Computational fluid dynamics simulations for composite rocket propellant optimization

F-M Dîrloman¹, L-C Matache², T Rotariu², T-V Țigănescu³, D Zvîncu², M-I Ungureanu¹ and O Iorga⁴
¹Military Technical Academy „Ferdinand I“, Doctoral School „Defense and Security Systems Engineering“, Blvd. George Coșbuc, No. 39-49, 050141, Bucharest, Romania
²Military Technical Academy „Ferdinand I“, Faculty of Integrated Weapons Systems, Engineering and Mechatronics, Blvd. George Coșbuc, No. 39-49, 050141, Bucharest, Romania
³Military Equipment and Technologies Research Agency, Aeroportului Street, No. 16, 077025, Clinceni, Ilfov, Romania
⁴Scientific Research Center for CBRN Defence and Ecology, Olteniței Street, No225, 041309, Bucharest, Romania
E-mail: florin.dirloman@mta.ro

Abstract. When designing a rocket engine configuration, both in terms of propellant grain, combustion chamber and nozzle geometry, one of the most convenient approach is using Computational Fluid Dynamics (CFD) Simulation. Numerical simulation is an alternative method of scientific investigation, which substitutes large number of experiments that often imply high financial burden and are also dangerous for the personnel involved. The numerical approach is often more useful than consecrated experimental method because it provides complete data that cannot be directly observed or measured, or it is difficult to highlight by other means. In this study we focused on applying CFD simulation to composite rocket propellants in a rocket engine with convergent-divergent nozzle configuration using Ansys Fluent Software. An ammonium nitrate (AN) based composite rocket propellant having four components was analyzed: oxidizer, metallic fuel, binder and catalyst agent. Explo5®, a thermochemical software, was also used to calculate the equilibrium compositions of the combustion products in the combustion chamber. It turned out that the results obtained on the basis of the simulation are consistent with those of the experimental testing. The data collected so far will be used to optimize the grain configuration of the composite rocket propellant.

1. Introduction
Solid rocket composite propellants are solid heterogeneous mixtures, consisting of three basic components: oxidizer, metallic fuel and binder. The usual oxidizer for solid rocket propellants is ammonium perchlorate (NH₄ClO₄), but in the last decades, ammonium nitrate (NH₄NO₃) and ammonium dinitramide, are under intense study due to their remarkable performance and green character [1]. In the case of metallic fuel, taking into account the compatibility with the oxidizer and the performance character, the most suitable solutions seems to be aluminum (Al) and magnalium (Al-Mg), an aluminum-magnesium alloy (50 : 50 wt.%) [1]. The last element of the propellants is the one creating the matrix that incorporates the oxidizer-metallic fuel mixture, providing homogeneity, mechanical strength and protection towards external agents. Currently the most widely used binders,
are hydroxyl-terminated polybutadiene (HTPB), an inert polymer and glycidyl azide polymer (GAP), an energetic polymer [1]. In addition to the aforementioned purpose, the binder also serves as combustible element.

In order to determine the most suitable heterogeneous mixture, before performing the experimental part, rocketry specialists use various optimization software programs. Computational Fluid Dynamics (CFD) Simulation represents one of the most convenient approach prior to propellant and motor rocket design. Numerical simulation is an alternative method of scientific investigation, which substitutes large number of experiments that often imply high financial burden and are also dangerous for the personnel involved.

The main purpose of this study was to determine the variation of some important parameters, pressure, temperature and gas flow velocity, for a proposed AN-based composite rocket propellant, in a rocket motor chamber with convergent-divergent nozzle configuration using Ansys Fluent Software [2, 3].

2. Computational procedure
Details on theoretical equations governing the rocket motor, internal geometry, mesh configuration, set-up conditions and combustion modeling of the employed composite propellant are given hereafter.

2.1. Mathematical model
Fluent software can solve the problem in two ways, based on pressure or density parameters. Given that the problem analyzed is of great complexity, it seems that the pressure-based solution seems to be the most reliable choice. Due to its design, it offers a faster solution to the problem. The mathematical model behind the program running in the Fluent Software is indicated below.

The mass conservation equation in the case of a two-dimensional, axial-symmetric configuration has the following form:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial \left( \rho v_x \right)}{\partial x} + \frac{\partial \left( \rho v_r \right)}{\partial r} + \rho v_r v \cdot \nabla \phi = S_m
\]  

(1)

where: \( t \) - axial coordinate; \( r \) - radial coordinate; \( v_x \) - axial velocity; \( v_r \) - radial velocity; \( \rho \) - propellant density; \( S_m \) - mass source of material.

