SIMULATION OF POTASSIUM NITRATE – SUGAR ROCKET MOTORS

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Introduction

At the end of seventies the state of KNO3-sucrose research by BVRO (Belgian Association For Rocket Research) was described in the Youth & Space book "The Potassiumnitrate-sugar propellant"[1]. At the beginning of the nineties this led first at NERO (essentially by John Koster) and later at VRO (under the impulse of Jan Volckaert) to the development of new motors based on potassium nitrate (KNO_3). In the mean time a large number of tests have been realized (more than 60) and KNO_3 based motors were used for flight purposes. The most spectacular one for VRO being the Golden Sky, measuring 2.5 m long with a diameter of 0.16 m and a total weight of 30 kg. The rocket reached 2.4 km and the whole flight was filmed from inside of the rocket.

The large number of data generated by all these tests give us the possibility to review the functioning of these motors. This would not be necessary if these motors would behave as expected. In many cases the measured thrust and pressure diagrams do deviate strongly from expectations. It is worth trying to understand the phenomena which occur in these motors.

In the first place we want to draw the attention to the following differences between the 3 motor types:

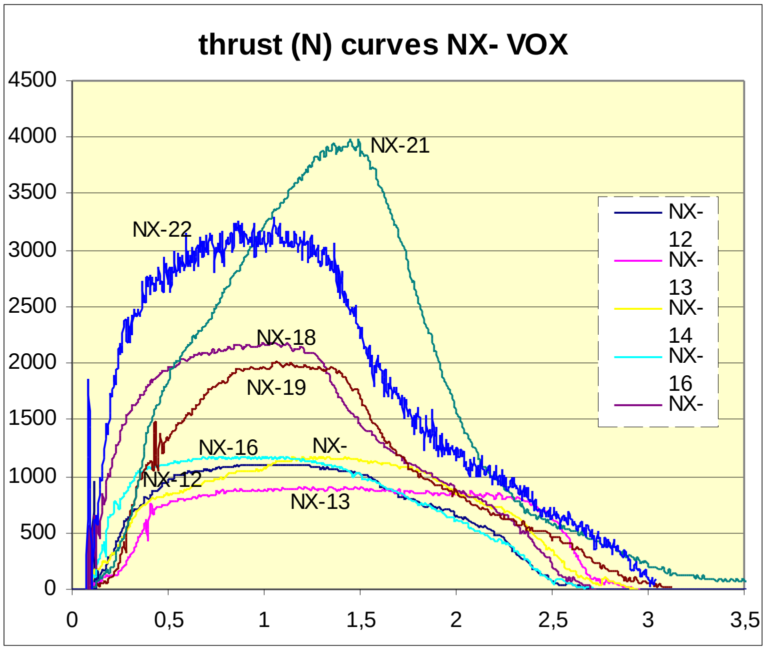
1. BVRO: although tests with sorbitol and mannitol were preformed back in the seventies, mostly KNO_3-sucrose (60/40) was used. Two different approaches were followed :

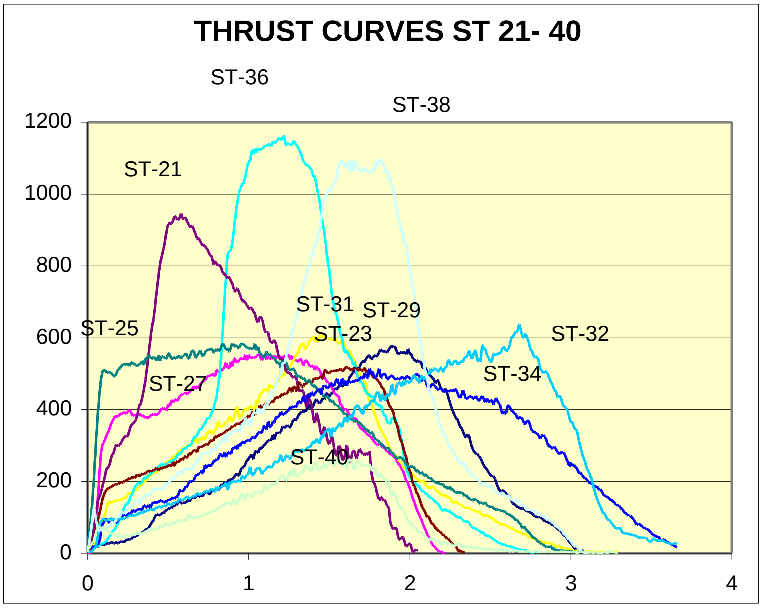
(a) The liquefied propellant was centrifuged in the coated motor. To assure a throughly connection between the coating and the propellant grain, a mixture of sucrose and salt, and in some cases only sucrose was used for the coating. Also the coating was centrifuged. In this way grains with a central cylindrical hole were realized.

(b) The liquefied propellant was pored in the coated motor provided with a cylindrical or cruciform central mandrel, which was withdrawn after full solidification.

Apart from the first few tests <u>all propellant blocks were case bond</u>.

2. John Koster used exclusively KNO_3-sorbitol in a ratio of 60/40, pored directly into the non-coated rocket motor provided with a cylindrical mandrel. Afterwards a layer of epoxy covered the nozzle end surface of the grain. So also the NERO motors were of the <u>case bond type</u> but without coating near the wall site.





3. Jan Volckaert from VRO uses a mixture of KNO_3-sucrose-sorbitol in the ratio of 67.5/17.5/15, and makes use of several modules, some made of an aluminum tube, coated with silicon on the inside. The grains have a cylindrical perforation. Up to 3 modules are used in a Bates configuration.

A Bates motor is expected to deliver an almost flat curve. A typical Bates curve is NX-13. From a grain that only burns from the inside to the outside (NERO) one can expect a continuous increase of the thrust, like ST-32. From the different thrust diagrams it is however clear that this is not always the case. At first sight there seems to be no logic behind it. The ratio of the initial burning area to the throat area is not always the determining factor in performance prediction!

