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NUMERICAL SIMULATION OF MICROSCALE COMBUSTION OF SOLID COMPOSITE ROCKET PROPELLANTS

Dr. Philip PIETREK† and Michael MOROFF**
** Fraunhofer Institute for Chemical Technology ICT*
Pfinztal, Germany
philip.pietrek@ict.fraunhofer.de, michael.moroff@ict.fraunhofer.de
† Corresponding Author

Abstract

The investigation of the pressure-dependent burning rate of solid rocket propellants is a critical aspect of their characterization and has significant implications for their practical applications. The combustion behavior of the propellant is influenced by environmental conditions such as pressure and temperature, which can be directly correlated with experimental results. Additionally, the composition of the propellant plays a vital role in defining its combustion characteristics. The primary components of a composite propellant include an oxidizer and a binder, along with additives such as curing agents, plasticizers, and bonding agents. These additives enhance the processability of the propellant while exerting minimal influence on the combustion process. The combination of these components results in a heterogeneous propellant, uniquely defined by the mass ratios and the shape and size of the oxidizer.

In this study, we employ a Coupled-Level-Set-and-Volume-Of-Fluid-Approach implemented in OpenFOAM to investigate the microscopic combustion of a composite propellant, specifically an AP/HTPB formulation. We examine the effects of mass fraction, size, and shape of the oxidizer particles on combustion behavior. An extended unit cell is defined within a two-dimensional model to describe the combustion process and its products, as well as the burning surface. This model facilitates the comparison of different compositions and their resultant average burning rates under varying pressure conditions, thereby enhancing our understanding of how the shape of the particles affect the burning behavior of the propellant. These findings contribute to the advancement of predictable, tailored designs for novel solid rocket propellants.

1. Introduction

The combustion behavior of solid rocket propellants influences the characteristics of solid rocket motors. Solid rocket propellants contain multiple components that contribute to the combustion process. This includes the main components: the oxidizer, binder, and other additives (catalysts, curing agents, etc.), which make the resulting composite propellant stable, homogeneous, processable, and applicable [5, 9, 15, 16]. The interactions between these chemical compounds are diverse and are still not completely understood. Since the compounds in these propellants are not miscible with each other, the resulting propellant is heterogeneous and not ideal. This heterogeneity also affects combustion, as various chemical and physical processes contribute to the actual macroscopic behavior.

This paper provides an overview of our ongoing work in the numerical investigation of the combustion behavior of heterogeneous solid propellants at a microscopic level. This includes the depiction of the evolution of the burning surface in combination with the chemical gas phase reactions and dynamics in a computational domain near the burning surface. The findings of this paper were produced using a Coupled-Level-Set-and-Volume-of-Fluid (CLSVOF) approach in OpenFOAM [12], which was expanded to include chemical reactions in the gas phase. In light of the development of new environmentally friendly propellants [2, 17], we focused on ammonium dinitramide (ADN) based propellants and the influence of their particle size on the gas phase reaction, the resulting flame region, and the pressure near the burning surface.

2. Numerical Setup

The CLSMVOF solver has been developed to depict the behavior of multi-material solid rocket motors on a system scale and was previously presented [12]. This solver is utilized in this paper to calculate the evolution of the burning surface and the released products at the burning surface. The chemical reactions of combustion at the microscopic scale of the propellant cannot be neglected; the model must address the transition from the condensed phase to the gas phase, as well as the possible reactions at the surface.

2.1. CLSMVOF-Solver

In this section, we present a concise overview of the fundamental equations governing the CLSMVOF solver. Comprehensive details regarding the solver can be found in [12]. The solver integrates the implicit Level-Set Method (LSM) to accurately represent the burning surface, alongside the signed distance function ϕ (SDF) and the Volume-of-Fluid (VOF) approach to differentiate between the solid and gas phases. The LSM facilitates a grid-independent representation and evolution of the burning surface.

