Numerical solution of moving boundary problem for deposition process in solid fuel gas generator

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Abstract. Moving boundary problem in application to process of depositions formation in gas generator are considered. Gas generator, as a part of fuel preparation system of high-speed vehicle, convert solid fuel into multicomponent multiphase mixture, which further burned down in combustion chamber. Mathematical model of two-phase “gas-solid particles” flow, including Navier-Stokes equations for turbulent flow in gas generator and mass, impulse conservations laws for elementary depositions layer are proposed. Verification of proposed mathematical model for depositions mass in gas generator conditions is done. Further possible improvements of proposed model, based on more detail accounting of particle-wall interaction and wall’s surface adhesion properties are analyzed.

1. Introduction
In moving boundary problem or similar Stefan problem, position of interfacial surface are considered and often this position can’t be determined a priori due the dependency of some other variable. Existing of locally changing in time and space interfacial surface is one of the main difficulties of such type problems and as a rule these problems have multidisciplinary and non-one dimensional nature. In particular, the great interest at nowadays is attached to systems, in which transition from solid to gas phase exist, example of such systems is burning surface of solid rocket fuel [1, 2, 3], and systems with gas-solid transition, for example, solid deposition formation in fuel lines of propulsion [4] or heat exchanger [5, 6] or in problems with icing [7]. Mathematical modelling of mentioned systems requires a description of a number of phenomena such as turbulent flow in complex geometries, heat transfer, chemical kinetics including combustion, discrete particles propagation, interaction of particles with solid surfaces and others. Modern CFD tools, providing advanced platform for solution of Navier-Stokes equations, can potentially take into account many of physical effects of the continuum media, though obtaining of physically correct solution often is a challenge. There are roughly two branches of methods within CFD, which can capture multiphase flow physics with moving interfacial surface. First branch is methods with Eulerian computational meshes, for example, immersed boundaries method, and second branch is dynamic meshes methods, which moves and recalculate mesh nodes positions in a way, that one or more of the mesh family lines always lie on the interfacial surface through the flow iteration. Last branch used in current work, two of the advantages of this branch of methods are in the absence of the special treatment of boundary conditions and relatively easy control of the near-wall mesh layer resolution.

In current work moving boundary problem in application to process of depositions formation
in gas generator are considered. Gas generator convert solid fuel into multicomponent multiphase mixture, which further burned down in combustion chamber. Two stages fuel combustion scheme improve operational characteristics of engine, but wherein burning of gas generator solid fuels can be accompanied by significant amount of condensed products, whose total mass fraction may reach about 5% from overall fuel mass in typical gas generator conditions, and about 50% for equilibrium conditions. Amount and properties of discrete phase essentially depends on fuel composition and conditions of gasification. Interaction of chemically active discrete phase particles with walls of gas generator under medium temperatures \( T \approx 800 \text{ K} \) leads to deposition of solid fraction and appearance of evolving with time interfacial surface \([4]\). Further depositions growth results in changes in heat transfer at walls and flow blockage in critical sections of gas generator, as shown at figure 1. Besides that, the depositions formation reduces the energy efficiency of the engine and could lead to a performance degradation.

The aim of this paper is to develop mathematical model of solid depositions formation process in solid fuel gas generator and to estimate by the proposed model typical full blockage time of the flow.

2. Mathematical model

Solid fuel gas generator mathematical model includes incompressible viscous fluid flow description in the channel with deformable boundary. Flow was considered in quasi-stationary formulation with time marching procedure: at first, velocity field in the channel with a certain geometry was obtaining, then deformation of boundary connected with depositions formation was computing, and after that, calculation was repeating for the modified channel geometry. Thus, gas flow governing equation system is of the form

\[
\nabla \cdot \mathbf{U} = 0,
\]

\[
\nabla \cdot (\mathbf{U} \mathbf{U}) = -\nabla p + \nabla \cdot (\nu \nabla \mathbf{U}),
\]

where \( \mathbf{U} \) is flow velocity, \( p \) is kinematic pressure, \( \nu \) is gas kinematic viscosity. Typical Reynolds number evaluation shows that there is developed turbulent flow in gas generator, hence equations (1)–(2) was calculated in Reynolds-averaged approach (RANS) with \( k-\omega\)-SST turbulence model \([8]\) for the computational cost reduction purposes. \( k-\omega\)-SST turbulence model combines \( k-\omega \) model features in near-wall regions and \( k-\varepsilon \) model features in free flow, hence allows to obtain more precise solution in entire channel in comparison with each model individually.