We can consider the impulse conservation equations, for:

- axial direction

\[
\frac{\partial \left( \rho v_x \right)}{\partial t} + r \frac{\partial \left( \rho v_x v_r \right)}{\partial r} = - \frac{\partial p}{\partial x} + r \frac{\partial \left( \rho v_x v_r \right)}{\partial r} \left[ \mu \left( \frac{\partial v_x}{\partial x} + \frac{\partial v_r}{\partial r} \right) - \frac{2}{3} \left( \nabla v \right) \right] + F_x
\]  

(2)

- radial direction

\[
\frac{\partial \left( \rho v_r \right)}{\partial t} + \frac{\partial \left( r \rho v_r v_x \right)}{\partial x} + \frac{\partial \left( r \rho v_r \right)}{\partial r} = - \frac{\partial p}{\partial r} + \frac{\partial \left( r \rho v_r v_x \right)}{\partial x} \left[ \mu \left( \frac{\partial v_x}{\partial x} + \frac{\partial v_r}{\partial r} \right) - \frac{2}{3} \left( \nabla v \right) \right] + \frac{\partial \left( r \rho v_r \right)}{\partial r} \left[ \mu \left( \frac{\partial v_x}{\partial x} + \frac{\partial v_r}{\partial r} \right) - \frac{2}{3} \left( \nabla v \right) \right] - 2 \mu v r \cdot v - \frac{2}{3} \mu v r \cdot v - F_r
\]  

(3)

where: \( F_x \) - axial force [N]; \( F_r \) - radial force [N]; \( \mu \) - dynamic viscosity of combustion products [Pa·s].

The energy conservation equation is represented as:
The mathematical model presented has a number of 5 equations with 5 indeterminate variables: $v_x$, $v_y$, $p$, $T$, $\rho$.

Compressible flows can be characterized by the value of the Mach number:

$$M = \frac{u}{c}$$

$$c = \sqrt{\gamma RT}$$

$$\gamma = c_v/c_p$$

where: $c$ - sound velocity in gas [m·s⁻¹]; $\gamma$ - specific heat ratio, $c_v$-specific heat capacity at constant volume [J·kg⁻¹·K⁻¹].

Typically, compressible flows are characterized by the maximum gas pressure and temperature, as follows:

$$p_0p^{-i} = \exp\left[\int_0^L c_v T^{-i} dTR^{-i}\right]$$

For $c_v$ = constant, the equation is reduced to:

$$p_0p^{-i} = \left(1 + (\gamma - 1)2^{-i}M^2\right)$$

$$T_0T^{-i} = 1 + (\gamma - 1)2^{-i}M^2$$

For compressible gases, the law of the ideal gas is represented in the form:

$$\rho = \left(p_{0\rho} + p\right)\left(8\pi M_w^{-i}T\right)^{-i}$$
where: $p_{op}$ - pressure under operating conditions; $p$ - relative static local pressure; $\mathcal{R}$ - universal gas constant; $M_w$ - molecular mass.

Due to the existence of turbulent flow in the combustion chamber, the kinetic energy dissipates into thermal energy, in other words the gas velocity is influenced by turbulence, in the sense of decreasing it compared to a laminar flow. The influence of turbulent flow is modeled in FLUENT with the transport equation for viscosity as:

$$
\frac{\partial}{\partial t}(\rho \tilde{v}) + \frac{\partial}{\partial x_i}(\rho \tilde{v} u_i) = G_v + \sigma_v \left( \frac{\partial}{\partial x_j} \left( \mu + \rho \tilde{v} \right) \frac{\partial \tilde{v}}{\partial x_j} \right) + C_{b2} \rho \left( \frac{\partial \tilde{v}}{\partial x_j} \right)^2 - Y_v + S_v \tag{14}
$$

where: $\tilde{v}$ - turbulent kinematic viscosity; $u_i$ - velocity of species i; $G_v$ - variable that represents the turbulence production due to kinematic viscosity; $Y_v$ - variable that represents the turbulence destruction due to kinematic viscosity; $\sigma_v$, $C_{b2}$ - constants; $S_v$ - heat source.

### 2.2. Internal motor and propellant geometry modeling

The 2-D sketch of the rocket motor internal geometry and propellant configuration was generated using Gambit Software. Depending on the desired propellant combustion mechanism: neutral, progressive or regressive, there are different types of grain configurations, such as circular, tubular, star shaped [1]. In this study circular grain geometry was used. The dimensions and the geometry of the sketch are depicted in table 1.

| Internal rocket chamber | Propellant configuration |
|------------------------|-------------------------|
| Characteristics        | Value                   | Characteristics | Value |
| Length                 | 80 mm                   | Length         | 40 mm |
| Diameter               | 50 mm                   | Outer diameter | 45 mm |
| Nozzle length          | 6 mm                    | Inner diameter | 10 mm |
| Throat diameter        | 4 mm                    |                |       |
| Divergence angle       | 150 degree              |                |       |
| Convergent angle       | 135 degree              |                |       |

### 2.3. Mesh generation

The rocket motor structure and the propellant configuration have been modeled with SHELL triangular elements, as shown in figure 2. The mesh characteristics are presented in table 2.

| Time (s) | Characteristics | Level | Cells | Faces | Nodes | Partitions |
|----------|----------------|-------|-------|-------|-------|------------|
| 0        |                 | 0     | 5380  | 8910  | 3843  | 1          |

### 2.4. Set up

In setup, single precision with serial processing option was selected. The general conditions, the material characteristics, the boundary conditions and the combustion models were solved as presented below.

