REVISTA
INTERDISCIPLINAR DE
PESQUISA EM
ENGENHARIA

CILAMCE
2016

XXXVII IBERIAN LATIN AMERICAN CONGRESS
ON COMPUTATIONAL METHODS IN ENGINEERING
BRASÍLIA - DF - BRAZIL

PRELIMINARY EVALUATION OF STRUCTURAL INTEGRITY OF THE SINGLE-PORT HDPE AND PARAFFIN GRAIN UNDER LOW TEMPERATURE CONDITIONS

Davi Gustavo Gomes Dias

Artem Andrianov

Manuel Nascimento Dias Barcelos Júnior

Olexiy Shynkarenko

davi.dias.411@gmail.com, andrianov@aerospace.unb.br, manuelbarcelos@aerospace.unb.br, olexiy@aerospace.unb.br

The University of Brasilia

Faculadade UnB Gama, 72444-240, Gama, Federal District, Brazil

Abstract. *The main aim of the paper is to verify the feasibility of application of such common materials as paraffin and polyethylene for a small-sized single-port fuel grain in hybrid rocket motors at low temperature conditions. The simplified analytical method of stress analysis had been used to calculate the stresses in the grain and afterwards was verified with results obtained by the finite element method. The results of calculation and simulation revealed that the structural integrity of the paraffin at low temperatures is in doubt, while the polyethylene may carry the loads induced by cold conditions.*

Keywords: *Structural integrity, Fuel grain, Hybrid rocket motor, Low temperature*

1 INTRODUCTION

Over the last few years the air launch of the rockets from a conventional aircraft or a high altitude balloon is of great interest. The altitudes of air launch may range from couple of kilometers to 30 km. According to the International Standard Atmosphere the temperature at some altitudes of the given range could be as low as $-56.5°C$. The low temperature conditions may considerably affect the structural integrity of the fuel grain of hybrid propellant rocket motors. Paraffin and high-density polyethylene (HDPE) are among various hydrocarbons that were used as a solid grain in hybrid propellant rocket motors (Altman and Holzman, 2007). There are a number of reasons for their use; among them are non-toxicity, low price and availability, friendliness to environment and good performance characteristics. Although the mechanical properties of both materials were studied in details, there is little information about their mechanical behavior as a component of solid-propellant grain.

The main aim of the paper is to carry out preliminary verification of the structural integrity of a small-sized one-port grain made from above mentioned materials in conditions of low temperatures common for altitudes 10-30 km using the simplified method described in (Balabukh, et al., 1984). The method is based on a number of simplifying assumptions; thereby its accuracy is not high. Nevertheless the method gives a good quantitative representation of the stress distribution and its order. In addition, the calculated results were verified with results obtained by the finite element method with use of ANSYS 14.5.

The load conditions at the moment of motor ignition are of primary interest. The geometry of the grain was defined by the performance characteristics of the hybrid propulsion system with nitrous oxide as oxidizer: total impulse 350 kNs and operation time 70 s. The design pressure in combustion chamber is 3 MPa.

2 PROCEDURE

Among various methods of grain placing into motor's case the worst condition is under analysis: cylindrical outer surface of the grain is bonded to internal surface of the casing. This approach for paraffin grain is reasonable, as far as it is usually made by pouring liquid paraffin wax into a motor casing, which serves as a mold. The bonding of HDPE grain to motor casing is questionable, since the adhesive bond of this material is a complex technological problem. However, equal boundary conditions are important for comparison of stress distribution for both materials.

There are two important load conditions for a one-port solid grain at the moment of ignition: internal pressure and thermal stress. The latter is caused by gradual cooling of the grain from normal temperatures to the temperature of the environment at the given range of altitudes considered as equal to $223°K$. This temperature was assumed as the worst case when the launch of the hybrid propellant rocket is made at night, i.e. there is no heat transfer due to radiation. At daytime the contribution of radiation may raise the temperature of a solid grain up to $293°K$.

According to (Balabukh, et al., 1984) the method is based on theory of thick-walled circular cylinder and the strength analysis for the given load conditions should be based on calculation of working stresses. Only elastic properties are considered, since pressure increases rapidly in 0.06 - 0.3 seconds according to (Fathrudinov and Kotelnikov, 1987) and the viscoelastic properties of the grain material can be neglected at low temperatures.

It was considered that proper strength criterion for HDPE grain at any temperature is equivalent (von-Mises) stress, since the brittle temperature of HDPE is minus $76°C$ or $197°K$ (Kitao, 1997). The strength criterion for paraffin grain is maximal principle stress, because recent work (Veale, et al., 2015) have shown experimentally that the material is highly brittle even at room temperatures.