Depositions formation occurs mostly due to convectional settling of particles from the flow. Therefore, depositions layer growth rate depends on mean velocity of the flow, which brings
settling particles and on turbulent pulsations which may increase probability of collision of near-wall particle and surface in comparison with the laminar flow. Probability of particle being captured by surface during the contact defined by many factors such as collision velocity, incidence angle, properties and features of surface, e.g. liquid film presence, etc. Problem of different factors influence estimation goes beyond the scope of the paper. Inertialess particles ($Sk \ll 1$) was considered as a first approximation of discrete phase model under the assumption that dispersed phase volume flow rate is small in comparison with carrying flow rate, $G_p \sim 0.01 G_g$, and the influence of dispersed phase on the flow is negligible. Then depositions growth rate $v$ is proportional to normal flow velocity in the near-wall region:

$$v = k_d U_w \cdot n,$$

where $U_w$ is gas flow velocity in the near-wall layer, $n$ is surface normal, $k_d$ is coefficient of probability of particle being captured by surface during collision.

Expression (3) defines velocity of computational mesh boundary nodes displacement during transition from one time step to the next one. This displacement corresponds to deposition growth (fig. 2). Time step $\Delta t = 10^{-4}$ was defined as lesser than typical convectional time and typical turbulent mixing time under the assumption that depositions growth is determined mostly by mass transport processes in gas. Discretization of numerical domain for modelling leads to forming of small-scaled highly indented surface (fig. 2(b)), that occurs even when nodes displacement velocity is smooth function as in (3). Local boundary irregularity increasing can lead to degeneracy of computational mesh because of negative volume cells formation. Smoothing procedures was applied to the interfacial surface for convergence improvement and avoiding of negative volume cells formation. Boundary-forming polygon was processed with Savitsky-Goley filter with window $n <= 9$ after boundary nodes displacement. Obtained boundary was used as initial geometry for the next step mesh generation (fig. 2(c)).

Solution of discrete equations was carried out by SIMPLE method on unstructured mesh. Gradient reconstruction was performed with the 2nd order approximation scheme. Resulting set of linear algebraic equations was solved with Gauss-Zeidel method and hybrid multigrid technology GAMG.

3. Simulation results and discussion
Model gas generator consists of two sequential cylindrical sections with diameter $D = 0.045$ m and $d = 0.019$ m, and conic junction between them as shown at fig. 3(a). Computational domain

![Figure 2. Depositions layer growth and roughness smoothing with Savitsky-Goley filter: (a) initial surface structure; (b) geometry deformation due to depositions formation; (c) deformed boundary after Savitsky-Goley filter smoothing with window $n = 7$.](image-url)
geometry is a copy of experimental model gas generator simplified by removing small constructive elements (device fragments pictures presented at fig. 1). The problem was considered in a 2D formulation for computational cost decrease purposes. Computational domain inlet boundary (left boundary at fig. 3(a)) coincide with solid fuel charge location, which is the source of gasification products. The location of this boundary was fixed, plain gas flow velocity profile $U_x = 1 \text{ m/s}$ was set on this boundary. The outlet boundary with soft boundary conditions was located on the distance of $5.5d$ downstream from channel step. Other boundaries was considered as solid surfaces with no-slip wall conditions.

Velocity field in non-deformed by depositions gas generator channel is presented on fig. 3(a). Uniform inlet flow forms two low-intensive zones with significant gas residence time in throat area of gas generator. Local flow acceleration with flow compression and two elongated recirculation zones occurs in a channel throat after the corner. Maximum reversed flow velocity is about $0.5 \text{ m/s}$, length of recirculation zone is about $d$. With depositions layers growth these recirculation zones tend to decrease in size and completely disappear eventually. After that flow without separation is developed, as shown at fig. 3(b). For initial stages of flow development outlet velocity profile has typical turbulent form with a large constant velocity flow core.

