2.221e-002	1.802e-002	1.516e-002	1.306e-002
c	Gas 7.828e-003	4.311e-003	2.946e-003	2.207e-003	1.741e-003	1.419e-003
ch2	Gas 2.798e-004	1.963e-004	1.519e-004	1.238e-004	1.042e-004	8.975e-005
ch3	Gas 5.603e-005	4.373e-005	3.571e-005	3.019e-005	2.616e-005	2.308e-005
cho	Gas 2.139e-005	2.642e-005	2.974e-005	3.247e-005	3.497e-005	3.739e-005
koh	Gas 1.015e-005	2.360e-005	3.885e-005	5.585e-005	7.478e-005	9.588e-005
ch3cl	Gas 5.875e-006	8.684e-006	1.067e-005	1.232e-005	1.382e-005	1.528e-005
ko	Gas 4.449e-006	9.420e-006	1.479e-005	2.060e-005	2.690e-005	3.378e-005
halo	Gas 2.016e-006	2.474e-006	2.758e-006	2.976e-006	3.164e-006	3.337e-006
ch4	Gas 1.352e-006	1.156e-006	9.777e-007	8.394e-007	7.313e-007	6.449e-007
o	Gas 1.108e-006	1.223e-006	1.296e-006	1.355e-006	1.407e-006	1.456e-006

c2h4	Gas	1.079e-006	9.410e-007	8.009e-007	6.884e-007	5.986e-007	5.258e-007
oh	Gas	9.662e-007	1.190e-006	1.333e-006	1.447e-006	1.547e-006	1.642e-006
h2o	Gas	6.841e-007	9.316e-007	1.101e-006	1.241e-006	1.369e-006	1.492e-006
ketene	Gas	4.858e-007	6.940e-007	8.451e-007	9.758e-007	1.100e-006	1.225e-006
co2	Gas	3.686e-007	7.674e-007	1.212e-006	1.710e-006	2.270e-006	2.901e-006
ch2o	Gas	1.909e-007	2.672e-007	3.208e-007	3.658e-007	4.074e-007	4.483e-007
alho2	Gas	1.419e-008	3.477e-008	6.019e-008	9.094e-008	1.279e-007	1.724e-007
alo2	Gas	2.195e-009	4.992e-009	8.322e-009	1.226e-008	1.692e-008	2.242e-008
ch2oh	Gas	7.208e-011	1.209e-010	1.594e-010	1.937e-010	2.267e-010	2.602e-010
o2	Gas	6.602e-012	1.517e-011	2.534e-011	3.731e-011	5.133e-011	6.779e-011
formac	Gas	2.217e-012	6.557e-012	1.259e-011	2.051e-011	3.072e-011	4.377e-011
ch4o	Gas	1.521e-012	2.876e-012	4.029e-012	5.104e-012	6.171e-012	7.277e-012
ho2	Gas	1.983e-014	5.421e-014	9.965e-014	1.573e-013	2.293e-013	3.188e-013
k2h2o2	Gas	1.099e-014	1.222e-013	5.191e-013	1.506e-012	3.567e-012	7.466e-012
h2o2	Gas	6.584e-016	2.037e-015	3.991e-015	6.574e-015	9.911e-015	1.418e-014
mgo2h2	Gas	2.388e-018	3.591e-018	4.496e-018	5.297e-018	6.069e-018	6.854e-018
mgo liqui		9.906e+000	9.906e+000	9.906e+000	9.906e+000	9.906e+000	9.906e+000
c(s) solid		9.736e-001	1.004e+000	1.019e+000	1.028e+000	1.035e+000	1.039e+000
mgo solid		0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000
*koh liqu		0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000
al2o3 sol		0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000
al2o3 liq		0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000	0.000e+000
Total Gas		1.198e+001	1.184e+001	1.174e+001	1.165e+001	1.158e+001	1.151e+001
Total Con		1.088e+001	1.091e+001	1.093e+001	1.093e+001	1.094e+001	1.095e+001

Product concentrations (mol/kg)

