Combustion in a solid fuel scramjet with channel geometry variation due to burnout

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Abstract. Stability of combustion in solid fuel scramjets is contingent upon proper geometry of fuel grain and availability of a flame holder. Flame stabilization is achieved in the recirculation zone developing due to sudden expansion behind the inlet. Previous experimental and theoretical works suggest that there exists an optimum range of length-to-diameter ratios for the flame holder. However, due to fuel burnout the channel and flame holder geometry change in the process of scramjet operation, the regression rate being variable both in time and length. The purpose of this work is to develop a computational model of a solid-fuel scramjet taking into account the geometry variation, as well as to obtain typical flow patterns at the different stages of combustion. The numerical model is based on a system of fully compressible RANS equations with k-epsilon turbulence model. Turbulent combustion is described by the Eddy Dissipation Concept (EDC) model. Stability of combustion in solid fuel scramjets is contingent upon proper geometry of fuel grain and availability of a flame holder. Flame stabilization is achieved in the recirculation zone developing due to sudden expansion behind the inlet. Previous experimental and theoretical works suggest that there exists an optimum range of length-to-diameter ratios for the flame holder. However, due to fuel burnout the channel and flame holder geometry change in the process of scramjet operation, the regression rate being variable both in time and length. The purpose of this work is to develop a computational model of a solid-fuel scramjet taking into account the geometry variation, as well as to obtain typical flow patterns at the different stages of combustion. The numerical model is based on a system of fully compressible RANS equations with k-epsilon turbulence model. Turbulent combustion is described by the Eddy Dissipation Concept (EDC) model.

1. Introduction
Recent few decades have seen an increasing interest towards the development of scramjet engines for unmanned aerial propulsion vehicles, see e.g. (Zvuloni, Gany, and Levy (1989); Ben-Yakar, Natan, and Gany A. (1998); Novozhilov et al. (2011)). A promising type of such engines is Solid-fuel ramjets, or SFRJ, with fuels not capable of self-sustained combustion (unlike the solid rocket fuels) and burning in the gas phase after gasification and mixing with incoming gaseous oxidizer. Solid-fuel ramjets and scramjets are of interest as thrusters, as well as a part of hybrid propulsion systems where the hot gases in the grain channel are created by burning a rocket fuel.

Engine performance depends significantly on the stability of combustion in the fuel grain. Combustion stabilization can be achieved by arranging flow recirculation near the oxidizer inlet due to
sudden expansion of the channel, acting as a flame holder. It was shown experimentally by Ben-Yakar, Natan and Gany (1998) that there exists an optimum range of length-to-diameter ratios providing stable combustion in a solid-fuel scramjet; in these experiments the length of fuel grain was about 170 mm, and PMMA was used as a fuel.

An important problem to be considered for solid-fuel ramjets and scramjets is that the shape of fuel grain changes with time due to fuel burnout. This applies not only to the main combustion chamber, but to the flame holder as well. Therefore, the initially optimum geometry may well become such that the flame holder no longer performs as expected, or other combustion instability types can develop. Therefore, it is necessary to develop numerical models capable of predicting the geometry variation due to fuel burnout, rather than based on assumptions that geometry evolves in self-similar manner, or burnout proceeds in parallel layers (uniform burnout rate). In the current paper, we present an approach developed recently, and demonstrate its capability on a simulation of small-scale supersonic SFRJ.

2. Problem statement
The mathematical model for transient internal reacting flow in the solid fuel scramjet is based on a system of fully compressible Reynolds-averaged Navier-Stokes (RANS) equations closed by the k–ε turbulence model with enhanced wall treatment.

We consider an axisymmetric fuel grain and introduce cylindrical coordinates \((r, z)\) with the origin located on the axis of symmetry near the inlet of combustion channel. In this coordinate system, the internal surface of the channel is generated by revolution of some curve, \(r_i(z,t)\), which varies with time due to solid fuel burnout. Evolution of burning surface is not prescribed; rather, it is obtained by solving a coupled problem.