The computer program

To be able to verify what is actually happening, a computer simulation program was set up. This program allows the following simulations:

- the use of several modules, with two possibilities: a) no burning of the top and bottom sites , b) burning at all none coated sites (Bates),
- cylindrical or crucifix shaped voids
- creation of cracks, partially or totally, at any time during burning (in the program these cracks go all the way through the grain)
- erosion
- ignition delay
- initial ignition

With erosion we mean the situation where the regression of the burning surface is faster than normal due to the high velocity flow of the reaction products over the burning surface. In our program we have used the following factor to the burning rate:

(1+ erosion coefficient x gas speed)

For the calculation of the burning rate (without erosion) use is made of the so-called St. Roberts burning law.

$$r = b + kP^n$$

In order not to complicate too much the simulations, "b" was always taken zero.The consequence of erosion is that the regression of the burning surface will not be the same at all locations in the grain. Some parts will burn away much faster than others, such that the void will soon deviate from a cylindrical shape. To cope with this effect the propellant length was divided into 50 segments of constant velocity.

The program also takes into account the changing situation of pressure and free volume. What is not taken care of is the pressure drop over the grain from bulkhead to nozzle.

For the thermodynamic values of the reaction products (molecular weight, temperature, ratio of the specific heat,…) the results from GUIPEP are used. The fact that accoding to the GUIPEP calculations a large part of the reaction products probably consists of condensable material (mainly K_2C0_3) is taken into account.

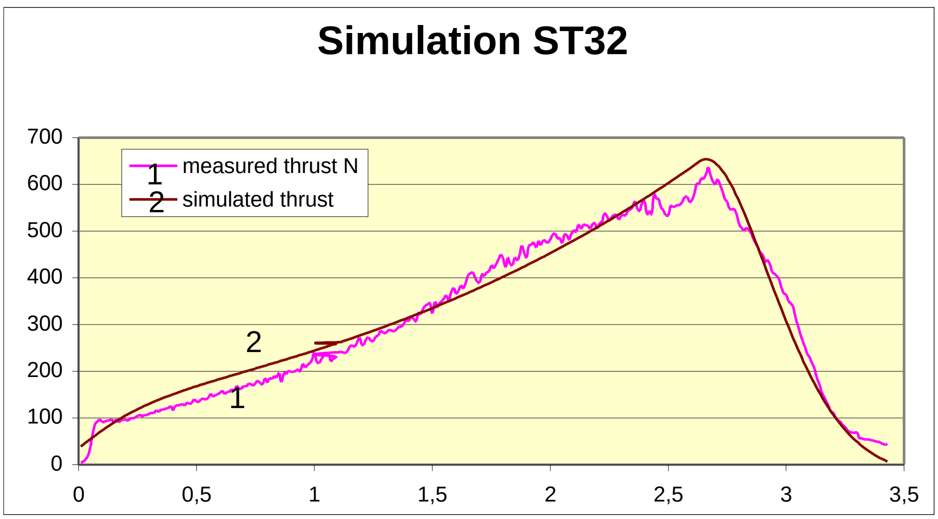
The results from the NERO motors

Let us first look at the results from the NERO motors. The next diagrams give the measured and the simulated thrust calculated with the computer program. As one can see that the results are quite reasonable, taking into account the fact that the parameters have to be found through trial and error. Also the fact that the used burning rate law will not be correct over the whole pressure range contributes to the deviation. Richard Nakka[2] has proven that the burning rate of KNO_3-sorbitol mixtures (in any case for 65% KNO_3-sorbitol) is very irregular. Also the erosion formula may not be sufficiently accurate. Finally, irregularities in the grain like differences in the density of the grains and air bubbles, or differences in KNO_3 concentrations may occur. Important is to show the tendencies in the thrust curves.

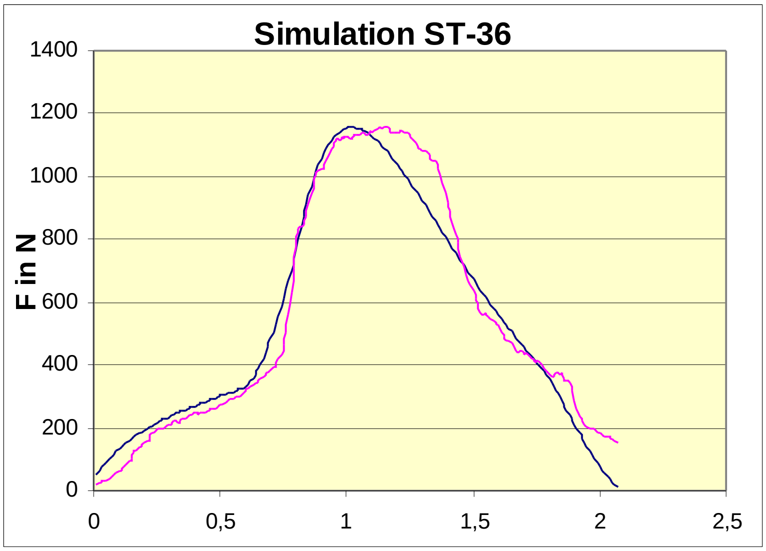
In the different thrust curves the actual values of the rocket (density of the propellant, length of the grain(s), inner and outer diameter of the grains,) are used and the best fitting values for “k” and “ε” (for erosion) are searched. “n” was taken at 0.41, because this is the exponent which was derived from the BVRO tests. Maybe n = 0.31 or 0.32 could have been a better choice. This is also the exponent found by Nakka for 65% KNO_3 and 35% sucrose.

Whenever felt necessary to explain the curves, cracks were introduced. As everything was done with trial and error better parameters can certainly be found.