As a result of different burning characteristics of HDPE and paraffin the dimensions of grain vary with material of propellant as it is shown in Table 1 to provide the same total specific impulse.

Table 1: Dimensions of one-port grains made from HDPE and paraffin

Material of the grain	External diameter, mm	Internal diameter, mm	Length, mm
Paraffin	344	100	244
HDPE	269	125	446

2.1 Analytical method

The following assumptions were accepted for calculation of working stress due to internal pressure: viscous-elastic properties of the grain material are neglected and motor casing is extremely rigid. The boundary conditions are: radial stress on inside cylindrical surface of the grain equal to the value of pressure; radial strain on outer cylindrical surface of the grain is zero. The equations for the radial stress σ_r, the hoop stress σ_θ and the axial stress σ_z are respectively

$$\sigma_r = \frac{m^2 P}{m^2 + 1 - 2\mu}(1 + \frac{r_2^2}{r^2}(1 - 2\mu)) \tag{1}$$

$$\sigma_\theta = \frac{m^2 P}{m^2 + 1 - 2\mu}(1 - \frac{r_2^2}{r^2}(1 - 2\mu)) \tag{2}$$

$$\sigma_z = -2\mu \frac{m^2 P}{m^2 + 1 - 2\mu} \tag{3}$$

where P is the pressure in chamber; r_1 and r are the inside and instant radio of the grain; m is the ratio between inside and outside radio $(= \frac{r_1}{r_2})$; and finally μ is the Poisson's ratio of the grain material.

The following assumptions were accepted for calculation of working stresses due to thermal change: viscous-elastic properties of the grain material are neglected; the grain is unstressed at initial temperature; the dimensions of the grain change only due to thermal deformations; the axial strain of the grain is determined by difference of thermal strain between grain and motor casing. The boundary conditions are: inside cylindrical surface of the grain is unstressed; total hoop strain of the grain on outer surface equals the thermal hoop strain of the motor casing. In this load condition the equations for the radial stress σ_r, the hoop stress σ_θ and the axial stress σ_z are respectively

$$\sigma_r = B(1 - \frac{r_1^2}{r^2}) \tag{4}$$

$$\sigma_\theta = B(1 + \frac{r_1^2}{r^2}) \tag{5}$$

$$\sigma_z = B(1 + m^2) \tag{6}$$

B is calculated by equation 7.

$$B = \frac{E(T - T_0)(\alpha_c - \alpha_g)}{m^2 + 1 - 2\mu} \tag{7}$$

Where E is the modulus of elasticity of the grain material; t and t_0 are respectively instant and initial temperature; α_g and α_c are respectively the coefficient of thermal expansion of the grain material and casing material.

2.2 Numerical simulation

Stress-strain equations for preliminary evaluation of grain integrity at various load conditions (restrained thermal shrinkage, internal pressurization, longitudinal accelerations) are based on assumptions of plane strain and a thin case (Noel, 1973). In the paper, the half-length axisymmetric 3D and 2D models were used in FEM analysis, since the plane strain does not predict the stresses and strains at the face ends of grain. According to (Noel, 1973) failures in solid propellant grains occur at high-strain regions of the free port surface and in grain-case interface. Sector with central angle 6° was under analysis in plane strain model. Aforementioned analytical method considers only elastic behavior of the grain's material, but it is known that HDPE exhibits non-linearity in the stress-strain relation. Thus, plastic material model was used in analysis along with elastic model of HDPE.

2.3 Material properties

Material properties are very important for numerical simulations as well as for analytical calculations. Equations of the method discussed in section 2.1 are very susceptible to the value of Poisson's ratio. For instance, at the Poisson's ratio equal to 0.5 according to (Rao, 2009), which is common for incompressible paraffin, all stresses turn to the value of pressure. Hence, the Poisson's ratio for paraffin is assumed to be in the range 0.490 - 0.499.

Moreover, recent work (DeSain, et al., 2009) have shown that mechanical properties of paraffin are not high (tensile strength 1.03 - 1.38 MPa, modulus of elasticity 200 MPa, percent elongation 0.6-0.8%). In the same reference, it was shown that addition of low density LDPE to paraffin in small quantities (2-4%) increases almost three times both strength and stiffness respectively; but absolute values of mechanical properties still remain small. The experimental work (Seyer and Inouye, 1935) on measurement of paraffin strength at various temperatures showed that the tensile strength increased rapidly below $303°K$ until about $278°K$. The maximum of tensile strength was found at $273°K$; at lower temperature $264°K$ it was impossible to measure tensile strength. Low strength was caused by the development of tiny cracks even visible with a naked eye at temperature 267°K. Thus, the given results prejudice the structural integrity of paraffin grain at low temperature.