The system of governing equations for non-swirling axisymmetric flow of reacting compressible gas takes the following form in cylindrical coordinates:

\[
\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{F}}{\partial r} + \frac{\partial \mathbf{G}}{\partial z} + S = \frac{\partial \mathbf{F}^D}{\partial r} + \frac{\partial \mathbf{G}^D}{\partial z} + R \tag{1}
\]

where \(\mathbf{Q}\) is the vector of conservative variables; \(\mathbf{F}, \mathbf{G}\) and \(\mathbf{F}^D, \mathbf{G}^D\) are “inviscid” and dissipative flux vectors in \(r\) and \(z\) directions, respectively, \(S\) and \(S^D\) are source terms arising in the cylindrical coordinates, while \(R\) is the vector of source terms due to gas-phase chemical reactions. For a gas composed by \(N\) species with mass fractions \(Y_i\), we have

\[
\mathbf{Q} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ E \\ \rho Y_i \end{pmatrix}, \quad \mathbf{F} = \begin{pmatrix} \rho u \\ \rho u^2 + P \\ \rho u v \\ (E + P)u \\ \rho u Y_i \end{pmatrix}, \quad \mathbf{G} = \begin{pmatrix} \rho u \\ \rho u v \\ \rho v^2 + P \\ (E + P)v \\ \rho v Y_i \end{pmatrix}, \quad \mathbf{S} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \rho u Y_i \end{pmatrix}, \quad \mathbf{R} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \dot{w}_i \end{pmatrix}
\tag{2}
\]

\[
\mathbf{F}^D = \begin{pmatrix} \tau_{rr} \\ \tau_{zz} \\ \tau_{rz} + \nu \tau_{zz} + \lambda T_r \\ \rho D Y_{r,r} \end{pmatrix}, \quad \mathbf{G}^D = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \tau_{rr} \end{pmatrix}, \quad \mathbf{S}^D = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}
\tag{3}
\]

The source term \(R\) involves the reaction rates for individual species. The source term \(R\) involves the reaction rates for individual species \(w_i\). We consider species as ideal gases, with the thermic
equation of state, specific internal energy $e$ (which includes the heat of formation for species) and specific heat capacity for multicomponent gas with variable ratio of specific heat capacities $c_p / c_v \neq \text{const}$.

Molecular viscosity, conductivity, and diffusivity of individual species, as well as corresponding multicomponent gas mixture properties can be evaluated from the classical molecular kinetic theory (Hirschfelder et al, 1964). However, for high-Reynolds number turbulent flows considered here, the turbulent transport coefficients exceed by far their molecular counterparts. This justifies a simplified approach to the calculation of molecular transport coefficients: the molecular gas viscosity $\mu$ is obtained from Sutherland’s formula with the coefficients corresponding to air, while the molecular conductivity $\lambda$ and diffusivity $D$ are evaluated then from the corresponding Prandtl and Schmidt numbers.

We rely on the standard high-Reynolds number $k - \varepsilon$ model of turbulence in which two equations for the turbulent kinetic energy and dissipation rate. The boundary conditions at solid walls are set by the “wall functions” approach taking into account the presence of log-law boundary layers where equilibrium between turbulence production and dissipation is assumed. This allows one to obtain the flow-wall interaction without the need of resolving the whole boundary layer (as is the case in so-called low-reynolds models). Wall functions are applied to calculate the wall shear stress, as well as the heat flux from the gas to the solid fuel surface.

We use a simple model for solid fuel gasification under the incident heat flux $q_s$. The model is based on energy balance; it takes into account heating of solid material from its initial temperature $T_0$ to the boiling temperature $T_s$ on the surface of decomposing material, as well as the heat necessary for its further gasification:

$$\dot{m} = \frac{q_s}{c_s(T_s - T_0) + \Delta H_G}$$  \hspace{1cm} (4)

Here, $c_s$ is the specific heat capacity of solid fuel, $\Delta H_G$ is heat of gasification. The heat flux $q_s$ can generally include the radiation part, but here it was not taken into account due to small sizes of the combustor considered. With the mass flux of fuel consumption (4), the linear velocity of fuel surface regression is defined by

$$v = \frac{\dot{m}}{\rho_s}$$  \hspace{1cm} (5)

where $\rho_s$ is the solid material density.

Polymethylmethacrylate (PMMA) was taken as the solid fuel with the following properties of in the gasification model (4): solid material density $\rho_s = 1.18$ g/cm$^3$, boiling temperature $T_s = 200$°C, specific heat capacity $c_s = 1500$ J/(kg·K), heat of gasification $\Delta H_G = 1591$ kJ/kg.

