Numerical Simulation of Multiphase Flows in Solid Rocket Motors

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The characterization of the two-phase flow in a heterogeneous solid-propellant rocket chamber and nozzle is crucial in ballistic/performance predictions, aeroacoustic studies, erosion analyses, slag accumulation rate estimates, predictions of thermal loads, plume analyses etc. In particular, aluminum particles initially embedded within the binder and injected in the flow during the burning of the grain, undergo mechanical and chemical interactions with the flow itself, and constitute a principal component of the condensed phase.

In the present work the attention has been focused on the numerical simulation of the internal fluid dynamics of solid rocket motors, with particular attention on multiphase features in the flow, related to the presence of aluminum particles as primary ingredient in the propellant.

Several simulation have been performed, both on very simple geometries (rockets with cylindrical grain) and on a real motor (Zefiro 9A SRM). The results show that the thermo-fluid dynamics features inside the chamber are strongly related to the behaviour of aluminum combustion and are very sensitive to initial dimensions of aluminum particles.

I. Introduction

The driving phenomena in a typical modern high performance rocket motor is the combustion of the heterogeneous aluminized propellant; worldwide, ammonium perchlorate and hydroxyl-terminated-polybutadiene composite mixtures, usually also containing aluminum powder and ballistic modifiers, are the most frequently used formulations in solid rocket propellants. Heterogeneous propellants are used instead of monopropellants because they permit to have an higher outflow velocity with consequent high specific impulse. Aluminum is used as an ingredient because of its high density, high heat release during oxidation, low cost and relative safety; because unaluminized propellant are fuel rich, it would seem that adding more fuel (aluminum) would be counterproductive, however aluminum oxidation reduces the oxidizer vapors (H₂O and CO₂) to better propulsive fluids (H₂ and CO). The aluminum also produces a large increase of temperature, so there is an increase in specific impulse of around 10%, along a net gain in propellant mass fraction of 15%. On the other hand, there are problems with the use of aluminum, such as smoky, luminous exhaust trails; contamination of launch sites with aluminum oxide; adverse effects on motor components in the extra-hot, two phase flow.

Understand the behaviour of heterogeneous aluminized propellant in the whole rocket and develop tools for the analysis and predictions of phenomena and performances are important tasks in the field of the rocket analysis and design.

In the present work the attention has been focused on the numerical simulation of the internal fluid dynamics of solid rocket motors. A numerical tool to simulate this kind of flows has been developed. The gas-dynamics modeling is based on the Euler system of equations for a mixture of gases; the combustion of

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the grain is taken into account with a model that correlate the burning velocity with the local pressure at the burning surface. A great care has been dedicated to the multiphase features of the flow; aluminum powders are widely used as one of the primary ingredients in modern propellants and their particular behaviour can drastically affect motor performances. It has been tried to model the multiphase aspects taking into account all the primary phenomena using direct calculation, limiting the use of simplifications. When propellant burns, aluminum particles added to the propellant melt and form puddles that are released from the surface with a complex mechanism that will be described in the following chapters, travel in the motor chamber and burn; these droplets have a characteristic dimension around 100 µ. From the propellant burning surface and from the combustion of the aluminum droplets very small particles of alumina smoke are generated. These smoke particles have characteristic dimension around 1 µ. These two kind of "condensed phases" have been treated using different approaches: the big particles have been described with a Lagrangian approach, that permits to track the position and velocity of objects that have different characteristics, as radius, temperature, composition, with the possibility of evolving these characteristics. So with this approach it has been possible to take into account the evolution of particle dimension, temperature, composition due to particle combustion, particle interaction with the alumina smoke field, heat exchange between gas and solid phase. Typically with the standard continuous approaches (Eulerian) it is necessary to introduce a set of additional equations (at least the three momentum equations for every grid point) for every particle family; a family means particles that have the same inertial characteristics, so the same radius, composition, temperature. Therefore the necessity to have a set of multidimensional partial differential equations for every radius makes the use of the Eulerian formalism not suitable if it is necessary to evolve particles characteristics, as size, composition, temperature. On the other hand alumina smoke has been described with an Eulerian formalism, that allows to track the enormous number of smoke particles. The Eulerian model is suitable for the simulation of a large number of object, instead of the Lagrangian approach that is limited by the amount of particles because with the Lagrangian method a system of ordinary differential equation is introduced for every particle (one equation for every particle property: position, velocity, temperature, mass, radius). The computational cost for the Eulerian method is independent of the number of particles. Given the models to describe every phase, a number of models to take into account the inter-phases exchanges have been introduced. One of the most important calculates the burn rate of the single Lagrangian particle, function of the local thermo-fluid dynamic state of the surrounding and permits to evaluate the effect of this combustion on the gas flow (mass and enthalpy exchange).

II. Combustion and Multiphase Phenomena in Solid Rocket Motors

A. Grain Combustion Mechanism and Flame Structure

The solid ingredients used most often in modern solid propellants are ammonium perchlorate (AP) and cyclotetramethylenetetranitramine (HMX) [or cyclotrimethylenetrinitramine (RDX)]. The two most common binder systems consist of either an inert binder system based on a polybutadiene polymer, typically hydroxy-terminated polybutadiene polymer (HTPB), with various plasticizers, additives, and cross-linking agent, or an active binder system based on energetic components such as nitroglycerin (NG) and nitrocellulose (NC) or with a polyester or polyether polymer (PE). In general, comparing the combustion characteristics of the monopropellants with the characteristics that occur when the monopropellants are combined with other ingredients to form propellants can lead to an understanding of the physical mechanism that are involved. The monopropellant burning rate of AP, HMX, and a typical NG/NC

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*Alumina is the combustion product of aluminum

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Actualy the approach followed is a simplified Eulerian approach, adopted to further reduce computational time; the method is described in the following sections
double-base propellant are similar. However, when a fuel and an oxidizer are mixed together, a diffusion flame usually results. In AP/HTPB this diffusion flame has a huge impact on the combustion process as a function of pressure.