On the other hand, according to (Vasile and Pascu, 2005) HDPE has exceptional impact strength, being one of the best impact-resistant thermoplastics available. The properties of HDPE are maintained even at extremely low temperatures and it has stress cracking resistance. The brittle temperature of HDPE lies between $-156°C$ and $-73°C$ (117°K and 200°K). The mechanical properties of HDPE at low temperatures, which have been used for analysis, are summarized in Table 2. For most of commercial HDPE the Poisson's ratio at normal temperatures is in the range 0.40-0.45, though at cryogenic temperatures 0 - 240°K it is in the range 0.30 - 0.35 according to (Perepechko, 1980). Thus, various values of Poisson's ratio were taken into consideration for the calculation case of grain cooling to 223°K. The modulus of elasticity varies in two times in the given range of temperatures.

Table 2: Mechanical properties of HDPE at low temperatures

Parameter	Temperature (°C/°K)					Reference
	-50/223	-35/238	-20/253	-5/268	25/298	
Tensile strength (MPa)	45.7	41.6	35.9	30.0	17.2	(Goldman and Grinman, 1974)
Coefficient of thermal expansion ($10^{-4}/K$)	1.175	1.40	1.51	1.73	1.6	(Zakin, et al., 1966)
Modulus of elasticity (GPa)	2	1.8	1.6	1.38	1	(Waterman, 1963)
Poisson's ratio	0.37	0.38	0.38	0.41	0.44	(Sahputra, 2013)

3 ANALYTICAL RESULTS

The stress distribution across the radius of the paraffin grain due to pressure in chamber is shown in Figure 1. Axial stresses are constant along radius of the grain and equal -2.38 and -2.92 MPa respectively for Poisson's ratio 0.490 and 0.499. All stresses due to internal pressure are compressive and the maximal value does not exceed the value of pressure in chamber.

Figure 2 shows distribution of stresses due to thermal change from normal temperature (298°K or 25°C) to a range of low temperatures (Poisson's ratio 0.5). Axial stresses (given in Table 3) are constant along radius of the grain. The coefficients of thermal expansion (CTE) for paraffin were taken from (Pereverzev, et al., 1973); it is necessary to note that some values were extrapolated. According to the given results stresses in the grain due to cooling are one order greater than stresses due to internal pressurization. Moreover, these stresses are greater than the strength of paraffin even modified with small amount of LDPE. The hoop stress increases with cooling and its maximal value is at the cylindrical surface of the port. These maximal values of principle stresses are dangerous since they may initiate the cracking of the grain surface.

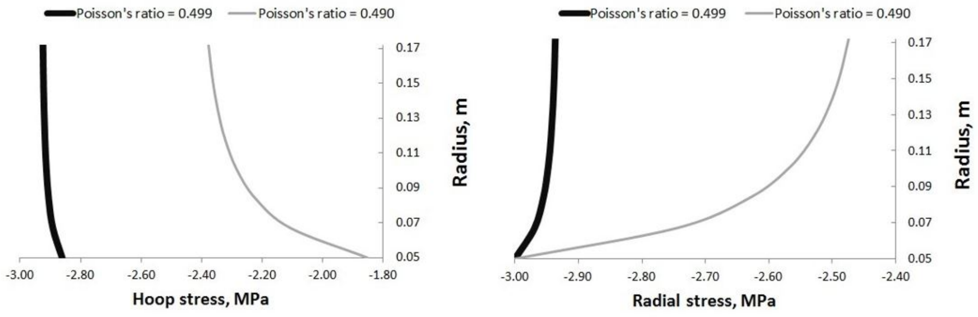

Figure 1: Stress distribution in paraffin grain due to internal pressure

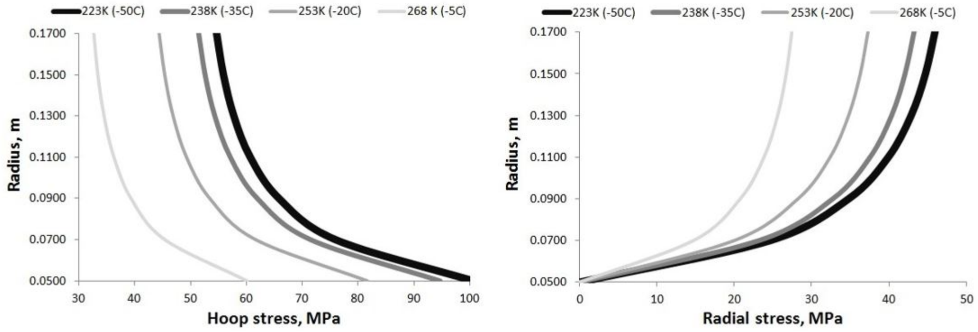

Figure 2: Stress distribution in incompressible paraffin grain due to temperature change

