Numerical modeling of gasification and combustion of solid fuels in a solid fuel ramjet combustor

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Abstract. In order to investigate features of processes inside a combustor of a solid fuel ramjet a numerical model was employed. The model is based on Reynolds-averaged Navier-Stokes equations along with turbulence and combustion models and considers solid fuel pyrolysis. Experimental data from an earlier work was used to validate the model. Dependencies of air mass flux on some combustor performance parameters were obtained for different solid fuels.

1. Introduction
A solid fuel ramjet (SFRJ) is the simplest design among air-breathing propulsion systems. Typically, as can be seen in figure 1, such an engine consists of an air inlet, a combustor with a solid fuel grain inside and a nozzle. Simplicity, high stored fuel density and high specific impulse at high flight speed make SFRJ an attractive design for supersonic propulsion systems.

During the flight of the aircraft with a SFRJ the incoming air is decelerated by shock waves in the inlet, yielding an increase of pressure and temperature. At the combustion chamber inlet, a diaphragm creates a sudden expansion of the incoming air, originating a recirculation zone, which provides flame stabilization. Inside the combustion chamber the solid fuel grain is pyrolyzed heat flux from diffusion flame caused by a reactions between gasified fuel and oxygen. Combustion of gasified fuel increases the internal energy of the flow which is converted to kinetic energy in the nozzle, yielding thrust. Polymers and their compositions with metal particles are considered [1] as solid fuels for ramjets. Performance parameters of a SFRJ depend on solid fuel regression rate, which, in turn, depends on parameters of the air flow at the combustor inlet. Thus, calculation of solid fuel regression rates is essential for investigation of the SFRJ performance.

The most detailed analysis of processes inside a SFRJ combustor can be performed by using computational fluid dynamics. There is a number of works which employed this tool to investigate some of SFRJ combustor performance features [2–8]. During the operation of SFRJ the combustion of non-premixed components takes place in the combustor. Since non-premixed flames are mostly controlled [9] by the mixing of reagents, different finite and infinite reaction rate approaches can be used to investigate features of flow field and solid fuel regression inside SFRJ combustor. Earlier works [2,3] employed Shvab-Zeldovich flame model. To consider influence of turbulence on combustion eddy-dissipation model can be used [4, 5]. A number of works considered finite rate kinetic models [7, 8, 10]. It was shown in [6], however, that the calculated regression rate is hardly influenced by the combustion model employed.
Figure 1. Schematic illustration of a SFRJ. Figure 2. Computational domain.

However, it is still little reported on some important features of SFRJ combustor performance. The aim of the present work is to devise a numerical model of processes inside a SFRJ combustor and to investigate some features of these processes for different types of solid fuels: polyethylene (PE), poly(methyl methacrylate) (PMMA) and hydroxyl-terminated polybutadiene (HTPB).

2. Model description
2.1. Case setup and computational domain
The model deals with the flow inside a typical SFRJ combustor which consists of a solid fuel grain and a flame stabilizer (figure 2). The solid fuel grain is a hollow cylinder made of hydrocarbon polymer. The flame stabilizer is a diaphragm placed before the fuel grain. A two-dimensional axisymmetric case is considered. Parameters of the air flow at the combustor inlet, e.g. temperature $T_0$, static pressure $P_0$ and air mass flux ($\rho V_0$) are the entry data of the model. It is assumed that solid fuel pyrolysis takes place at the grain surface consuming all the heat supplied from the gas phase and yielding monomer.

2.2. Flowfield calculation
The flow is governed by system of mass, momentum, energy and species conservation equations:

$$\frac{\partial Q}{\partial t} + \frac{\partial F_i}{\partial x_i} = \frac{\partial G_i}{\partial x_i} + S,$$

where $Q$, $F_i$, $G_i$, $S$ are vectors of conserved variables, convective fluxes, viscous fluxes and source terms respectively:

$$Q = \begin{pmatrix} \rho \\ \rho v_j \\ \rho E \\ \rho Y_n \end{pmatrix}, F_i = \begin{pmatrix} \rho v_i \\ \rho v_i v_j + P \delta_{ij} \\ (\rho E + P) v_i \\ \rho v_i Y_n \end{pmatrix}, G_i = \begin{pmatrix} 0 \\ \tau_{ij} \frac{\partial v_i}{\partial x_j} \\ \frac{\partial Y_n}{\partial x_i} \\ \rho D \frac{\partial v_i}{\partial x_i} \end{pmatrix}, S = \begin{pmatrix} S_{\text{mass}} \\ 0 \\ S_{\text{energy}} \\ S_n \end{pmatrix}.$$

Here $\rho$ is density, $v$ – flow velocity, $P$ – static pressure, $E$ is the sum of the specific internal energy and specific kinetic energy, $\tau_{ij}$ is the shear-stress tensor and $Y_n$ is the mass fraction of the n-th specie. These equations are closed by equation of state of a perfect gas.