Understanding of the combustion mechanism that determine solid propellant burning rates have evolved over the past 30 years. In the 1960s, emphasis was determining the critical mechanism that controlled the burning rate and most attention was given to AP composite propellant. A typical example of identifying a single critical mechanism that would describe combustion behavior was the Summerfield granular diffusion flame model (GDF). That model was based on the concept that fuel and oxidizer gasify at the burning surface, leaving the surface in pocket of gases that diffuse together and react. This interpretation was too narrow in concept to describe the great variation in burning rates observed with AP propellants for varying pressure, oxidizer particle size, and loading. In general finer AP particle size causes an increase in burning rate, but at very low or high pressure this effect is diminished. Similarly, increased AP concentration tends to increase the burning rate, but this effect is also reduced at extreme pressures. The GDF model was not comprehensive enough to explain such wide range of behavior.

Hermance proposed a model of heterogeneous reaction at the burning surface between oxidizer and binder, creating an increased, reacting surface area. Although this concept resulted in a mathematical model that correctly gave the increased burning rate with decreasing particle size, some experiments failed to show the postulated undercutting of oxidizer crystals.

In the early 1970s, Beckstead et al. published their multiple-flame model (BDP). This model proposed a complex interaction between the oxidizer monopropellant flame and two different diffusion flame occurring above the oxidizer binder interface. Figure 1 from Ref. illustrate this. This physical picture was sufficiently comprehensive to be able to explain most of the observed phenomena and to create and validate simple models that have to be used in the rocket scale simulation.

B. Multiphase Features

Aluminum powder is frequently used as solid propellant ingredient to increase performance of the solid rocket motor. Aluminum has a high density, a large oxidation reaction energy (without any adverse effects on the detonation characteristics of the propellant) and its oxidation reduces the amount of $H_2O$ and $CO_2$ to better propulsion fluids as $H_2$ and $CO$. As the propellant burns, the propellant-combustion interface regresses and aluminum particles enter in the core chamber flow. A detailed summary of the history of aluminum particles originating at the propellant surface and entering in the chamber is discussed in Price and Sigman. Figure 2 shows the burning surface of two propellant with and without aluminum particles.

![Figure 2. Composite propellant without aluminum (left) and with aluminum (from Ref.4)](image)

The physics of aluminium combustion is very different from other propellant ingredients such as polymeric binder and ammonium perchlorate. Aluminum particle are less volatile so do not burn instantaneously at the propellant surface. The melting of aluminum particles at the surface can lead to the formation of agglomerates that ignite (on or after leaving the surface). The droplet combustion produces aluminum oxide ($Al_2O_3$) smoke that are carried out into the flow field. The presence of these droplets contributes to the motor performance loss because can cause a decrease in the nozzle efficiency, possible surface damages from droplet impingement, slag accumulation in submerged nozzles and can have a significance effect on combustion stability. Because of the physical properties of aluminum and its oxide, a large fraction of aluminum remains unreacted and in liquid state at the burning surface. Several liquid droplets coalesce
into large “agglomerates” (often on the order of 100 – 200 \(\mu m\)). These agglomerates leave the propellant surface and continue to burn relatively slowly due to low volatility of aluminum. The vaporized aluminum reacts with the oxidizing species in the gas phase forming \(Al_2O_3\). A part of the formed oxide is captured on the agglomerates surface and condenses to form an oxide shell. The formation of aluminum oxide shell contributes to the “slowness” of aluminum combustion. Instead it is generally accepted that the reaction rate for the remaining propellant constituents is rapid. Typical values of the mean diameter are 1.5 \(\mu m\) for the small particles (smoke) and 150 \(\mu m\) for the larger agglomerates.

The whole concentration, agglomeration, ignition, burning sequence is dependent on a whole range of propellant formulation and combustion environment variables:

- size distribution of oxidizer particles
- size distribution and amount of aluminum particles
- kind of oxidizers and binder
- presence and composition of ballistic modifiers
- fluid dynamics state of the gas in the combustion zone

A related issue is the effect of aluminum on propellant burning rate. Because the aluminum combustion usually occurs outside the normal combustion zone, it does not enhance burning rate much. However introduction of aluminum is at the expense of the oxidizer, and as a result it is difficult to determine an aluminum effect unambiguously.

The physical process by which the \(Al\) droplets form at the propellant-combustion interface and get injected into the flow are still not fully understood.\(^\text{10}\) Models for the droplets injection into the chamber have not been well quantified. Sabnis\(^\text{11}\) have proposed a simple model based on a predetermined number of “pulses” of new computational droplet at appropriate spatial locations during a certain time period. The overall mass rate of \(Al\) injection is well defined from the local burn rate of the propellant and the mass fraction of \(Al\) in the propellant. What is not well understood is the size, velocity and composition (\(Al\) vs \(Al_2O_3\)) spectra of the injected droplets. The popular approach is to use a lognormal bimodal distribution. Recently Jackson, Najjar and Buckmaster\(^\text{7}\) proposed a more realistic modification to that procedure.