Formation of cracks on the surface of paraffin grain with black pigment and carbon black was observed after transferring of paraffin grain from low ($-195°C$ or $78°K$) to normal temperature environment ($25°C$ or $298°K$) (Salvador, et al., 2007). Authors of the paper also observed crack formation in the paraffin grain with small additives of pigment in the combustion chamber after exposure to cooled nitrous oxide during couple of seconds (Figure 3) imitating ignition failure at normal temperature. In the first case, the grain was manufactured by centrifugation process, in the second - by casting.

Table 3: Axial stress in the paraffin grain for various temperatures

Temperature, $°K$ ($°C$)	223 (-50)	238 (-35)	253 (-20)	268 (-5)
Axial stress, MPa	54.6	51.3	44.3	32.6

The stresses due to internal pressure in HDPE grain are not high (up to the value of pressure in chamber); however, the stresses due to cooling to $223°K$ are one order of magnitude greater according to the calculation results shown in Figure 4. The maximal hoop stress 63.6 MPa at $223°K$ is greater than tensile strength of HDPE 45 MPa. At other temperatures the maximal principle stress as well as equivalent stress is also greater than the strength of polyethylene (Figure 5).

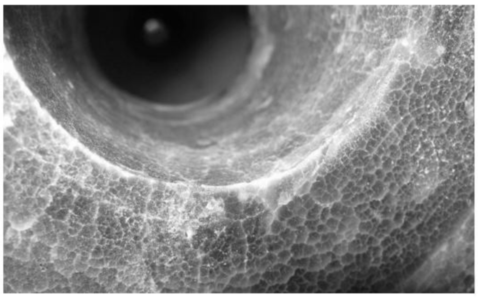

Figure 3: Cracks in the paraffin grain after exposure to cooled nitrous oxide

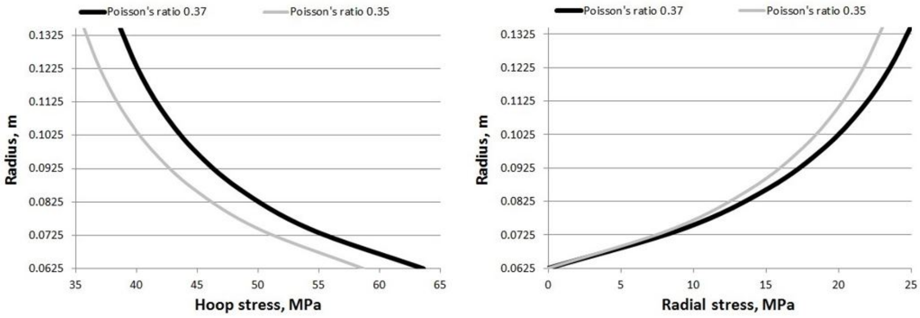

Figure 4: The effect of Poisson's ratio of HDPE on stress distributions along radius of the grain due to temperature change from $298°K$ $(25°C)$ **to** $223°K$ $(-50°C)$

4 RESULTS OF NUMERICAL SIMULATION

Since some simplifications were introduced in analytical method it is worth to verify obtained results with numerical simulation. In the actual conditions, outer surface of the grain is bonded to internal surface of the casing making equal the strain in all directions of both grain and casing at the connection. Thus to check the feasibility of suggested numerical model for further analysis it is necessary to put both analytical and numerical models into the same conditions. The equal conditions were realized by putting zero value for CTE of steel in equations of section 2.1 and making deformations of the outer surface of the grain model completely restrained in all directions (hoop, radial and axial). Strictly, these conditions are not completely the same since in the analytical method the axial strain of grain is determined just by difference of thermal strain between grain and casing and thereby the axial stress is constant along radius. Figure 6 shows stress distribution for this case due to cooling to $223°K$ of the HDPE grain. The stress data of numerical simulation was collected along radius of the cross-section in the middle of grain's length. The model was 1/64 of the cylindrical grain with edges filleted by radius 5 mm. It was meshed predominantly by 5.5 thousands elements SOLID186.