From the simulation one can see that ST 32 is quite normal. This is not the case for ST 21 where 3 cracks occurred after about 0.3 s, and ST 36 with even 6 cracks. One has to keep under consideration that when cracks are simulated, they are situated at equidistances. In reality it may well happen that one crack is situated closer to the other. Also cracks are considered to happen all over the thickness of the grain, although this need not be the case in reality.



Not all-19 measurements of John Koster’s motors have been analyzed. Such an analysis is very time consuming and not always necessary for our conclusions.



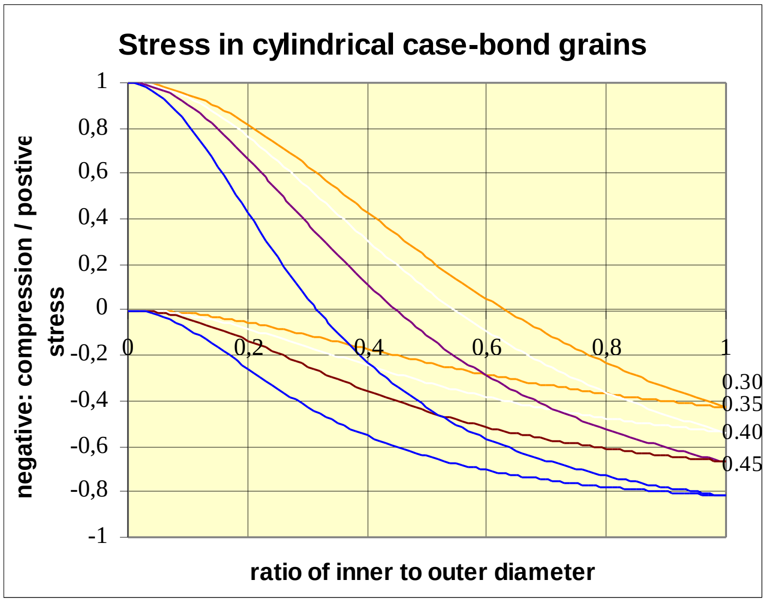
We come to the following results:

	ST-21	ST-32	ST-36
k	0.0014	0.0016	0.00135
n	0.42	0.42	0.42
ε	0.005	0.004	0.006

The erosion is important and will, essentially at the start when the inside diameter is still small, generate high burning rates. They can go up till about 2 times the normal value. Gas speeds of more than 100 m/s are found in the initial phase of burning. This means that when the burning rate at the front site is 10mm/s, the burning rate at the nozzle site becomes 20 mm/s. As a consequence the cylindrical void soon turns into a conical shape and the flames will reach the wall at the nozzle site much sooner than at the bulkhead site. The thrust curve reaches a maximum much sooner than expected, but the total duration will remain as long as in a normal case, since this is determined by the burning rate of the grain close to the bulk head, which is not subjected by erosion.

The reason why the NERO motors give such a wide range of results has probably to do with a too low ratio of the inner diameter to the outer diameter of the grain. Indeed in case bond propellants large tensile strengths can occur at the inside of the grain. This phenomena is essentially determined by the above mentioned ratio and the Poisson number of the material. This is clearly demonstrated by the following figure with gives the internal tress as a function of both parameters.[3] The upper series of curves give the tangent stress at the inner side of the cylindrical void. Each curve corresponds to a given Poisson ratio (ratio between shrinkage and elongation). The horizontal axis gives the ratio between inner and outer diameter. When the inner diameter is very small, the ratio between inner stress and pressure approaches 1, meaning that the stress is almost equal to the gas pressures. The smaller the Poisson number the larger the stress at any given ratio of inner to outer grain diameter. To be save this ratio should lie between 0.4 for a Poisson number of 0.45 and 0.8 for a Poisson number of 0.3. For KNO_3 propellants the Poisson number is not known. As a general rule the inner diameter should be about half the outer diameter. In the NERO motors the ratio of the inner to the outer diameter is situated between 3.4 and 3.7. This yields stresses between 0.2 an 0.6 times the gas pressure in the

motor. Although the tensile strength measured by Nakka is about 7.6 N/mm² (for KN-sorbitol 65/35 at a density of 1820 kg/m³), cracks can occur much sooner due to lack of elasticity of the material. In the seventies the occurrence of cracks was already described in KNO_3-sucrose propellant grains as a possible explanation of the observed results with these motors. That some grains, with a too low value of the ratio of inner to outer grain diameter, sometimes escape from cracks, is probably due to the fact that, thanks to a low ratio of inner grain surface to throat area, only low initial pressures are built up, which keeps the internal stresses within save limits.
The bottom series of curves give for the same Poisson number the tangent stress at the outer diameter (against the wall). Negative values mean compression of the grain.



The results from the VRO and KAPPA motors

The VOX-motors have a ratio of internal diameter to outside diameter of 0.47 to 0.54. This means that they are situated in the relatively safe region where compression is more likely than stress. The VOX motors use a conception, which is beneficial to avoid important stress. Separate modules are used which allow counter pressure of the combustion gases at their outer surface. As a consequence all sides of the grain are subjected to the same pressure. As the envelope is weaker the grain is less subjected to stress and becomes a freestanding grain. Hence a weak but good heat resistant coating is to be preferred above a strong coating which does not allow compression.