1. \textit{Aluminum}

Aluminum has several peculiarities as propellant ingredient:

- It does not decompose to a vapor at the burning surface. Its boiling point is 2749 \(K\) (pressure dependent)
- The usual temperature of propellant burning surface is around 870 \(K\), 60 \(K\) below the 940 \(K\) melting point of aluminum
- The density is around 1750 \(Kg/m^3\), 1.3 times that of AP and 3 times that of typical binders.
- The particle surface are coated with an impervious refractory coating of \(Al_2O_3\) that for a 25 \(\mu m\) particle constitutes about 0.5\% of the particle mass
- At high temperature the droplets contains both aluminum and molten \(Al_2O_3\), which tend to separate into lobes of droplets because \(Al\) and \(Al_2O_3\) are insoluble
- At temperature between the aluminum and the oxide melting points, leaking of \(Al\) from the oxide coating can lead to sintering in assemblages of particles.
C. Droplet burning

The combustion of Al droplet consists of a very complex process. Empirical correlation may be used in order to predict the time required for the aluminum particles to burn, but data collected from rocket motors measurements are not available because of the inaccessibility of the motor environment. Most empirical correlation have therefore been derived from carefully controlled lab experiments.

When the single particle of aluminum ignites, the heat of reaction is so great that the aluminum boils and thus remains at about 2800 K (at 1 atm). The flame around the particle has a diameter of 2 − 4 times the diameter of the particle. In this flame zone a homogeneous reaction takes place between the aluminum and available oxidizers. Figure 3 shows a representation of the vapor-phase aluminum combustion process. In the flame zone, the oxidized products consist of Al$_2$O$_3$.

Once the ambient temperature exceeds the oxide melting point, the oxide shell around the droplet cracks and liquid Al is exposed to the gas. Aluminum vaporizes and reacts with the oxidizers (O$_2$, H$_2$O, CO$_2$) that are present. The primary product of the combustion process is aluminum oxide.

Because the oxide melting temperature, 2327 K, is higher that the melting temperature of aluminum, 933 K, the aluminum is assumed to be fully melted on ignition. The molten aluminum droplet surface burns at a temperature between the oxide melting temperature, ~2300 K, and ~2700 K, the aluminum boiling temperature. Although the global oxidation reaction of aluminum produces alumina, Al$_2$O$_3$ and many suboxides exist in the flame zone. The condensation of alumina at its estimated boiling point, ~3800 K, sets the approximate temperature of the oxide cloud because Al$_2$O$_3$(l) condenses directly from the association of the suboxides and the idealized gas Al$_2$O$_3$(g), immediately dissociates in AlO and O$_2$. The submicrometer alumina particles can radially diffuse both outward and inward, where they can accumulate in the oxide cap on the molten aluminum surface. The entire reaction is considered diffusion controlled because the species are reacting much faster than the diffusion rates at the elevated temperature.

1. Accumulation and agglomeration

When a particle of aluminum is reached by the propellant burning surface, it is usually not yet melted and is in pyrolyzing fuel environment, usually a binder melt. The particle is not immediately carried away because it is stuck in the binder melt. It is not ignited because of the fuel-rich environment and because it has a solid Al$_2$O$_3$ coating. In typical propellant aluminum particles are small compared to the oxidizer particles hence they are concentrated in pockets between oxidizer particles. Aluminum particle continues to emerge and collect on the receding surface until the environment causes ignition and/or detachment from the surface. The size distribution of the agglomerates depends on:

- features of the Al particles packing in the propellant
- surface retention characteristics of the binder
- the susceptibility of individual particle to ignition

![Figure 3. Representation of the vapor-phase aluminum combustion process](image)

![Figure 4. Schematics of the zone of propellant combustion](image)
The stoichiometry of the AP/binder system dictates that a maximum achievable content of AP be used consistent with required propellant processing and mechanical properties. A coarse AP portion is combined with finer particles to fill the spaces left between coarse particles. Such propellant are still somewhat fuel rich. When aluminum is added to the formulation, it is necessary to reduce AP content to accommodate aluminum. The Al size is typically smaller that the coarse AP particles dimension. Thus the aluminum particles are preconcentrated in pockets in the coarse AP pattern. The foregoing description is oriented around the idea that there are pockets in the AP packing pattern where aluminum particles are already preconcentrated in the mix, pockets that would be occupied by fine AP if no aluminum were used. However combination of AP and aluminum particles sizes can be chosen in which the preconcentration of aluminum in the packing array are more tenuous and may or may not lead to agglomeration, depending on proximity of ignition source.

Once a particle is free of the surface the vapors from the other pyrolyzing ingredients carry it away with the outward vapor flow. However there is evidence that emergence of the particle is complicated by surface retention forces, leading to aluminum concentration on the surface. There are several reasonable mechanisms: particle adhesion in a binder melt layer, direct adhesion (sintering) to underlying Al particles, centrifugal forces in spinning motors. The relative roles of these mechanisms probably depend on type of binder, amount of Al, Al particle characteristics, and extent of fine AP or carbon powder in the Al-binder matrix.

Aluminum is extremely reactive in oxidizing environment, but ignition is impeded by the refractory oxide shell until conditions are reached that cause the skin to break down. Temperature at the propellant surface is typically 900 \( K \), whereas the melting point of the oxide is around 2350 \( K \). Unless an individual particle emerges at a site where oxidizer vapors are present and high heat flow from a close-by hot oxidizer-binder vapor flamelet are present, the particle will not ignite. If it does ignite, its temperature will quickly become so high that residence on the surface will end. Particles that do not ignite reside on the surface and tend to be joined by underlying particles. The presence of Al pockets gives rise to large areas of relatively small amount of ignition of individual particles.

An accumulate typically originates from the preconcentration of aluminum in the pockets of the packing pattern. When such sites emerge at the burning surface, binder provides an adhesive surface and a nonoxidizing environment. Only particle on the periphery of the pocket are exposed to oxidizing vapors and high heat flux from hot flamelets. As surface regresses the accumulate is progressively exposed and then the accumulate that has survived to this point ignites or leaves the surface. If ignition conditions are poor the outcome is a detaching accumulate, if ignition conditions are good, a detaching agglomerate.

Accumulates lead to agglomerates by a complex process involving local thermal breakdown of the protective oxide and progressive inflammation from such local sites. This ensures that the molten aluminum will coalesce into a burning droplet.