**2.4.1 General.** In order to calculate the compressible effects, due to the C-D nozzle, Density-based solver type was selected. The flow is symmetric about X axis so 2-D space was set to Axisymmetric.
The effects of the gravity were neglected. The energy equation was turned ON for the all analysis; viscous model is S-A (Spalart–Allmaras).

2.4.2 Material characteristics. The analysis was carried out for both Air and Gas as working fluids. The characteristics of the working fluids are depicted in table 3.

| Characteristics                  | Gas                                      |
|----------------------------------|------------------------------------------|
| Density (ρ)                      | ideal gas                                |
| Thermal conductivity (k)         | user defined (Appendix 1)                |
| Molecular viscosity (μ)          | user defined (Appendix 1)                |
| Ratio of specific heats (ϒ)      | piecewise-linear                         |

2.4.3 Boundary conditions. The following boundary conditions were used for the analysis (table 4):

| Characteristics                  | Values                                      |
|----------------------------------|---------------------------------------------|
| Inlet (Mass flow-Inlet)          | user defined (Appendix 2)                   |
| Inlet Temperature                | user defined (Appendix 3)                   |
| Operating conditions pressure    | 0bar                                        |
| Outlet Pressure, temperature     | 1bar, 300K                                  |

2.5. Combustion modeling
The combustion process of a rocket composite propellant is a complex process. In order to evaluate the combustion products a thermochemical software, Explo5®, was used [4]. The analyzed propellant formulation is: NH₄NO₃ (49%), KNO₃ (10%, potassium nitrate), GAP (20%), Al (20%) and Fe₂O₃ (iron oxide-1%). NH₄NO₃ is the oxidizer which evolves in gases species (NO₂, O₂, N₂O) necessary for combustion of Al, metallic fuel, and GAP, binder and organic fuel. The iron oxide is used as catalytic agent. The results are presented in figure 1, for the chamber, inlet, throat section and outlet.

![Figure 1](image-url) Mass fraction of the combustion products.
3. Results and discussions

The flow simulation was carried out under Steady state condition. Contours of pressure, temperature and velocity were obtained in different points of interest by using four gauges, depicted in figures 3 to 5. The positions of the gauges, ignition charge and propellant are given in figure 2.

The pressure and temperature are maximum at the inlet and begin to decrease until the outlet. The maximum values are 46.4 bar and 2700 K, while the minimums are 0.465 bar and 865 K.

When it comes to velocity, it can be concluded that this parameter is inversely proportional to the two discussed above, because it is minimal near the convergent zone and starts to increase to the end of the divergent zone, while in the throat section it is nearly Mach 1. The maximum values obtained for magnitude velocity is 2640 m/s.
Based on the simulation, the variations of pressure and temperature versus time were recorded, as presented in figure 6.

In order to validate the pressure values obtained based on the simulation, some experimental tests were carried by real firing of a propellant grain on a stand burner. The experiments were performed on a sub-scale Rocket Motor Tests TRM 35 and the composite propellant samples were ignited with 1 gram of black powder. The testing installation is depicted in figure 7.
The time dependence of pressure determined in the experiments is presented in figure 8, where can be observed that the maximum experimental pressure recorded was 48.92 bar. But this value sums up the contribution corresponding to the ignition charge. Considering that, to determine the average pressure value of the propellant, this value was not taken into account. The average pressure value in the combustion chamber was 44.56 bar. Thus the pressure obtained by Computational Fluid Dynamics (CFD) is a good approximation of the experimental one, the difference being of about 4%.

![Figure 8. Pressure-time dependence.](image)

4. Conclusions and perspectives
A numerical simulation model was developed for the calculation of the gas flow dynamic in the rocket motor, which was applied to a propellant formulation consisting of PSAN, GAP, Al and Fe₂O₃. It turned out that the results obtained are in accordance with those resulted from experimental tests.

The data obtained so far create a perfect background for a more extensive computational simulation, to determine the combustion behavior more accurately. In the development phase of composite mixtures, the model can be applied to a variety of configurations and the results can be compared for optimization. Numerical modeling of green solid composite propellants for civilian and military applications based on various components can be further performed.