We will discuss now 3 simulations each with a specific character. Because of its nearly ideal behavior NX-13 is a good reference. The simulation of the NX-13 is almost perfect with the following parameters:

- k = 0.0026 m/s
- n = 0.32 (this is arbitrary chosen)
- ε = 0.005 – 0.007
- ignition delay = 0.25 s (m=1)
- initial ignition = 40%

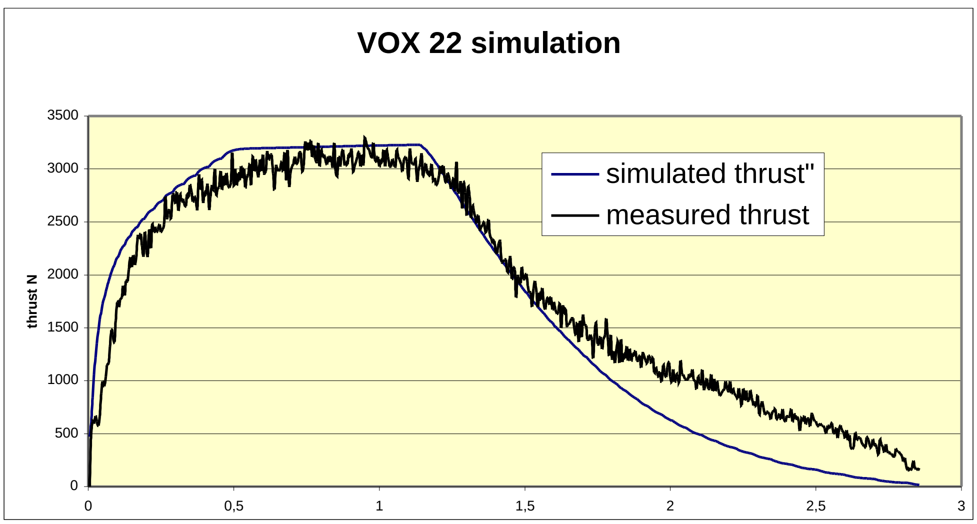
The last 3 values need clarification. The tail off of the thrust curve determines to a certain extend the erosion coefficient. When the burning surface reaches the wall at the same moment everywhere, the tail-off is very short and is only determined by the gases left over in the rocket motor at that moment. Erosion creates a conical shape of the grain, such that some parts of the burning surface closer to the nozzle, reach the wall sooner than other parts. The consequence is a longer tail off.

The curves of the NX and to an even stronger extend, the KAPPA[2], cannot be explained without the assumption that the full burning surface of the grain is not ignited at ones and that an ignition delay occurs. In our simulation we start from the idea that part of the grain already burns when the diaphragm burst. This we call here "initial ignition". Since the grain is divided into 50 equal parts, an initial ignition of 40% means that only 40% of the surface is ignited at the start.

In the simulation program the delay caused by the incomplete ignition of the grain is calculated as follows: when the number of the grain part (numbered 1 to 50), is larger than the value derived from the following formula,

$$\text{time}^{m} * \text{ignition delay} + \text{initial ignition}$$

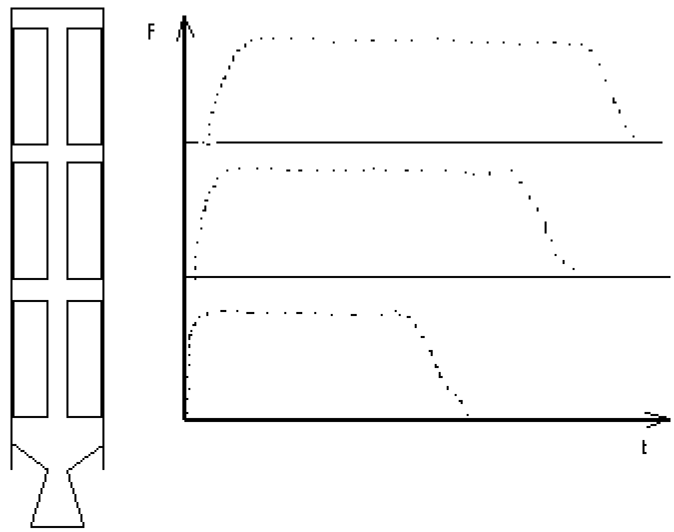
there is no ignition of that part of the grain. Within a certain delay, all parts of the propellant grain will ignite.



The simulation of the NX-22 is given. The NX-22 was chosen because it is very representative for the VOX motors. From the simulation one can see that in reality the digressive part of the curve is situated at somewhat higher values. When the thrust gets its downward knick (at about 1.3 s), the burning surface at the nozzle site of the grain has reached the wall and the shape of the grain is more or less conical. Following results have been obtained:

- $k = 0.0028$ m/s
- $n = 0.32$
- $\varepsilon = 0.025$
- ignition delay = 0.61 s ($m=0.3$)
- initial ignition = 16

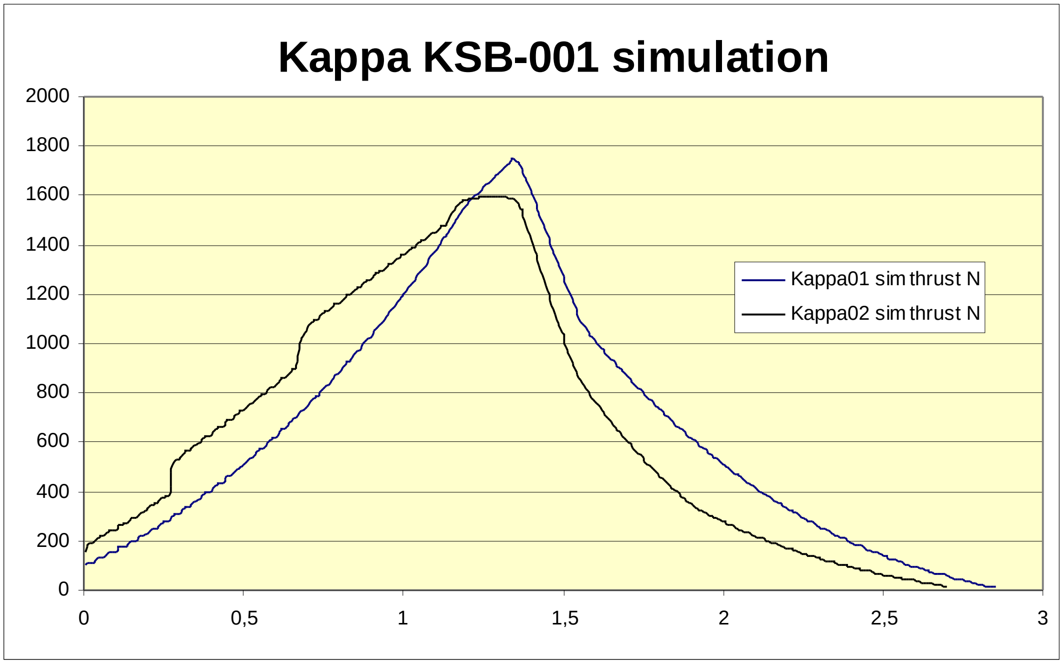
The NX-21 is largely different from the other curves. Only one reasonable explanation could be found: the different propellant modules do not burn at the top and bottom surfaces, but only at the inside. But does it make any sense to suppose that some parts of the surface do not burn at all? In any motor it takes some time to get the total burning surface ignited.