Since flows inside SFRJ combustor are highly turbulent ($Re > 10^5$), $k-\Omega$ shear stress transport [11] two-equation turbulence model was employed in present work. This model was proven [8,10] to be reliable in simulating flows inside SFRJ combustors.

In this work combustion processes are taken into account by using the laminar finite chemical reaction rate model. Various simplified gas-phase kinetic schemes are employed to describe combustion of different solid fuels. These schemes are taken from [10] in case of PE combustion, from [12] in case of PMMA combustion and from [13] in case of HTPB combustion.
Dirichlet boundary conditions are set at the combustor inlet for the most of flow parameters. At the centerline a symmetry boundary condition is specified for every variable. It is assumed that every wall of the domain including grain surface is impermeable and does not conduct heat. A no-slip boundary condition is specified on the walls for velocity.

Numerical results were obtained on a rectangular mesh by using OpenFOAM [14] toolbox which is based on the finite volume method of solving partial differential equations. Mesh cells were clustered near walls in order to ensure the resolution of the laminar sublayer.

2.3. Modeling of solid fuel gasification
In order to calculate the temperature of the grain surface and fuel injection rate one must couple energy balance equation of the grain surface with the Arrhenius law, which governs solid fuel regression rate [15]:

\[ U = A \exp \left( -\frac{E_A}{R \mu T_s} \right), \]  

where \( E_A \) is the activation energy of solid fuel pyrolysis, \( A \) is the pre-exponential factor, \( R \mu \) – universal gas constant and \( T_s \) is temperature of the grain surface. In present work the solid fuel gasification is dealt with by introducing additional corresponding source terms for energy, mass and fuel transport equations in cells adjacent to the grain surface:

\[ S_{\text{energy}} = -\frac{F_{\text{sur}}}{V_{\text{cell}}} [H_{\text{pyr}} + C_p(T - T_{\text{in}})] \rho_{\text{fu}} A \exp \left( -\frac{E_A}{RT} \right), \]

\[ S_{\text{mass}} = S_{\text{fu}} = \frac{F_{\text{sur}}}{V_{\text{cell}}} \rho_{\text{fu}} A \exp \left( -\frac{E_A}{RT} \right), \]

where \( F_{\text{sur}} \) – area of the cell face which belongs to the grain surface, \( V_{\text{cell}} \) – cell volume, \( H_{\text{pyr}} \) is standard enthalpy of pyrolysis, \( C_p \) is specific heat of gasified fuel and \( T_{\text{in}} \) is temperature inside the grain, which is considered constant and equal to 298 K, \( \rho_{\text{fu}} \) – density of solid fuel. Parameters of solid fuel pyrolysis employed in the present work are provided in table 1.

| Solid fuel   | \( A, \, \text{m/s} \) | \( E_A \, \text{kJ/Mole} \) | \( H_{\text{pyr}}, \, \text{MJ/kg} \) |
|--------------|------------------------|------------------------------|----------------------------------|
| PMMA [16]   | \( 72 \times 10^{-3} \) | 53.1                         | 1.03                             |
| PE [17]     | 4780                   | 125.05                       | 3.79                             |
| HTPB [13]   | \( 11.04 \times 10^{-3} \) | 20.52                        | 2.06                             |

2.4. Combustor performance parameters
With the temperature field calculated the longitudinal distribution of solid fuel linear regression rate is obtained by using (1). With this distribution known the overall solid fuel consumption rate is obtained by integrating linear regression rate along the grain:

\[ G_{\text{fuel}} = \Pi \rho_{\text{fu}} \int_0^L U \, dx. \]

The equivalence ratio can be obtained from:

\[ \alpha = \frac{G_{\text{air}}}{\nu G_{\text{fuel}}}, \]

where \( G_{\text{air}} = (\rho V)_{\text{air}} \Pi \pi R^2 \) is air supply, \( \nu \) is the amount of unit mass of air required to completely burn a unit mass of solid fuel.
In present work, considering relatively low fuel injection rate, combustion efficiency is evaluated by
\[
\eta = \frac{G_{\text{air}} c_p^{\text{air}} (T_{\text{out}} - T_0)}{G_{\text{fuel}} H_u},
\]
where \(c_p^{\text{air}}\) is air specific heat, \(T_{\text{out}}\) is flow temperature averaged across outlet section and \(H_u\) is the heat of combustion of solid fuel employed.