While gasification of PMMA, as a complex polymer, produces whole spectrum of gas components, in this study we take a simple model that PMMA, upon thermal decomposition, gives rise just to gaseous methylmethacrylate (MMA) represented by chemical formula $C_5H_8O_2$. Combustion of MMA in the gas phase is described by a one-step irreversible gross reaction (Bedir and T’ien, 1998):

$$C_5H_8O_2 + 6O_2 \rightarrow 5CO_2 + 4H_2O + \Delta H_c$$  \hspace{1cm} (6)

with the reaction rate for $i$-th species

$$\dot{\omega}_i = B \cdot T \cdot W_i \cdot \rho Y_i \cdot \exp \left( -\frac{E_i}{RT} \right)$$  \hspace{1cm} (7)
where $Y_F$ and $Y_O$ are the mass fractions of fuel (MMA) and oxidizer, respectively; $s_i$ is the mass stoichiometric coefficient of $i$-th species (for fuel $s_F = -1$), $W_{O_2}$ is the molar mass of oxygen. The kinetic parameters in (7) are: pre-exponential factor $B = 6.6 \times 10^6$ m$^3$/(mol s K), activation energy $E_a = 144$ kJ/mole. The heat of combustion per unit mass of fuel is $\Delta H_c = 25.6$ MJ/kg.

The turbulent combustion rate is obtained from the Eddy Dissipation Concept (EDC) model by Gran and Magnussen (1996) (see also Magnussen, 2005).

3. Numerical implementation

This work is aimed at numerical simulation of combusting gas flows in a solid fuel grain, taking into account the variation of channel geometry due to fuel burnout. As the approach, we apply the Cartesian grid method with “embedded” boundaries in which the sharp interface between the solid material and gas is described as a zero level set of a signed distance function (the level set method, see Osher and Fedkiw, 2003). The advantage of level set method is that simulations are performed on a fixed Cartesian grid where high-order numerical schemes are available for gas flow; the moving boundary is implemented by considering the signed distance function as time-dependent, with the surface receding in the normal direction at the local burnout velocity.

The system of governing equations and turbulence model equations are integrated on a uniform Cartesian grid. All variables are collocated, i.e., defined at the centers of numerical mesh cells. The solution procedure is based on splitting by physical processes and is performed in sequential fractional steps: i) solution of the reactive subsystem, ii) solution of “inviscid” subsystem with fluxes $F$ and $G$ form; iii) taking into account dissipative terms with fluxes $F^D$ and $G^D$ form.

At the chemical reaction substep, the kinetical equations in the context of EDC turbulent combustion model are integrated by stiff ODE solver VODE. At the inviscid substep, we solve the system of Euler equation for compressible multicomponent gas, taking into account the fluxes $F$ and $G$, as well as term $S$ due to cylindrical coordinates. The “inviscid” fluxes are approximated by the scheme HR-SLAU2 by Kitamura and Hashimoto (2016). HR-SLAU2 scheme belonging to the AUSM family of numerical schemes, with modifications making it an “all-speed” numerical scheme applicable to wide range of Mach number flows. Viscosity, diffusion, and heat conduction terms are approximated by the standard second-order central difference scheme.

The surface is a body of revolution described by its generatrix in the meridian plane, defined as a zero level set of a time-dependent signed distance function. The overall approach to numerical approximation in the presence of embedded boundaries corresponds to the conservative method by Hu et al (2006). Grid cells are classified according to their location (in the freestream, in solid body or cut by the boundary) and size (small or large cut cells depending on the volume fraction in the flow). The viscous and inviscid fluxes are multiplied by the corresponding apertures on each cell boundary; fluxes from the pieces of boundary are added in the cut cells. Depending on the availability of cells near the boundaries, the approximation order for the fluxes is lowered to one if necessary.

The wall functions of $k-\varepsilon$ turbulence model were implemented for the embedded boundaries by extending a normal from the surface into the flow, setting the wall laws along this normal, and subsequent interpolation of the boundary layer variables back onto the Cartesian grid. This approach allows one to eliminate the difficulties of posing the boundary conditions in cut cells for which the distance from the cell centroid to the surface can vary randomly, see (Berger and Aftosmis (2012)).

For supersonic flows in small-size engines, the characteristic residence time and characteristic combustion times are much smaller than the characteristic times of fuel burnout. Therefore, simulation of the whole combustion process (dozens of seconds) with the time step governed by gas dynamics (of the order of $10^{-5}$ s) would require enormous CPU times. To overcome this difficulty, simulations were carried out in the quasi-static manner: the gas dynamics solver was run to steady state in the current geometry (requiring about $10^4$ iterations), the heat fluxes obtained were used to evaluate the local surface propagation velocity $V_s$ (see equations (4) and (5)) then the geometry was altered by
propagating the surface in the normal direction according to this velocity. Then the gas dynamics solver was run again until a new steady state solution was obtained etc. The typical surface propagation time was chosen to be 0.1 s, and this propagation was performed with time step of 0.01 s.