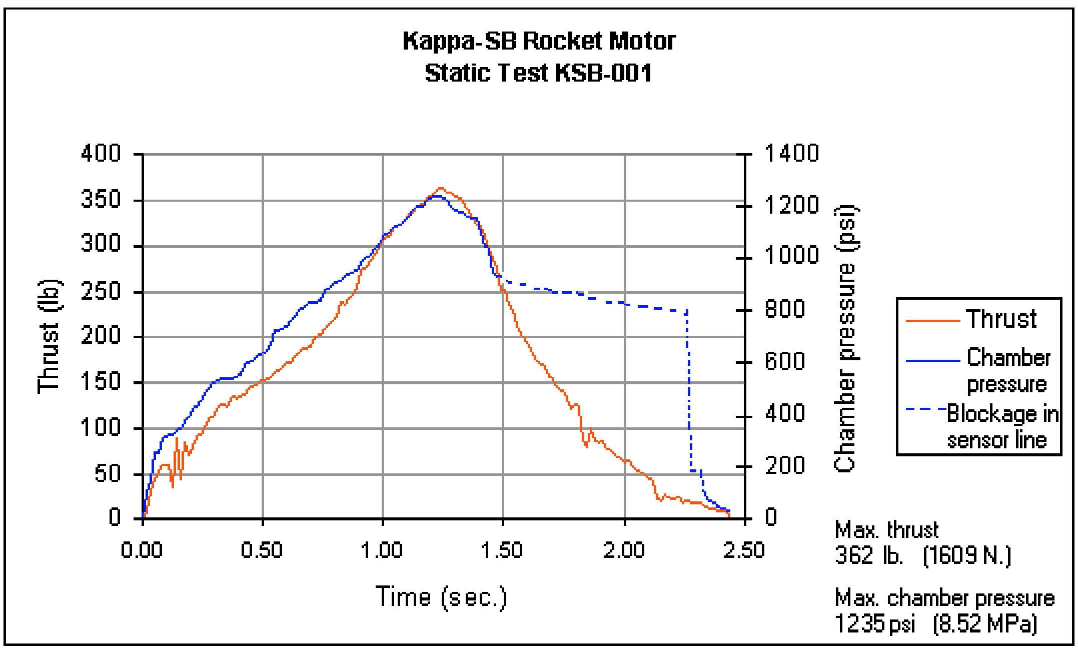


From the KAPPA motor it is known that ignition takes place at the bulkhead such that flames can reach the whole surface (probably with the exception of the top and bottom surfaces of the individual grains). In both the KAPPA and VOX motors it takes some time (0.25 to 0.8 s) before normal thrust is reached. From tests with the VOX it is known that a more powerful igniter indeed results in a faster initial thrust increase. So the ignition systems plays a very important role. But between slow ignition and no ignition at all there is much difference. Some parts of the surface seem to ignite later than others. This is also the point of view of Hans Olaf Toft, from the Danish rocket club DARK, who performed a simulation of the thrust of the KAPPA. In his approach the thrust curve can be completely explained by this effect. According to this theory, the grain module closest to the nozzle, ignites first, than the second, the third and finally after about 0.8 s the module near the bulkhead is completely ignited. This could be a possible explanation for the sometimes-stepwise shape of the digressive phase (the phase we still have some problems with). One can image the thrust curve to be made up from a number of thrust curves generated by the different modules, shifted in time through ignition delay. However, if this where the only reason as Toft suggests, than the top of the curve should be determined by the theoretical combustion time for the propellant module closed to the nozzle. Indeed, it is this module that first reaches the wall according to his theory. As from that moment the thrust decreases. From simulations based on the measured burning rate for 65% KNO_3-35% sorbitol, it is however clear that the top of the curve is too much to the right as compared to the measured thrust curve (in other words it takes too much time). Only if also erosion is assumed, we come to acceptable results.

The simulation of KAPPA gives the following results:

- k = 0.0032
- n = 0.31
- ε = 0.008
- ignition delay = 1.17 s (m=1)
- initial ignition = 30%