5. References
[1] Jai Prakash Agrawal 2010 High Energy Materials, Propellants, Explosives and Pyrotechnics (Weinheim: WILEY-VCH Verlag GmbH & Co.KGaA) chapter 6 pp 209-316.
[2] 2013 Ansys Fluent User’s Guide, Available online: http://www.pmt.usp.br/ACADEMIC/martoran/NotasModelosGrad/ANSYS%20Fluent%20Users%20Guide.pdf (accessed 19.01.2020).
[3] 2013 Ansys Fluent UDF Manual, Available online: http://www.pmt.usp.br/academic/martoran/notasmodelosgrad/ANSYS%20Fluent%20Theory%20Guide%2015.pdf (accessed 19.01.2020)
[4] SUCESKA, M., Explo 5 Users Guide, Version 6.05 /Edition 1/2018.
Appendix 1

DEFINE_PROPERTY(cell_thermal_conductivity, c, t) {
    real T, lam;
    real p1 = -9.004e-17;
    real p2 = 2.077e-12;
    real p3 = -1.748e-8;
    real p4 = 1.256e-4;
    real p5 = 3.243e-3;

    T = C_T(c, t);
    lam = p1*pow(T, 4) + p2*pow(T, 3) + p3*pow(T, 2) + p4*pow(T, 1) + p5;
    return lam;
}

DEFINE_PROPERTY(cell_viscosity, c, t) {
    real mu, T;
    real p1 = -1.158e-19;
    real p2 = 1.984e-15;
    real p3 = -1.299e-11;
    real p4 = 6.5e-8;
    real p5 = 7.019e-6;

    T = C_T(c, t);
    mu = p1*pow(T, 4) + p2*pow(T, 3) + p3*pow(T, 2) + p4*pow(T, 1) + p5;
    return mu;
}
Appendix 2

DEFINE_PROFILE(Ma_flu_elp, t, nv)
{
    float time, m_flux, x0, y0, x1, y1, d0, temp, Sx, Sy, Xcc, Ycc, Dar, Psi, R, pres, ropb, vardo, niu, Alelp_real, Alelp_sim, rap_Alelp;
    int Kid;
    int Ntrs = 0;
    int Nelp = 1;
    int Nel_red;
    int in_int3 = 13;
    real Ar;
    real Aria = 0;
    real xbaza = 0;
    real ybaza = 0;

    Domain *d;
    Node *v;
    face_t f;
    cell_t c0;
    Thread *tb;
    real NV_VEC (area);
    vardo = 0.084e-06;
    niu = 0.726;
    ropb = 1.60*1e+3;

    time = RP_Get_Real("flow-time");
    Sx = 0;
    Sy = 0;
    Kid = 0;

    begin_f_loop(f,t)
    {
        Kid = Kid + 1;
        v = F_NODE(f,t,0);
        x0 = NODE_X(v);
        y0 = NODE_Y(v);
        Sx = Sx + x0;
        Sy = Sy + y0;
    }
    end_f_loop(f,t)

    Xcc = Sx/Kid;
    Ycc = Sy/Kid;

    Sx = 0;
    Sy = 0;

    begin_f_loop(f,t)
    {
        v = F_NODE(f,t,0);
        x0 = NODE_X(v);
    }
    end_f_loop(f,t)
y0 = NODE_Y(v);

v = F_NODE(f,t,1);

x1 = NODE_X(v);

y1 = NODE_Y(v);

Dar = ((x1-Xcc)*(y0-Ycc)-(x0-Xcc)*(y1-Ycc))/2;

Aria = Aria + Dar;

end_f_loop(f,t)

Aria = Aria*1e6;

Nel++;

if(Nel==1)

Aria0 = Aria;

begin_f_loop(f,t)
{
    pres = F_P (f,t);
    temp = F_T(f,t);

    if(Aria>=1)
    {
        if(temp>=500&&pres>0)
        {
            m_flux = ropb*vardo*pow((pres),niu);
        }
        else
        {
            m_flux = 1e-6;
        }
    }
    else
    {
        m_flux = 1e-6;
    }

    F_PROFILE(f,t,nv) = m_flux;
}

end_f_loop(f,t)
Appendix 3

DEFINE_PROFILE(Temp_elp, t, nv)
{

    cell_t c0;
    Thread *t0;

    face_t f;
    real NV_VEC (area);

    float time, temp0, temp1;
    real Temp_c, Pres_c;

    time = RP_Get_Real("flow-time");

    begin_f_loop(f,t)
    {
        c0 = F_C0(f,t);
        t0 = F_C0_THREAD(f,t);
        Temp_c = C_T(c0,t0);
        Pres_c = C_P(c0,t0);
        temp0 = F_T(f,t);

        if(temp0>500)
        {
            temp1 = temp0+100;
            if(temp1>2300)
                temp1 = 2300;
            else
                temp1 = 0.2*Temp_c+0.8*temp0;
        }
        F_PROFILE(f,t,nv) = temp1;
    }
    end_f_loop(f,t)
}