3. Verification of the numerical model
In order to validate the numerical model and the computational algorithm let us compare numerical results with experimental regression rate data from [8]. In figure 3 there are shown calculated fuel regression rate longitudinal distribution in comparison with experimental data. Data was obtained for combustion of cylindrical grains of PE with \(L = 0.3\) m, \(R = 0.035\) m, \(h = 0.0175\) m in air flow with inlet temperature \(T_0 = 540\) K, static pressure \(P = 0.66\) MPa and mass flow rate \(G_{\text{air}} = 0.3\) kg/s. It can be seen that calculated results agree with experimental data and do capture main features of the processes under investigation. Average fuel regression rate grows with air mass flux growing due to intensification of heat transfer between the flame and the grain surface. Local regression rate drastically grows along the grain where the recirculation zone takes place reaching maximum at the flow reattachment point and then it slowly decreases with boundary layer thickness growing and cross section average mass fraction of oxygen decreasing.

4. Results and discussion
A working process inside the combustion chamber of a SFRJ was simulated for different types of solid fuel and parameters of the inlet air flow. The chamber under consideration (see figure 2) has following parameters: the length of the grain \(L = 0.5\) m, inner radius of the grain \(R = 0.05\) m and the height of the flame stabilizer \(h = 0.025\) m. The incoming air has temperature 500 K, static pressure 5 atm and mass flux varying between 10 kg/(m\(^2\)s) and 400 kg/(m\(^2\)s).

A typical for SFRJ situation can be observed in figure 4 which shows distributions of temperature and mass fractions of oxygen and gasified fuel inside the combustion chamber with grain of PE under air mass flux of 100 kg/(m\(^2\)s). A flame is forming above the grain surface behind flame stabilizer and divides the flow into an oxygen-rich region and a fuel-rich region below the flame. Fractions of these species become thinner when closing to the flame as
Figure 4. Temperature field, distribution of oxygen and gasified fuel mass fractions inside a SFRJ combustor with grain of PE.

Figure 5. Dependencies of fuel consumption on air supply for different types of solid fuels.

Figure 6. Dependence of equivalence ratio on air supply for different types of solid fuels.

Figure 7. Dependence of combustion efficiency on air supply for different types of solid fuels.
they consumed by the combustion process while fraction of fuel is highest near the grain surface where it yields during solid fuel pyrolysis. The temperature is highest near the flame and drops near the grain surface due to endothermicity of solid fuel pyrolysis.

Dependencies of air mass supply on solid fuel mass regression rate are shown in figure 5. It can be seen that consumption of solid fuel grows with air supply growing for every type of fuel. It also can be seen that regression rate of PE, which has the highest enthalpy and activation energy of pyrolysis, in general is the lowest among considered fuels, while kinetic parameters and the lowest enthalpy of PMMA pyrolysis makes it regress most intense. It can be seen in figure 6 that under conditions considered there is no drastic change of equivalence ratio for PE combustion while ratios for HTPB and PMMA combustion slightly increase with air supply growing. In every case a drastic increase of air supply does not affect equivalence ratio significantly. It can be attributed to dependency of regression rate on air mass flux close to linear for subsonic flows inside combustion chamber. While no obvious correlation between air supply and combustion efficiency can be observed in figure 7, combustion efficiency within grain in case of PE and PMMA is significantly higher than one in case of HTPB lying between 0.4–0.5. This makes PE more preferable than PMMA (which has twice as low heat of combustion) and HTPB as a fuel for propulsion systems with limited length.

5. Conclusion
A model of gasification and combustion of solid fuel grain in a ramjet combustor is presented and validated by comparison of numerical results with available from literature experimental data. The model is able to predict SFRJ combustor performance parameters. Dependencies of these parameters were obtained for different fuel types. It was shown that for subsonic flows equivalence ratio and combustion efficiency do not vary significantly within wide range of air mass fluxes. In conditions simulated among fuels considered HTPB has the least combustion efficiency within the grain, which makes it less preferable for system with limited length.

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