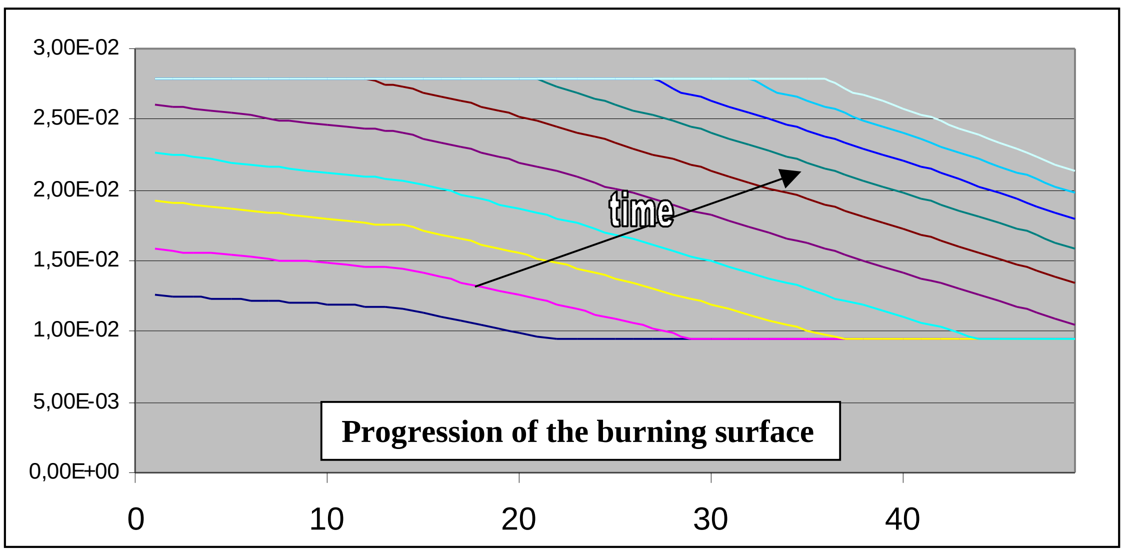


In the diagram the simulation is represented for the case when all surfaces burn (KAPPA 02) as for the case where no burning occurs at the top and bottom surfaces of the 4 propellant grains (KAPPA 01).

The “k” and “n”-values for the burning rate are close to the measurements of Nakka.

How to explain that the 65% KNO_3 - 35% Sorbitol propellant is so difficult to ignite and that in the NX-21, during more than 2.5 s, the top and bottom surfaces of the grains are not ignited? There is more and more evidence now that KNO_3-sorbitol propellants are much more difficult to ignite than KNO_3-sucrose mixtures. So it is not completely unexpected that when instead of sorbitol alone, also a mixture of sorbitol and sucrose is used, as in the NX motors, ignition problems occur. Moreover, it is possible that at ignition, thanks to the low viscosity of liquid sorbitol and its resistance to decomposition, a thin film of sorbitol is created on the outside of the grain. This thin film may isolate the propellant surface and protect the KNO_3 grain. It is also possible that this thin sorbitol layer is created during manufacturing. To prevent this problem the burning surface should be made rough (which is always a good procedure). Another possibility is that liquid K_2CO_3 or KOH, produced during the combustion, condenses on the “cold” and isolated surface of the grain.

The next figure shows how the burning surface progresses in time. The x-ax is the length of the total grain (50 units), the y-axis the radius in m. The largest value is the wall.



Not only there are limits for the inner diameter of the grains for case-bonded grains, also the erosion puts limits. This time however to the total length of the grain. With increased length of the grain (at constant internal cross section) the speed of the gases will increase and consequently also the erosion. As a consequence, part of the wall (or coating) will be unprotected for the flames. When neglecting the effect of erosion during motor design, the chamber pressure can become unexpectedly large and even lead to explosion.

What happened to the BVRO NEBEL[2] motors in the seventies?

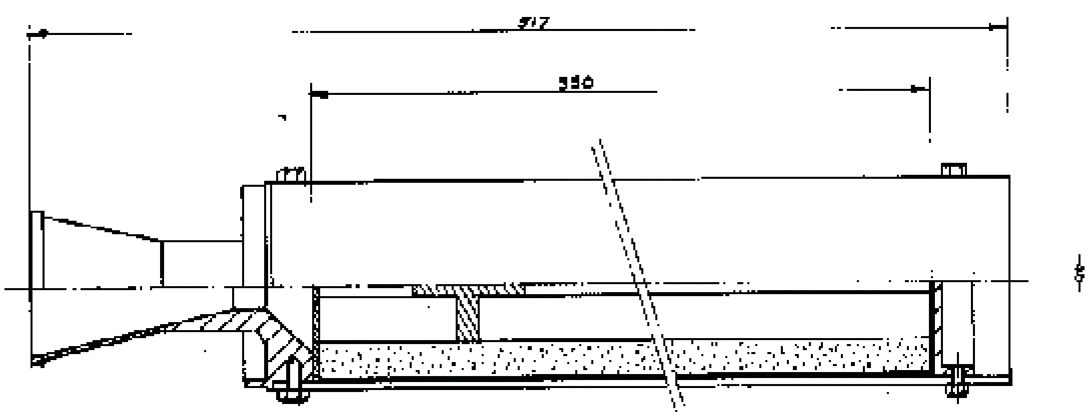
In the seventies BVRO experimented with 60% KNO_3-40% sucrose case bond propellant grains. One type of propellant grain was provided with a crucifix shaped hole, the other type with a cylindrical hole of different diameters, mostly prepared by the centrifugation of the liquid propellant. Although most of the time these motors worked very well, both types led to explosions. Most explosions occurred with the centrifuged propellants.

For the thrust curves of the NEBEL motors with crucifix hole we did not succeed in finding out how these grains actually burn. Several hypotheses were proposed, all based on the occurrence of cracks in the propellant, but none gave satisfaction. Cracks were supposed because they explained very well what happened in the motors with a cylindrical hole, and a crucifix shaped hole was expected to generate important stress. That we could not find the solution was quite remarkable, and frustrating, because this type of motors produced all the time more or less the same shape. So there was undoubtedly always the same thing happening. No cracks was not imaginable because in that case the thrust had to show an increasing thrust curve, at least of a long period. At that time we were convinced that erosion could not be the cause.