The difference between analytical and numerical data is in the range 2.6 - 3.7% for hoop stress, up to 9.4% for radial stress and up to 4.5% for equivalent stress. Small difference between stresses obtained by analytical and numerical methods is an evidence of the feasibility of FEM model for further analysis.

Further analysis was fulfilled for conditions close to real-life application, where HDPE grain is enclosed in steel casing with certain properties and supported at normal condi-

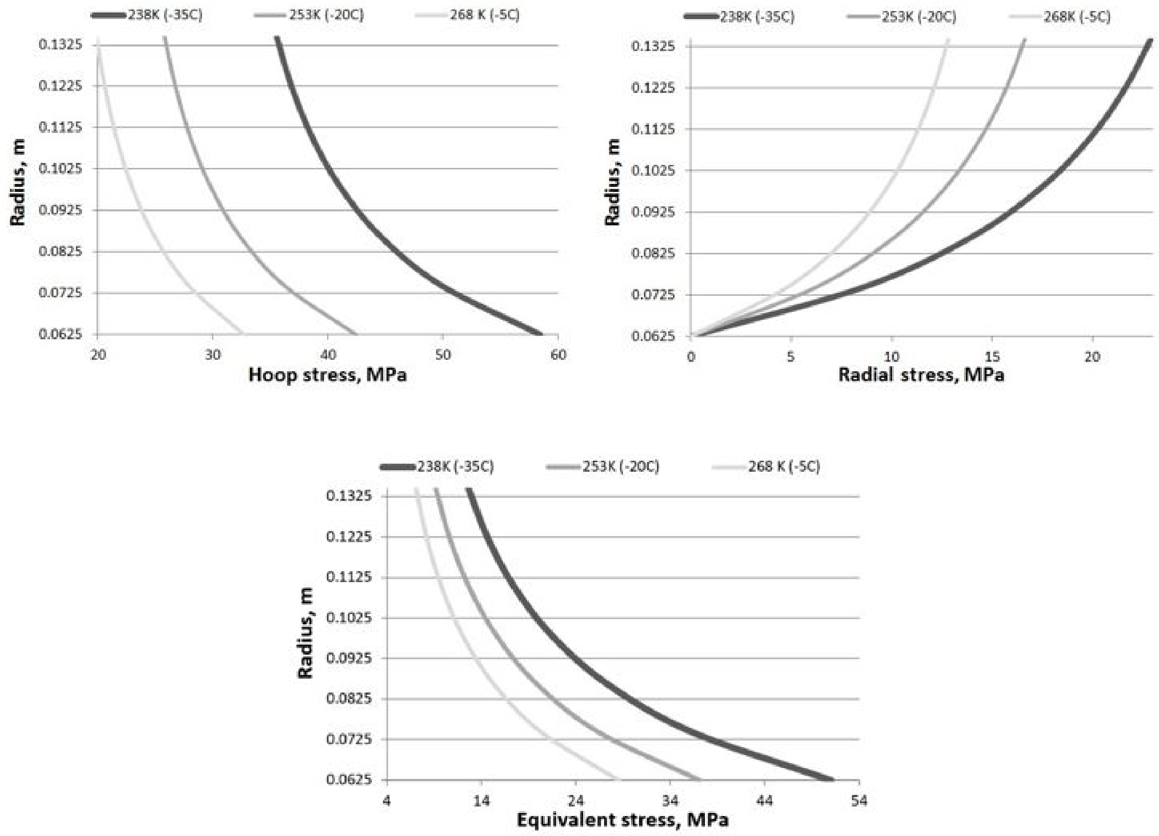

Figure 5: Stress distribution in HDPE grain due to temperature change

tions by plane circular surfaces of rigid heat-insulation. It is important to note that two boundary conditions were analyzed. It was considered that external cylindrical surface of the grain was not bonded to the casing of the motor at the first condition and was bonded by mechanical (non-adhesive) connection at the second condition. The thickness of the casing was defined by the given internal pressure and safety factor 2.5 taking into consideration that material of the casing is steel S17400 tempered to H1150 (ASTM 630-03).

Axisymmetric two-dimensional model with edges filleted by radius 2 mm was used for analysis. Compression only constraint was applied at the peripheral ring surface of the grain's face to simulate lateral support of heat insulation. The model was meshed predominantly by 65 thousands elements PLANE183.

Preliminary analysis have shown zero stresses due to cooling from $298°K$ ($25°C$) to $223°K$ ($-50°C$) at first "non-bonded" condition, since there were no constrains applied to the grain and the grain was free to shrink. However, external surface of the grain detached from the internal surface of the casing and as a result, the gap 1.2 mm have appeared. This gap may cause burning of the uninsulated external cylindrical surface of the grain with subsequent overheating and destruction of the chamber's casing.