The following generalization can be asserted:

- Large agglomerates result in large residual oxide droplets
- High aluminum content in the propellant leads to large agglomeration
- Factors that increase burning rate reduce size of agglomerates
- Crossflow environment tend to decrease agglomeration
- Size distribution of other propellant ingredient has a big impact on agglomeration (coarse AP particles leave space for preconcentrated pocket of Al particles)

III. SRM Numerical Simulation Model

A. Gas Phase Equations

The evolution of mass, momentum and total energy are governed by the time-dependent compressible Euler Equations:
Supposing we have $N_{\text{species}}$ different gas species, the mass fraction of $s^{th}$ specie is defined as:

$$Y_s = \frac{\rho_s}{\rho}$$  \hspace{1cm} (1)

where $\rho_s$ is the density of $s^{th}$ specie and $\rho = \sum_{s=1}^{N_{\text{species}}} \rho_s$, the equations of mass fractions conservation are:

$$\frac{\partial (r \rho Y_s)}{\partial t} + \frac{\partial (r \rho Y_s u)}{\partial x} + \frac{\partial (r \rho Y_s u_r)}{\partial r} + \frac{\partial (\rho Y_s u_\theta)}{\partial \theta} = 0$$  \hspace{1cm} (2)

Assuming that the species are calorically perfect gases in thermal equilibrium with specific heat constants $C_v$ and $C_p$, we obtain

$$C_p = \sum_{s=1}^{N_{\text{species}}} Y_s C_{ps} \quad C_v = \sum_{s=1}^{N_{\text{species}}} Y_s C_{vs}$$

where $C_{ps}$ and $C_{vs}$ are the specific heats of $s^{th}$ specie. As a common practice we integrate directly the conservation of specific densities $\rho_s$ and then with the values of $\rho_s$ it is possible to calculate the mass fractions and the specific heats.

The Euler system for a mixture of gas become:

$$\frac{\partial (r \rho u)}{\partial x} + \frac{\partial (r \rho u_r)}{\partial r} + \frac{\partial (r \rho u_\theta)}{\partial \theta} = 0 \quad s = 1, 2, ..., N_{\text{species}}$$

$$\frac{\partial (r \rho u_r)}{\partial x} + \frac{\partial (r \rho u_r u)}{\partial r} + \frac{\partial (r \rho u_r u_r)}{\partial r} + \frac{\partial (\rho u_r u_\theta)}{\partial \theta} = p + u_r^2$$  \hspace{1cm} (3)

$$\frac{\partial (r \rho u_\theta)}{\partial x} + \frac{\partial (r \rho u_\theta u)}{\partial r} + \frac{\partial (r \rho u_\theta u_r)}{\partial r} + \frac{\partial (\rho u_\theta u_\theta)}{\partial \theta} = -\rho u_{r \theta}$$

And in compact form:

$$U = \begin{bmatrix} \rho_1 \\ \vdots \\ \rho_{N_{\text{species}}} \\ \rho u \\ \rho u_r \\ \rho u_\theta \\ \rho E \end{bmatrix}$$  \hspace{1cm} (4)

$$F_x = \begin{bmatrix} \rho_1 u \\ \vdots \\ \rho_{N_{\text{species}}} u \\ \rho u^2 + p \\ \rho u u_r \\ \rho u u_\theta \\ \rho u H \end{bmatrix} \quad F_r = \begin{bmatrix} \rho_1 u_r \\ \vdots \\ \rho_{N_{\text{species}}} u_r \\ \rho u_r u_r \\ \rho u_r^2 + p \\ \rho u_r u_\theta \\ \rho u_r H \end{bmatrix} \quad F_\theta = \begin{bmatrix} \rho_1 u_\theta \\ \vdots \\ \rho_{N_{\text{species}}} u_\theta \\ \rho u_\theta u_r \\ \rho u_\theta^2 + p \\ \rho u_\theta u_\theta \\ \rho u_\theta H \end{bmatrix}$$  \hspace{1cm} (5)

$$S = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \rho u_{r \theta}^2 + p \\ -\rho u_{r \theta} \rho u_\theta \\ 0 \end{bmatrix}$$  \hspace{1cm} (6)
and again the compact Euler system is:

$$\frac{\partial (rU)}{\partial t} + \frac{\partial (rF_x)}{\partial x} + \frac{\partial (rF_r)}{\partial r} + \frac{\partial F_\theta}{\partial \theta} = S$$  \hspace{1cm} (7)

To take into account the effect of aluminum particles on the flow behaviour it is necessary to introduce in the equations a set of source terms. In particular in the system 7 an additional vector of source terms is added:

$$\frac{\partial (rU)}{\partial t} + \frac{\partial (rF_x)}{\partial x} + \frac{\partial (rF_r)}{\partial r} + \frac{\partial F_\theta}{\partial \theta} = S + rS^p$$ \hspace{1cm} (8)

where

$$S^p = \begin{bmatrix} S_{\rho_1} \\ \vdots \\ S_{\rho_{N_{species}}} \\ S_{\rho u_1} \\ S_{\rho u_2} \\ S_{\rho u_3} \\ S_e \end{bmatrix}$$ \hspace{1cm} (9)

All the solid phase effects are taken into account in the gas phase evolution introducing the following source terms in the gas equations:

$$S_{\rho} = S^a_{\rho} + S^p_{\rho}$$

$$S_{\rho u,i} = S^a_{\rho u,i} + S^p_{\rho u,i}$$

$$S_e = S^a_e + S^p_e$$

The source terms represent both the effect of the droplet described with the Lagrangian approach and the smoke described with the Eulerian formulation.

### B. Grain Combustion Model

The combustion surface is considered infinitely thin and the combustion reaction fast, so the combustion surface is a boundary condition for the equations that describe the flow in the rocket; simple models are necessary to evaluate the fluxes at the surface and the theories described in the previous section can be used to create and validate these models.