4. Results

4.1. Geometry and parameters
The initial fuel grain geometry was set according to the experimental paper by Ben-Yakar, Natan, Gany (1988); it is sketched in figure 1, with all linear sizes summarized in table 1. In order to obtain supersonic inlet conditions, a converging-diverging nozzle was added on the left boundary, with flow choking in the critical cross-section; the flow conditions at the subsonic inlet of the nozzle were set according to the total pressure 16.7 atm and total temperature of 1156 K (corresponding to experiment No. 5 by Ben-Yakar, Natan, Gany (1988), where stable combustion was achieved).

![Figure 1. Initial geometry of the grain.](image)

Table 1. Summary of geometry parameters.

| Parameter | Value |
|-----------|-------|
| \(d_{f,0}\), mm | 30 |
| \(d_{in}\), mm | 12.45 |
| \(L_{f,0}\), mm | 50 |
| \(L_{cyl}\), mm | 35 |
| \(d_{cyl}\), mm | 14.5 |
| \(L\), mm | 170 |

4.2. Combustion in the initial geometry
In figure 2, the steady-state flowfield calculated in the initial geometry is presented. The streamlines clearly show the recirculation zone developing near the inlet due to the presence of flame holder.

![Figure 2a. Temperature of gaseous mixture in the initial geometry. Streamlines show the recirculation zone.](image)

The distributions of mass fractions of fuel (MMA) and oxygen show that combustion in the engine is of diffusion type. Hot temperature zones are developing in the flame holder where combustion
products are recirculating, causing gaseous fuel production at the surface, as well as in the channel near the wall where fuel mixes with oxygen from the main stream.

![Mass fraction of gaseous fuel MMA](image1)

![Mass fraction of oxygen in the initial geometry](image2)

**Figure 2 b, c.** Mass fraction of gaseous fuel MMA (b), and mass fraction of oxygen in the initial geometry (c).

### 4.3. Geometry and parameters
As combustion proceeds in the scramjet engine, the shape of the channel is gradually changing. In this section, we show the distributions of temperature (figure 3) and Mach number (figure 4) in the course of the time-dependent fuel burnout. Distributions are shown at times of 1, 2, 3, and 4 seconds after ignition. The shape of the fuel channel is visible by the outer boundary of the flow domain.

![Temperature distributions with moving solid boundary](image3)

**Figure 3.** Temperature distributions with moving solid boundary in a different times: a) after 1 s, b) after 2 s, c) after 3 s, d) after 4 s.
Figure 4. Mach number distributions with moving solid boundary in a different times: a) after 1 s, b) after 2 s, c) after 3 s, d) after 4 s.

The results of the calculations are in qualitative agreement with the experimental data by Ben-Yakar, Natan, Gany (1988) and show that over time, the channel of the solid fuel grain is levelled, acquiring a cylindrical shape. This indicates that the regression rate of the solid fuel in the channel is significantly higher than the regression rate in the flame holder.

5. Conclusions
The fuels used in the solid-fuel scramjet do not contain (or contain insufficient amount of) oxidizer, and they are not capable of self-sustained combustion. Because of this, decomposition of the solid fuel occurs in forced regime due to heat flux from the gaseous combustion products while combustion of fuel in the gas phase occurs in mixture with the ambient air oxygen. This leads to a mutual influence of gas-dynamic and thermal processes in the charge channel and the decomposition process of solid fuel.

The model and CFD code developed allow one to calculate both stationary and nonstationary processes in a scramjet taking into account burnout of solid fuel grain and change of the channel geometry.

Comparison of the results of simulations for this model with experiments by Ben-Yakar, Natan, Gany (1988) showed that the calculated data are in qualitative agreement with the experimental data, but the calculated rate of decomposition of solid fuel is approximately 2 times greater than the experimental one. This indicates the need to improve the solid-fuel decomposition model (4), which seems to be too simplistic.

From this point of view, it seems necessary to describe in more detail the processes in the condensed phase of the solid fuel near the burning surface, in particular, the melting of the fuel, the excitation of waves on the surface of the melt, formation and detachment of melt droplets from the surface of the waves, and combustion of fuel droplets in the air stream. These issues are expected to be considered in the following articles.

Note finally that the model and CFD code developed can also be used to calculate hybrid rocket motors.

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