Figure 7a shows equivalent stress distribution in non-bonded grain due to simultaneous action of thermal load (cooling from $298°K$ to $223°K$) and internal pressure 3 MPa. This condition simulates the loading of the cooled non-bonded grain at the moment of

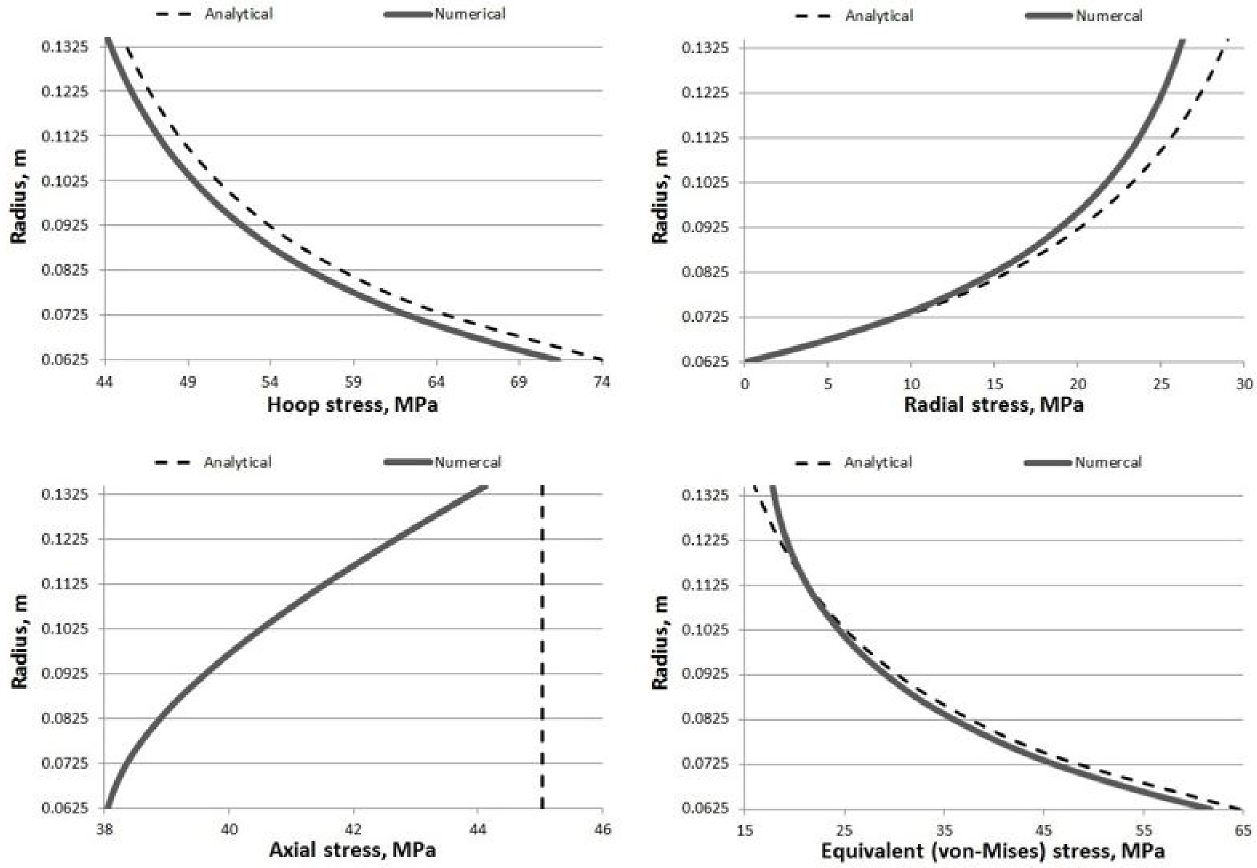

Figure 6: Stress distribution due to cooling from $298°K$ ($25°C$) to $223°K$ ($-50°C$) obtained from analytical and numerical models for the case of restrained outer surface of HDPE grain

ignition. Due to internal pressure, the gap diminishes to 1 mm that still compromises the structural integrity of the casing. However, the stresses are not high (the maximum equivalent stress is 7.7 MPa on internal cylindrical surface of the grain).