Most of the simple models are based on a simple relation between the burning rate and the pressure; the formula is obtained with a correlation of experimental data, that are typically available performing static firing tests of small motors (BARIA).

$$r_b = Ap^n$$ \hspace{1cm} (10)

where $r_b$ is the burn rate of the propellant. The coefficients $A$ and $n$ depend on the propellant characteristics.

Using that formula the fluxes can be evaluated at the burning surface; typically the mass is injected with a small velocity (often simply equal to 0), and the temperature of the injected gas is fixed to the flame temperature of the reaction, evaluated with an equilibrium calculus. If the simulation of the internal flow is performed taking into account the effect of the solid particles (aluminum) in the core flow, the equilibrium calculus to evaluate the temperature of the injected gas is performed considering that in the reaction the aluminum must not be included because its behavior is explicitly treated in the core flow simulation.
C. Equations for the Multiphase Phenomena

1. Lagrangian Evolution of Aluminum Droplet

The most important parameter for the transport of the single droplet is the particle Reynolds number:

\[ Re_p = \rho \parallel u(x_p) - v_p \parallel \frac{d_p}{\mu} \]  

(11)

Originally Basset\(^1\) and later Boussinesq\(^3\) and Oseen\(^9\) examined the motion of a sphere settling out under gravity in a fluid that was otherwise at rest. The disturbance flow produced by the motion of the sphere was assumed to be at sufficient low Reynolds number that the fluid force on the sphere could be calculated from the results of unsteady Stokes flow.

Considering the Lagrangian approach to model particles behaviour the temporal evolution of the characteristics of particles are described by a set of ordinary differential equations:

\[ \frac{dx_p}{dt} = v_p \]  

(12)

\[ \frac{dv_p}{dt} = \frac{1}{\tau_p} [u(x_p) - v_p] \]  

(13)

\[ \frac{dT_p}{dt} = \frac{1}{\tau_{p,\theta}} [T(x_p) - T_p] \]  

(14)

where \( \tau_p = \frac{\rho_p d_p^2}{18 \mu f(Re_p)} \)  

(15)

\[ \tau_{p,\theta} = \frac{c_{p,p} \rho_p d_p^2}{12 k f_\theta(Re_p)} \]  

(16)

Because the Reynolds number of the droplet is expected to be larger than unity a standard correction to the Stokes drag is used.

\[ f(Re_p) = 1 + 0.15 Re_p^{0.687} \]  

(17)

\[ f_\theta(Re_p) = 1 + 0.3 Re_p^{4/5} Pr^{1/4} \]  

(18)

The droplet are generally multicomponent (Al\(^1\) and Al\(_2\)O\(_3\) cup) so the composition of the droplet is tracked:

\[ \frac{dm_{Al}}{dt} = -\dot{m}_{bu} \]  

(19)

\[ \frac{dm_{Al_2O_3}}{dt} = \dot{m}_{dep} \]  

(20)

where the right-hand sides represent respectively the burning and evaporation of aluminum and a model of the behaviour of the oxide cup.

So the density and the diameter of the droplet can be evaluated:

\[ \rho_p = (m_{Al} + m_{Al_2O_3}) \left( \frac{m_{Al}}{\rho_{Al}} + \frac{m_{Al_2O_3}}{\rho_{Al_2O_3}} \right)^{-1} \]  

(21)

\[ d_p = \left( \frac{6}{\pi} \left( \frac{m_{Al}}{\rho_{Al}} + \frac{m_{Al_2O_3}}{\rho_{Al_2O_3}} \right) \right)^{1/3} \]  

(22)
2. **Eulerian Evolution of Smoke Particles**

The smoke particles of alumina are very small and their number is enormous so they can’t be treated in a Lagrangian manner; the best approach could be an Eulerian modelling. In the limit of very fine particle, one can use the modified density approach to evolve the smoke concentration field. In this case, one assumes that the smoke advects with the surrounding gas velocity; thus only the smoke concentration field needs to be evolved as a scalar field. This approach has the great advantage that one avoids solving additional momentum equations for the smoke phase. However this approach ignores inertial effects such as accumulation and wall impactions. A fully Eulerian approach to the smoke field avoid this drawback by computing the smoke phase velocity separately from the gas velocity. However additional momentum equations must be solved (in 3D, the additional equation are 3 for every different size of smoke particle). A possible way to take into account all the phenomena and preserve an acceptable computational efficiency is to evolve only the smoke concentration and use an expansion of the gas velocity to calculate the solid phase velocity via algebraic relations. So the only differential equation to be solved is the convective equation of the concentration of the smoke particle:

\[
\frac{\partial C_s}{\partial t} + \frac{\partial}{\partial x_j} (C_s w_j) = S_m
\]

(23)

where \( w \) is the velocity of the smoke, expressed as an explicit expansion in term of the local gas velocity:

\[
w = u - \tau_s \frac{D}{D_t} u
\]

(24)

and the time scale of the smoke particle is

\[
\tau_s = \frac{\rho_s d^2_s}{18 \mu}
\]

(25)

where \( C_s \) is the field of the concentration of the smoke and \( S_m \) is a term that take into account the coupling between the big particle, modelled with the Lagrangian approach, and the small particle of alumina smoke.

3. **Aluminum Combustion Model**

On the scale of the rocket the combustion process can only be treated in a Lagrangian point of view, because the necessary level of detail to resolve the chemical kinetics of the reactions involved in the combustion of the droplet is not reached using the coarse grids that permit to perform simulations of the whole rocket. In particular the combustion model acts as source terms in the equations of the gas phase, taking into account the generation of mass of gas and energy during the reactions. The burn rate of the droplet is assumed to follow a power-law relation dependent on droplet state and gas pressure and temperature in the droplet location. Widener and Beckstead\(^ {13} \) proposed the following correction of the Hermsen model:\(^ 6 \)

\[
\dot{m}_{bu} = c \rho_{Al} T^{1.57} (x_p) p^{0.2} (x_p) \chi_{eff} D_{rel} d_p^{1.1} \psi_{Al}
\]

(26)

where the constant \( c \) has the value \( 2.885 \cdot 10^{-13} \) (in SI units).