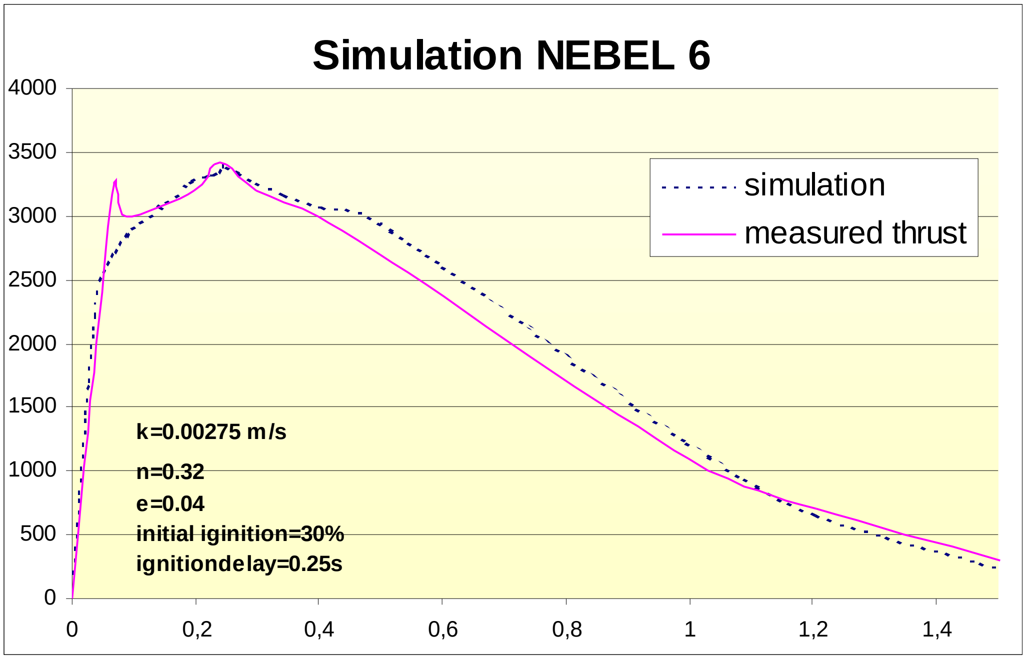
Based on the developed computer model first NEBEL 3 with cylindrical perforation was recalculated. The thrust curve could be very well simulated without cracks and with following parameters:

- k = 0.0029
- n= 0.32
- ε = 0.003 – 0.005

The values for "n" and "k" were used on NEBEL 2 were a good match was found if several cracks occurred. Finally it was applied to grains with crucifix holes. It was shown that with increasing value of the erosion coefficient "ε", curves of the type NEBEL 8 (ε = 0.02), NEBEL 6 (ε = 0.04) and NEBEL 9 (ε = 0.045) were generated. Contrary to what was thought during such a long time, these motors behave "normal", that is without cracks.



The reason for the very strong erosion may be found in the high ratio of total burning surface to the cross section area of the void (65 to 70). After about 0.3 to 0.5 seconds the burning surface reaches the wall at the nozzle side. The burning rate during that period ranges between 3 to 5 cm/s <u>or 2 to 4 times faster than the burning rate without erosion</u>. As one can see the simulation of the NEBEL motors is of very good quality.



This however does not solve the problem of the explosions. In 1978 out of a series of 4 NEBEL motors, 3 exploded one after the other. From these NEBEL motors one was provided with a crucifix shaped hole (NEBEL 10 a rocket intended to flight, but exploded during the first moments of lift-off), and 3 (NEBEL 11, 12 and 13) provided with a cylindrical hole, manufactured through centrifugation. In all exploded motors, the propellant density was extremely low: 1.54 – 1.57. From centrifuged propellant grains one can expect the density to decrease with decreasing radius because of lower centrifugal forces. Whether KNO_3, which is heavier than sucrose, migrates towards the outer regions of the grain has never been measured. If this happens it would contribute to even higher differences in density over the radius. Knowing that the burning rate increases with decreasing density, and that strength decreases, may explain much. One NEBEL explosion, NEBEL 7 (crucifix), has another reason. The motor worked perfectly till about 0.75 s. The reason for explosion here lays probably in the used coating. After 0.75 s a large part of the propellant is already consumed and the flames have reached the coating over a certain distance. Since at that time we used sucrose as coating material (because it would perfectly integrated with the propellant), it is highly probable that this material, becoming quickly liquid, has been driven to the nozzle where it blocked the throat. On the pressure and thrust diagram a sudden drop in thrust goes together with a steep rise in pressure. This kind op problems can easily we solved when using other liners.

Somme concluding remarks:

- ***characteristic velocity:***

For the different propellant formulations used and discussed in this article we have the following values of the characteristic velocity:

Propellant composition	Theoretical characteristic velocity m/s	Measured characteristic velocity m/s
65 % KNO_3-35% sucrose	1003.5	-
60% KNO_3-40% sucrose	991[4]	979
65% KNO_3-35% sorbitol	938	880[5]
60% KNO_3- 40% sorbitol	-	797

The characteristic velocity is a value which only depends upon the propellant and its chemical reaction efficiency, and not on the conversion in the nozzle.

The use of sorbitol:

The use of sorbitol as fuel, alone or in combination with sucrose has positive and negative effects.

Negative:

- Decrease in specific impulse.
- increased ignition problems
- lower density: sorbitol: 1.489 , sucrose: 1.58
- if only sorbitol is used (at least for 65/35), the burning rate- pressure relation is not a smooth curve, instead it shows plateau's and dips.

Positive:

- decrease in melting temperature. Sorbitol melts at 110°C while sucrose melts at 185°C.
- On the other hand the use of sucrose makes the propellant very hygroscopic and makes storing over large periods difficult.
- Densities are closer to the theoretical values (see also table)

The increase of KNO_3 content also increases the content of condensable material (K_2CO_3 and KOH). The usage of nozzles with very small divergent angle (7 – 8°) may increase the specific impulse, although no tests have been reported so far.