Figure 7b shows equivalent stress distribution in the grain bonded to steel casing at the same loading conditions as for non-bonded grain (cooling from $298°K$ to $223°K$ and internal pressure 3 MPa). To mitigate overestimation of stresses at the fillet of the grain (singularity condition) plastic material model was used in simulation. Plastic material model was fulfilled in ANSYS by multilinear isotropic hardening model together with data of stress-strain relation of HDPE at various temperatures taken from work (Goldman and Grinman, 1974). It was found that equivalent stresses at the middle-length section of the grain are two times less than those predicted by analytical model. It is necessary to note that stresses at port surface of axisymmetric model are 14% greater, than stresses predicted by plane strain condition (Figure 8a). This difference have provoked interest to compare the stress-strain parameters at critical areas calculated by axisymmetric 2D model in mid-length section of the grain and plane strain model (Table 4), though it was not an objective of the work.

Values of equivalent stresses estimated by both models are less than values of tensile strength of HDPE at minus $50°C$ ($223°K$). Moreover, strains calculated for plane strain model (Figure 8b) are less than true yield strain for HDPE at minus 50°C (0.02 mm/mm).

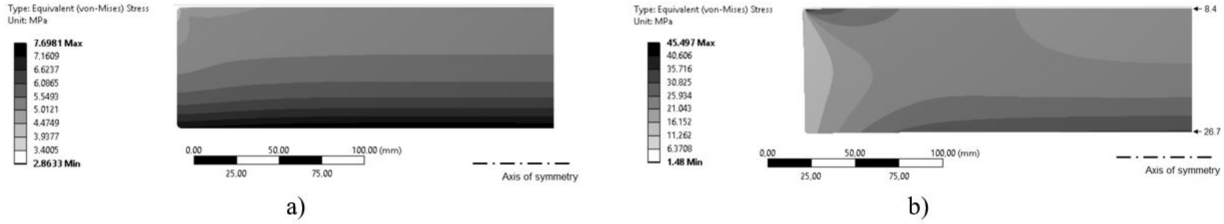

Figure 7: Equivalent stress distribution in axisymmetric 2D model due to thermal load (cooling to $223°K$) and internal pressure 3 MPa for non-bonded (a) and bonded (b) grain

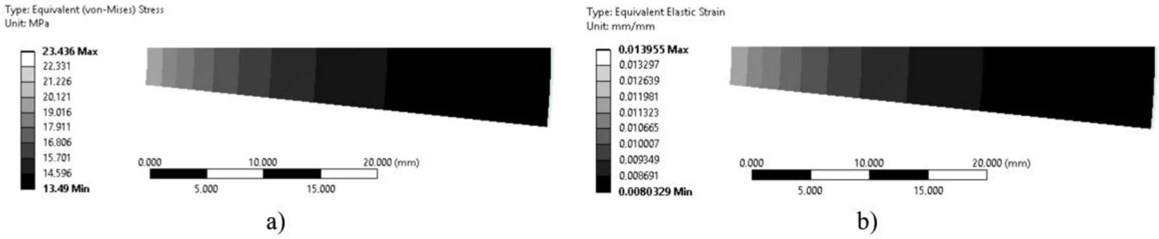

Figure 8: Equivalent stress (a) and strain (b) distribution in plane strain model due to thermal load (cooling to $223°K$) and internal pressure 3 MPa for bonded grain

5 CONCLUSIONS

The preliminary analysis of paraffin grain have shown that its structural integrity is compromised, since stresses in the grain are much higher than strength of the paraffin. In the analysis neither analytical methods no numerical simulations took into consideration viscoelastic properties of paraffin, at the same time experiments revealed crack formation in the volume of paraffin grain. However, here the question should be raised: will these cracks affect the characteristics of the burning process and structural integrity of the combustion chamber? In reference (Czysz, P.A. and Bruno, C., 2009) it was mentioned that integrity of paraffin grains are not susceptible to cracks and imperfections, but no results of experiments at cold conditions were published. This may serve as a main reason for further study of structural integrity of the paraffin grain.

The structural integrity of HDPE grain is also compromised, but for the worst ”theoretical” condition, when outer cylindrical surface is bonded to steel casing, which does not undergo deformations due to temperature change. In conditions close to real ones, when the outer surface of the grain is not bonded to steel casing, the stresses are not high. However, the gap appears between grain and casing. Oxidizer entering this gap provokes burning of the external grain surface that finally may considerably affect the structural integrity of combustion chamber. Thus, some technical solution should be found to avoid this problem. One of the possible solutions might be bonding of external surface of grain to steel casing. In this case, stresses and strains are moderate, but realization of common adhesive bonding is complicated. Thus, a mechanical connection should be developed to