\( \chi_{eff} \) is the effective oxidizer mass fraction that is defined in term of the single components:

\[
\chi_{eff} = \chi_{O_2} + 0.58 \chi_{H_2} + 0.22 \chi_{CO_2}
\]

(27)

and \( D_{rel} = 1 + 2.7 \chi_{H_2} \).

The term \( \psi_{Al} \) takes into account the fact that part of the droplet is in the form of the oxide cap; the burning rate is scaled with the volume fraction of aluminum:

\[
\psi_{Al} = \frac{\phi_{Al} \rho_{Al2O_3}}{\phi_{Al} \rho_{Al2O_3} + (1 - \phi_{Al}) \rho_{Al}}
\]

(28)

where

\[
\phi_{Al} = \frac{m_{Al}}{m_{Al} + m_{Al2O_3}}
\]

(29)
The energy balance of the combustion process is:

$$h = -h_{ev} + h_{reac} + h_{cond} + h_{solid}$$  \(30\)

where:

- $h_{ev}$ is the heat of evaporation from $Al(l)$ to $Al(g)$
- $h_{reac}$ the heat of reaction from $Al(g)$ to $Al_2O_3(g)$
- $h_{cond}$ the heat of condensation from $Al_2O_3(g)$ to $Al_2O_3(l)$
- $h_{solid}$ the heat of solidification from $Al_2O_3(l)$ to $Al_2O_3(s)$

If the local temperature exceed the boiling temperature of $Al_2O_3(g)$ ($T_{b,Al_2O_3}$) the condensation process can’t occur, so the different eventuality must be considered. The aluminum oxide, product of the reaction, can be in gas or in solid phase (so it must be considered as a component of the gas mixture and as smoke).

The reaction can be symbolically represented as:

$$2Al(l) + 3O(g) \rightarrow \alpha Al_2O_3(s) + (1 - \alpha)Al_2O_3(g) \quad 31$$

where $\alpha$ is the fraction of aluminum oxide that condenses and solidifies as smoke particles. This fraction depend on the local temperature; if $T > T_{b,Al_2O_3}$ then $\alpha = 0$, because all the oxide remain in gas phase. When $T \ll T_{b,Al_2O_3}$ then $\alpha = 1$, all the oxide solidifies in oxide smoke particles. When $T$ is just less then $T_{b,Al_2O_3}$ $\alpha$ must be evaluated to reach the local temperature to the value of $T_{b,Al_2O_3}$.

In the absence of this regulation procedure an excessive amount of energy could be provided to the gas mixture with possible non physical temperature peaks.

4. Model for the oxide cap growth

The oxide cap grows because the particle collides with the oxide smoke that is in the chamber. The collision is regulated by the relative velocity and local concentration of smoke. So the deposition rate can be expressed proportionally to the volume swept by the particle and the local concentration $C_s$:

$$\dot{m}_{dep} = \pi \frac{d_p^2}{4} \| \mathbf{u}(x_p) - \mathbf{v}_p \| C_s \eta_{c}$$  \(32\)

The term $\eta_{c}$ is a correction that could take into account the fact that because of the local hydrodynamics not all the smoke particle will end up colliding and agglomerating on the particle. For lack of good understanding of the complex phenomenon in the literature it will be assumed simply $\eta_{c} = 0.25$.

5. Coupling between Gas and Solid Phase

The source terms in the gas phase equations are evaluated using the following formulas, typical expressions widely used in literature (Refs.\textsuperscript{118}). Considering the effect of the single $i^{th}$, for the mass equation:

$$S_{p,i} = L\dot{m}_{bu}(1 - M_R) \quad 33$$

where $L$ is the ratio of real droplet to the computational one. For computational efficiency is not possible to follow the dynamics of every droplet, so every computational droplet is a cluster of real droplet and so its effect is multiplied for that ratio. $M_R = M_{Al_2O_3}/2M_{Al}$ corresponds to the molecular weight ratio.

$$S_{pu,i} = LF_{p,i} + L\dot{m}_{bu}v_{p,i} + S_{p,i} \cdot u(x_{p,i}) \quad 34$$

where

$$F_{p,i} = -\left(\frac{\pi}{6}\right)\frac{d^3_{p,i}}{p_{i}^{\rho_{i}}/\tau_{p,i}}(v_{p,i} - u(x_{p,i})) \quad 35$$

Finally for the energy source term:

$$S_{e,i} = S_{pu,i} \cdot u(x_{p,i}) + L\dot{m}_{bu}h_b \quad 36$$

where
\[ h_b = \alpha h + (1 - \alpha)(-h_{ev} + h_{reac}) \]  

(37)

To have the source terms for the gas phase equations the contribution of the single particle are summed for all the particle in the computational cell.

6. Coupling between Big Particle and Alumina Smoke

The Lagrangian treatment of the big particle must be coupled with the Eulerian smoke; when it burns, every doplet act as a source on the smoke field and is a sink through the fact that during the motion of the particle the smoke can settle on the particle.

\[ S_{m,l}^p = \dot{L}m_{bu}M_R - \dot{L}n_{dep} \]  

(38)

7. Particle injection

An important aspect in the Lagrangian representation of particles is an appropriate description of the injection process of particles from the grain. Typically, in the literature, the injection process is imposed to be at a fixed rate both in space and time. The experiments show that the complex phenomena that occur on the burning surface, characterized by the interaction of pyrolysis and burning of perclorate ammonium and HTPB, melting and agglomeration of aluminum particles, produce an injection process that is random in space and time.