Calculation results in deformed by depositions gas generator channel are presented on fig. 3(b). Solid depositions are formed mostly in cylindrical part of channel with diameter
Figure 4. Influence of the depositions growth on gas generator parameters: diameter of the flow section (a), total pressure loss (b).

$d$, solid depositions layers have conic form in inlet and outlet parts of the channel. However, flow in the inlet part differs from the outlet part considerably: there are typical stable confuser flow and unstable flow with separation correspondingly. Further at time depositions cone angle at the outlet part of the channel exceeds critical value (8°) with the following stability loss, after that maximum velocity zone of the flow starts to oscillate. Flow instability leads to formation of inhomogeneities at the depositions layer surface. “Pockets” are forming in the cylindrical depositions layer, this process could lead to computational domain connectivity increasing, for example, if parts of depositions layer leaved the solid surface or if cavities formed in the depositions layer volume. With growth of depositions layer velocity magnitude in the paraxial zone of the channel is increased and for fig. 3(b) it equals to 11.2 m/s. For near blockage time the mass of the depositions in the inlet part of the gas generator with the diameter $D$ is insignificant and depositions layer has wave-like form.

There are many important characteristics of gas generator, among them are the flow section of long cylindrical part and overall device hydraulic resistance. Time dependences for minimal channel flow section and total pressure losses in comparison with their initial values are presented on fig. 4. Calculation results show that minimum diameter of flow section decreases monotonously in time and at for shown at 4 time moment equals to 4.4 mm (approximately five times smaller than initial value). Further depositions growth leads to full blockage of the gas generator channel, and the corresponding moment in time could be estimated at fig. 4(a) as abscissa value at intersection point between the curve and abscissa axis. Minimal flow section locates at the distance of about 0.7$d$ from the beginning of the smaller cylindrical part of the gas generator and moves downstream with the growing of depositions layer until the distance of 2.5$d$. Monotony of $d(t)$ dependence can be explained by absence of global flow separation in the flow domain. Time dependence behavior of total pressure losses differs from minimal flow section one. Curve at fig. 4(b) could be divided into three parts: initial part until $t/t_f \approx 0.5$ with approximately constant pressure loss value, rapid growth part until $t/t_f \approx 0.9$, and last part at $t/t_f > 0.9$ with significant pressure oscillations related to flow instability. Net increase of relative total pressure losses equal to 12 for near blockage time.

Experimental data for solid fuel gas generator with a similar geometry at operational time 9.51s show about 2.6% reduction of relative minimal flow section, while numerical simulation results show value in 2.1% for the same parameter. Experimental growth rate of the depositions layer corresponds to coefficient value of $k_d = 521$. The main reasons of differences between
experimental and numerical results are in discrepancy of quantitative parameters of depositions
growth mechanism and neglecting of heat effects, which could alter adhesive properties of
particles and surface. Nevertheless, proposed mathematical model can qualitatively describe
solid depositions formation at gas generator walls and can estimate depositions influence on
flowfield. Approximation of frozen particles can be in natural way replaced by lagrangian
massive particles model and that should allow to simulate influence of particle inertia and
weight distribution on depositions formation. Capturing gas-solid surface with dynamic mesh
approach allow in a direct way to extend model for accounting thermo-physical properties of
solid surfaces, that can be do by wall boundary conditions modification in computational cells
with depositions. Future improvements of proposed mathematical model can include mesh
deformation small-scale smoothing procedure, which should give correct correlation between
physical inhomogeneities scales of depositions surface and computational mesh ones (filter
window width and depositions roughness scale correspondence); exact formulation for mass
conservation law for solid depositions (this property could be expressed using geometrical
conversation laws [9]).

4. Conclusion
In this paper description of proposed mathematical model of two-phase flow “gas-solid particles”,
including Navier-Stokes equations for turbulent flow and mass, impulse conservations laws for
elementary depositions layer are given. Despite the simplicity of the proposed model, it allow
with sufficient for engineering applications accuracy describe evolution of interfacial surface.
Comparison between numerical and experimental data show, that discrepancy don’t exceed
40% for total depositions mass. Further possible improvements of proposed model, based on
more detail accounting of particle-wall interaction and wall’s surface adhesion properties are
analyzed.

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