Table 4: Stress-strain parameters of the bonded grain at critical areas calculated by axisymmetric 2D model at mid-length section of the grain and plane strain model

Parameter	Location	Axisymmetric model	Plane strain model
Equivalent stress, MPa	Free port surface	26.7	23.4
Equivalent stress, MPa	Grain-case interface	8.4	13.5
Hoop stress, MPa	Free port surface	27.7	19.8
Radial stress, MPa	Grain-case interface	8.2	6.0
Equivalent strain, mm/mm	Free port surface	0.016	0.014
Hoop strain, mm/mm	Free port surface	0.014	0.008
Radial strain, mm/mm	Free port surface	-0.011	-0.011

meet the following requirements: no gap formation between grain and casing; preservation of structural integrity of both grain and combustion chamber as a whole.

Marked difference was found between stress-strain parameters calculated by two models of bonded HDPE grain: axisymmetric 2D and plane strain. The results can be validated only by experimental tests; nevertheless, both models consider structural integrity of the HDPE grain at accepted assumptions.

REFERENCES

Altman, D. and Holzman, A., 2007. ”Overview and history of hybrid rocket propulsion”. Fundamentals of Hybrid Rocket Combustion and Propulsion. Progress in Astronautics and Aeronautics, Vol. 218, pp. 1 - 36.

Balabukh, L.I., Alfutov, N.A. and Usyukin, V.I., 1984. Structural Mechanics of Rockets. High School Edition, Moscow.

Czysz, P.A. and Bruno, C., 2009. Future Spacecraft Propulsion Systems. Praxis Publishing, Chichester, UK, 2nd edition.

DeSain, J.D., Brady B.B., Metzler, K.M., Curtiss, T.J. and Albright, T.V., 2009. ”Tensile tests of paraffin wax for hybrid rocket fuel grains”. 45th AIAA/ASME/SAE/ASEE Joint Propulsion Conference & Exhibit. Denver, Colorado.

Fathrudinov, I.H. and Kotelnikov, A.V., 1987. Design and project of solid propellant rocket motors. Machine-Building Edition, Moscow.

Goldman, A.Ya. and Grinman, A.M., 1974. ”Variant of temperature-time analogy for partially crystalline polymers (High-density Polyethylene)”. Polymer Mechanics, Vol. 2, pp. 261 - 269.

Kitao, K., 1997. ”A study of brittle-ductile transition in polyethylene”. Polymer Engineering and Science, Vol. 37(5), pp. 777 - 788.

Noel, J.S., 1973. Solid Propellant Grain Structural Integrity Analysis. NASA SP-8073.

Perepechko, J., 1980. Low-Temperatures Properties of Polymers. Pergamon Press, MIR Publishers, Moscow.

Pereverzev, A.N, Bogdanov, N.F. and Roshchin, Yu. N., 1973. Production of paraffin waxes. Publishing house ”Chemistry”.

Sahputra, I.H. and Echtermayer, A.T., 2013. ”Effects of temperature and strain rate on the deformation of amorphous polyethylene: a comparison between molecular dynamics simulations and experimental results”. Modelling and Simulation in Materials Science and Engineering, Vol. 21, p. 065016.

Salvador, C.A.V., Netto D.B. and Costa, F.S., 2007. ”Production and testing of paraffin grains for hybrid rockets”. In Proceedings of the 19th International Congress of Mechanical Engineering - COBEM2007. Brasilia, Brazil.

Seyer, W.F. and Inouye, K., 1935. ”Tensile strength and density at various temperatures”. Industrial and Engineering Chemistry, Vol. 21, No. 5, pp. 567 - 570.

Vasile, C. and Pascu, M., 2005. Practical guide to polyethylene. Rapra Technology, Shawbury, Shrewsbury, Shropshire, UK.

Veale, K.L., Brooks, M.J. and de la Beaujardiere, J.P., 2015. ”Structural Performance of Large Scale Paraffin Wax Based Fuel Grains”. In Proceedings of the 51st AIAA/SAE/ASEE Joint Propulsion Conference. Orlando, Florida.

Waterman, H.A., 1963. ”Determination of the complex moduli of viscoelastic materials with the ultrasonic pulse method (Part II)”. Colloid and Polymer Science, Vol. 192, Issue 1, pp. 9 - 16.

Zakin, J.I., Simha, R. and Hershey, H.C., 1966. ”Low-temperature thermal expansivities of polyethylene, polypropylene, mixtures of polyethylene and polypropylene, and polystyrene”. Journal of Applied Polymer Science, Vol. 10, pp. 1455 - 1473.