From measured data in experiments, it is possible to obtain an indication of the probability density function that describe the dimension of the particles that leave the propellant surface; given that PDF a collection of particle is generated and depending on the burning rate of the propellant the particles are injected randomly in space. In particular the mass of aluminum that must be injected during a certain time is calculated, then during that interval the mass is injected with the desired PDF of dimension and randomly in space and time.

The typical probability density function that can be found in the literature is a Logarithmic normal distribution:

\[ Pr(d) = \left( \frac{1}{\sqrt{2\pi}\sigma d} \right) \exp \left\{ -\frac{1}{2\sigma^2} \left[ \ln \left( \frac{d}{d_{med}} \right) \right]^2 \right\} \]  

(39)

where \( d_{med} \) is the mean diameter and \( \sigma \) is the standard deviation.

Figure 5 contains the imposed Lognormal probability density function and an analysis of the dimension of the particles effectively injected in the field during the simulation.

IV. Numerical Simulation Results: Cylindrical Port Area Rocket

The calculation were initiated by specifying the mass flux at the burning surface and imposing the flame temperature to the injected gas. A simple geometry were chosen to simply analyze the effects of the different physical phenomena and the performance of the mathematical methods. In fig. 6 is reported the geometry used (a simple cylindrical port rocket with a convergent-diverging nozzle). For all the lateral walls of the cylindrical zone the boundary condition is related to the pressure dependent combustion of the grain.
Several simulations have been performed and in the following a resume of the obtained results will be presented. First of all, the simulation of the cylindrical rocket have been performed without taking into account the distributed combustion of aluminum droplets. At the grain surface the fluxes are assigned considering all the amount of the burned propellant in gas phase; no solid particle are injected. The flame temperature is set to the value that is obtained considering the total burning of aluminum at the propellant surface. In particular this temperature is around 3530 K.

Then simulations taking into account the particle have been performed; the mass flux at the boundary is recalculated considering the fraction of mass that is injected in the form of solid particle. The flame temperature to calculate the energy flux has been set to a lower value, evaluated without adding the contribute due to the enthalpy of reaction of aluminum combustion. This temperature is around 2850 K. Comparing the fields obtained in the two different cases it is possible to analyse the effect of distributed aluminum burning in the chamber.

An analysis of the effect of initial dimension of the particles is also described. Simulations with different value for the mean of the lognormal distribution of the injected particles have been performed and compared.

A simulation without the multiphase effect have been performed. In that situation the fluid dynamics variable have very small variation inside the motor chamber; it will be shown in the following section that this fact in absolutely not true if the combustion of aluminum particle is considered in detail and the correct burning time of droplet is considered.

A simulation has been performed including the aluminum particles; in particular the solid droplets have been modelled with the Lagrangian approach. From the grain surface the particle are injected depending on the burn rate of the propellant, evaluated knowing the local pressure.

The simulation has been performed considering the motion of the particles due to the drag forcing term; the effect of the particles on the flow has been taken into account considering the exchange of mass, momentum and energy.

The figure 7 shows the instantaneous positions of the droplets in the chamber; the color of the particle represents their diameter. It can be observed the evolution of the diameter, that is related to the aluminum combustion. From the grain surface to the core of the chamber the diameter of the particle decreases and a long time (so a long space) is necessary for the burning of the major part of the particle so the temperature field is characterized by large variation in the chamber (effect of aluminum burning). Moreover the particles that are injected in the zone of the grain near the nozzle can be quite big and with a large amount of residual not burned aluminum when they enter in the nozzle. This fact can significantly decrease the combustion efficiency of the propellant and of the motor. The fact that a certain number of not completely burned particles can be found near the nozzle can be an effect also on the nozzle throat ablation and erosion. Regarding the ablation, if the burning of aluminum occurs very close to the throat, the local composition can be quite different to the one in the case in which the particles burn on the surface of the propellant; with regard to the erosion, the dimension of particle can have an important role when they impact on the nozzle. So it is important to analyse which can be the characteristics of the particle.
particles that enter the nozzle.

In the two figures 8(a) and 8(b) a comparison of the two cases, with and without distributed aluminum burning, is shown; in particular isosurfaces of temperature have been drawn. The temperature fields in the two cases are very different, the maximum value of the temperature in the case of distributed combustion is reached only near the axis of the chamber and in some zones near the nozzle entry. The pressure of the chamber depends on the total temperature before the nozzle, so the fact that a certain amount of energy is not released by the particles because the combustion of aluminum is not complete, can affect the pressure in the motor.

The effects of distributed combustion on the Mach number field are shown in the figure 8(b). It can be observed that there are only small differences between the two cases analysed.

![Figure 8. Effect of distributed combustion](image)

(a) Temperature isosurfaces. Comparison of fields with (top) and without (bottom) distributed combustion

(b) Mach number isosurfaces. Comparison of fields with (top) and without (bottom) distributed combustion

A. Effect of the injection dimensions of the particles

The effects of the initial dimensions of the particle on the flow field features have been analysed. In particular three different mean value for the initial particle dimension have been considered. The typical value for the mean $d_{med}$ that can be found in the literature is around 45 micrometer; the analysis has been performed comparing the results for that value with the results obtained with a smaller and a larger value (20 and 100 micrometer). The effects of the different initial particles dimensions can be easily observed in the temperature field. Figures 10(a), 10(b), 10(c), 10(d) show the temperature fields for the case without particles burning and with particles with the three different injection sizes; for the smallest sizes case the temperature reaches the values that can be observed without taking into account the distributed combustion; no distributed combustion means that all the reaction enthalpy is provided at the propellant burning surface, instead of adding it along the chamber in function of the combustion rate of the aluminum contained in the particles. In the limit of very small particles the combustion of aluminum