Name	7.)	8.)	9.)	10.)	
al2o	Gas	4.447e+000	4.447e+000	4.447e+000	4.447e+000
k	Gas	2.620e+000	2.509e+000	2.401e+000	2.296e+000
cl	Gas	1.880e+000	1.872e+000	1.865e+000	1.860e+000
hcl	Gas	1.729e+000	1.737e+000	1.743e+000	1.749e+000
k2	Gas	4.625e-001	5.184e-001	5.729e-001	6.261e-001
co	Gas	2.086e-001	2.086e-001	2.086e-001	2.085e-001
kh	Gas	6.345e-002	6.270e-002	6.180e-002	6.080e-002
h	Gas	1.479e-002	1.252e-002	1.072e-002	9.252e-003
c2h2	Gas	1.146e-002	1.019e-002	9.159e-003	8.304e-003
h2	Gas	9.683e-003	8.418e-003	7.393e-003	6.545e-003
c	Gas	1.182e-003	1.000e-003	8.565e-004	7.397e-004
koh	Gas	1.195e-004	1.459e-004	1.757e-004	2.094e-004
ch2	Gas	7.856e-005	6.961e-005	6.227e-005	5.613e-005
ko	Gas	4.130e-005	4.956e-005	5.868e-005	6.876e-005
cho	Gas	3.982e-005	4.234e-005	4.498e-005	4.778e-005
ch3	Gas	2.064e-005	1.866e-005	1.702e-005	1.564e-005
ch3cl	Gas	1.675e-005	1.826e-005	1.986e-005	2.157e-005
co2	Gas	3.615e-006	4.425e-006	5.345e-006	6.395e-006
halo	Gas	3.501e-006	3.663e-006	3.825e-006	3.990e-006
oh	Gas	1.734e-006	1.827e-006	1.922e-006	2.021e-006
h2o	Gas	1.616e-006	1.745e-006	1.879e-006	2.023e-006
o	Gas	1.504e-006	1.552e-006	1.601e-006	1.651e-006
ketene	Gas	1.354e-006	1.493e-006	1.643e-006	1.809e-006
ch4	Gas	5.743e-007	5.153e-007	4.653e-007	4.222e-007
ch2o	Gas	4.899e-007	5.333e-007	5.796e-007	6.294e-007
c2h4	Gas	4.656e-007	4.148e-007	3.713e-007	3.336e-007
alho2	Gas	2.258e-007	2.903e-007	3.683e-007	4.630e-007
alo2	Gas	2.894e-008	3.668e-008	4.590e-008	5.691e-008
ch2oh	Gas	2.951e-010	3.325e-010	3.732e-010	4.182e-010
o2	Gas	8.710e-011	1.098e-010	1.366e-010	1.682e-010
formac	Gas	6.045e-011	8.174e-011	1.090e-010	1.440e-010
k2h2o2	Gas	1.440e-011	2.621e-011	4.580e-011	7.765e-011
ch4o	Gas	8.459e-012	9.750e-012	1.118e-011	1.280e-011
ho2	Gas	4.299e-013	5.679e-013	7.393e-013	9.528e-013
h2o2	Gas	1.961e-014	2.652e-014	3.531e-014	4.651e-014
mgo2h2	Gas	7.681e-018	8.571e-018	9.547e-018	1.063e-017
mgo liquid		9.906e+000	9.906e+000	9.906e+000	9.906e+000
c(s) solid		1.043e+000	1.045e+000	1.048e+000	1.049e+000
mgo solid		0.000e+000	0.000e+000	0.000e+000	0.000e+000
*koh liquid		0.000e+000	0.000e+000	0.000e+000	0.000e+000
al2o3 solid		0.000e+000	0.000e+000	0.000e+000	0.000e+000
al2o3 liquid		0.000e+000	0.000e+000	0.000e+000	0.000e+000
Total Gas		1.145e+001	1.139e+001	1.133e+001	1.127e+001
Total Cond.		1.095e+001	1.095e+001	1.095e+001	1.096e+001

References

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- (2) Laurence E. fried, W. Michael Howard, P. Clark Souers (20 August 1998): Cheetah 2.0 User's Manual: *UCRL-MA-117541 Rev. 5*, Lawrence Livermore National Laboratory.

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