The density of the propellant:

It is interesting to have a look at the values for the density:

Composition	Theoretical	Measured	Difference %	source
67.5 KNO_3 – 17,5 sucrose – 15 % sorbitol	1.88	1.72	8.5%	VRO -VOX
65 KNO_3- 35 % sorbitol	1.84	1.82	1.1%	NAKKA
65 KNO_3 – 35 % sucrose	1.89	1.80	4.8%	NAKKA
60 KNO_3-40% sorbitol	1.81	1.72	5%	NERO
60% KNO_3-40% sucrose	1.86	1.66	10.7%	BVRO '70-'80)

It is clear that in all cases Nakka comes to the highest densities, essentially for 65% KNO_3-35% sorbitol, he gets extremely good figures. Higher density gives better mechanical strength. It probably also influences the burning rate: it can be expected that lower density propellants burn faster than high density ones. The figures also show clearly that in the seventies the BVRO had poor control over the density (in some motors we only got 1.54 or 17% deviation from the theoretical value), which is probably the reason for some malfunctions.

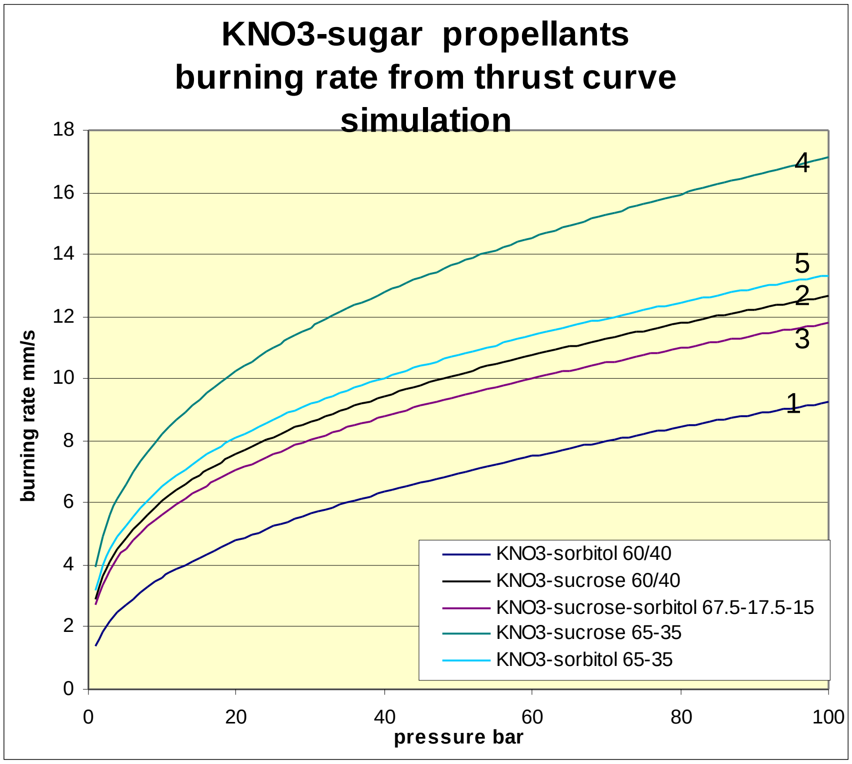
The burning rate of the different propellant compositions:

The simulations allow us to compare the burning rate (without erosion) of the different propellant compositions. What we find is in good agreement with what can be expected in general:

- higher KNO_3 content (until a maximum value) will increase the burning rate.
- higher sorbitol content decreases the burning rate.

The propellant composition 65% KNO_3-35% sucrose (as measured by R.Nakka) gives the highest burning rate. 60% KNO_3 – 40% sorbitol gives the lowest rate. The other compositions are situated in between both rates. 67.5 KNO_3- 17.5 sucrose-15% sorbitol (simulation) is situated in between 65% KNO_3- 35 % sucrose and 65% KNO_3-35% sorbitol. Hence, the amount of sorbitol (15%) decreases the burning rate more than the increase (2,5%) in KNO_3. The situation of the burning rates is a good indication of the reliability of the simulation method used. At the same pressure, the highest burning rate is about 2 times larger than the slowest! The specific impulse of 65% KNO_3-35%surcrose and density are also higher.

Propellant composition	k in m/s (pressure in bar)	n
65 KNO_3 – 35 % sucrose	0.00395	0.319
65 KNO_3- 35 % sorbitol	0.0032	0.31
60% KNO_3-40% sucrose	0.0029	0.32
67.5 KNO_3 – 17,5 sucrose – 15 % sorbitol	0.0027	0.32
60 KNO_3-40% sorbitol	0.0014	0.41



It should be emphasized that the burning rate trajectories are only global. It should be remembered that we started from the St.Roberts equation for the whole trajectory. As has been demonstrated by Nakka, some propellants not always obey this law.

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[1]. "The Potassiumnitrate-sugar propellant" Tony Vyverman, Youth & Space 1978 (available at www.VRO.be or Chris.Steyaert@vvs.be). This book contains details about the NEBEL motors and many other experiments with this propellant.

[2] www.nakka-rocketry.net. This excellent website contains a wealth of information about potassium nitrate sugar propellants

[3] "Fabricage en mechanische eigenschappen van een vast brandstofblok" Chris Steyaert – BVRO Bulletin 1978

[4] In the "The Potassiumnitrate-sugar propellant" book a thermodynamic calculation of the propellant was made. It was assumed at that time that K_2CO_3 is decomposed at the conditions in the rocket motor and hence not produced during combustion, in contradiction with the GUIPEP calculations. This assumption was taken because of the large gap between the theoretical calculations with formation of K_2CO_3 (like GUIPEP does) and the measured results and because of the similarity of K_2CO_3 to $CaCO_3$, with almost the same melting point, which decomposes completely. The value of 994 m/s for the characteristic velocity of 60%KNO_3-40%sucrose was obtained under this assumption. For 65%KNO_3-35%sucrose, GUIPEP predicts a specific impulse of 166 s while the measured specific impulse is about 130 s. The values for the other compositions were calculated with GUIPEP.

[5] This value was calculated by the author based on the pressure curve from the KAPPA002 test.

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