For the initial particle distribution the lognormal distribution has been considered:

$$Pr(d) = \left( \frac{1}{\sqrt{2\pi}\sigma_d} \right) exp \left\{ -\frac{1}{2\sigma^2} \left[ \ln \left( \frac{d}{d_{med}} \right)^2 \right] \right\}$$

Figure 9. Probability density functions of the initial particles dimension for the three different cases analysed

\[\text{Figure 9. Probability density functions of the initial particles dimension for the three different cases analysed}\]
finishes in a quite thin layer close to the propellant surface, so a very small amount of unburned aluminum exits the motor. All the available energy contained in the aluminum is added to the chamber flow and the temperature reach his maximum values. For very big particles a certain amount of aluminum doesn’t burn in the chamber so the temperature is, in average, lower.

The temperature level can have an effect on the pressure of the motor; table A contains the pressure level that has been obtained at the head end region of the motor in the four cases analysed. For very small particle the effect on the pressure of distributed combustion is very small, but for very big particles the effect is important.

Table 1. Head end pressure at steady state obtained from simulations with different injected particles dimensions

<table>
<thead>
<tr>
<th>Particle diameter $d_{med}$</th>
<th>Time averaged head end pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td>No distributed combustion</td>
<td>70 Bar</td>
</tr>
<tr>
<td>20 µ</td>
<td>69.4 Bar</td>
</tr>
<tr>
<td>45 µ</td>
<td>68.9 Bar</td>
</tr>
<tr>
<td>100 µ</td>
<td>65 Bar</td>
</tr>
</tbody>
</table>

Figure 10. Temperature isosurfaces
V. Numerical Simulation Results: ZEFIRO 9 A SRM

The new ZEFIRO 9 A motor is an improved version of the ZEFIRO 9 motor, a solid rocket motor designed, developed and tested by AVIO Group SPA. The ZEFIRO 9 motor should have been the third stage of the VEGA launcher, but its new improved version will be used.

Figure 11 contains a schematics of the motor geometry in its initial configuration. The motor is characterized by a cylindrical zone with a small radius followed by an enlargement of the port area (conical zone) and a finocyl zone characterized by a star-shaped geometry with 11 fins. It is a quite short motor, with a small initial free volume compared with the initial burning surface, a large submerged region. The shape in the finocyl region is characterized by a periodicity due to the fact that all the fins can be considered equivalent; to reduce the computational time of the simulation it has been decided to reduce the computational domain to a 22nd of the entire motor on the azimuthal coordinate. So half of a fins has been considered and for the boundaries in the azimuthal direction a slip wall condition has been imposed. The simulation domain is the red zone in fig. 11.

Figs 12(a), 12(b), 12(c) and 12(d) contain some of the fundamental fluid dynamics variables obtained from the simulation. The pressure in the motor is quite constant, as typically is supposed when simple ballistic models are adopted. The pressure is higher in the submerged zone and decrease approaching the nozzle for the injection of mass from the grain.

The temperature is very inhomogeneous in the flow field, phenomenon related to the distributed combustion. The Mach number is quite low, it is at most around $0.15 - 0.2$. In this kind of motors, with a very large submerged zone, connected to the motor core with narrow channels, the Mach number in the zone between submerged and cylinder regions can be very high. The velocity magnitude is shown in figures 12(d) and 14(a); in particular fig 14(a) contains an enlargement of the star-shaped zone. The values of the velocity are quite high only in the core of the flow that is approaching the nozzle entrance.

Particles instantaneous position is shown in figures 13(a) and 13(b); the colour of the particles indicate the diameter. It can be noticed that the residual diameter of particles entering the nozzle is quite large; the particles contain both alumina (combustion product of aluminum combustion) and an amount of unburned aluminum. Anyway it is clear that particle combustion is distributed in the motor.

Figure 14(b) contains some streamtrace in the star-shaped zone; it can be observed that the flow is regular in this zone, without large scale vortices.

Figure 15 contains the probability density function of the dimensions of particles at the nozzle entrance, compared with the statistics of the injected particles. At the nozzle entrance the average dimension of the particles is quite large; these particle are constituted by alumina and a certain amount of unburned aluminum, so there is a certain amount of unused fuel energy. The characteristic particles dimensions distribution at the nozzle entrance has also a primary influence on the nozzle throat evolution, because the impacts of particles on the nozzle thermal protections can cause a significant erosion; this fact has a particular importance in that class of motors, because analysing data from static firing tests it has been observed a critical level of throat area enlargement, with large effects on motor performances.
Figure 12. Zefiro 9A SRM, fluid dynamics fields in the combustion chamber

(a) Isosurfaces of pressure
(b) Isosurfaces of temperature
(c) Isosurfaces of Mach number
(d) Isosurfaces of velocity magnitude

Figure 13. Zefiro 9A SRM, instantaneous particles position. The colours indicate the particles diameter

(a) Whole motor
(b) Star-shaped region
Figure 14. Zefiro 9A SRM, instantaneous particles position. The colours indicate the particles diameter

Figure 15. Probability density function of particles diameter of injected particles (green dashed line) and at the nozzle entrance (red solid line)
VI. Conclusion

A description of the flow field in the combustion chamber of solid rocket motors has been presented; particular care has been devoted to the multiphase features of the flow, using detailed models to describe phenomena related to motion and burning of aluminum particles. The effects of aluminum distributed combustion have been underlined and the relations between initial particles size, a characteristic of the propellant that is typically hard to specify, and flows features and performances have been analysed; in particular several simulations with different initial size distribution have been performed to calculate the amount of unburned aluminum and the dimension distribution at the nozzle entrance, features that have a primary importance to characterize throat erosion and ablation.

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References