The integration of the LSM within the VOF framework is accomplished by coupling the volume fraction α with the surface within a designated computational cell. This coupling leads to modified conservation equations, which are essential for accurately modeling the dynamics of the combustion process.

Mass conservation equations:

$$\frac{\delta \rho_\alpha}{\delta t} + \nabla(\rho_\alpha \vec{u})_f = \dot{q}_{mass} \tag{1}$$

Momentum conservation equation:

$$\frac{\delta \rho_\alpha \vec{u}}{\delta t} + \nabla\big((\rho_\alpha \vec{u})_f \cdot \vec{u}\big) + \nabla\left(\rho_\alpha \nu_{eff} \nabla(\vec{u})\right) + \nabla\left(\rho_\alpha \nu_{eff} \vec{u}\right) = -\alpha_\phi \nabla p + \dot{q}_{impulse} \tag{2}$$

Energy equation:

$$\frac{\delta \rho_\alpha h}{\delta t} + \nabla\big((\rho_\alpha \vec{u})_f \cdot h\big) + \frac{\delta \alpha \rho K}{\delta t} + \nabla\left((\rho_\alpha \vec{u})_f \cdot K\right) + \alpha \frac{\delta p}{\delta t} = \dot{q}_{energy} \tag{3}$$

With the kinetic energy $K = u^2 / 2$

$$\frac{\delta Y_i}{\delta t} + \nabla\big((\rho_\alpha \vec{u})_f \cdot Y_i\big) + \frac{\delta \alpha \rho K}{\delta t} + \nabla\left((\rho_\alpha \vec{u})_f \cdot K\right) + \alpha \frac{\delta p}{\delta t} = \dot{q}_{energy} \tag{4}$$

Pressure equation:

$$\nabla \frac{\rho_\alpha}{A} \alpha_\phi \nabla p = \frac{\delta p}{\delta t} + \nabla \frac{\rho \mathrm{H}}{A} - \dot{q}_{mass} \tag{5}$$

A and H are gained by writing the momentum conservation equation as:

$$\mathrm{M}(\vec{u}) = -\alpha_\phi \nabla p \tag{6}$$

The matrix $\mathrm{M}(\vec{u})$ can be written as: $\mathrm{M}(\vec{u}) = \mathrm{A}\vec{u} - \mathrm{H}$. A contains the diagonal and H the off-diagonal contributions. It is mentioned, that at this point of the development the energy equation of the solid phase is not yet implemented. Hence the temperature within the solid propellant cannot be investigated. In the current stage of development, the solver does not account the interaction of the phases in terms of energy, hence temperature conduction within the solid propellant is not depicted.

2.1. Numerical model

As mentioned earlier, the numerical model must accurately depict various processes occurring at microscopic length and time scales. This necessitates a small, representative volume of the composite propellant and its components. In this study, we investigate a composite propellant composed of ammonium dinitramide (ADN) and glycidylazid polymer (GAP).

The combustion characteristics of ADN and GAP differ significantly; thus, the reactions occurring in the gas phase are crucial for understanding the pressure, temperature, and concentration dynamics near the burning surface. In the following sections, we describe the phase transitions between the solid and gas phases, including the intermediate products, and outline the gas phase reactions considered in this work.

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ADN is an energetic material with high reactivity due to its substantial oxygen content. Its combustion has been extensively studied in the literature [2, 4, 7, 8, 11, 13, 14]. We employed the reaction mechanism proposed by Kore [8], which identifies key reactions in ADN combustion, including the initial decomposition of ADN into $HN(NO_2)_2$ and NH_3 at the surface, followed by the two-step decomposition of $HN(NO_2)_2$ into OH and N_2O. For this analysis, we assumed that the solid ADN produces $HN(NO_2)_2$ and NH_3 at a surface temperature of 810 K [13] across all examined pressures.

In contrast, the combustion of GAP has not been as thoroughly investigated as that of ADN, primarily due to its limited oxygen content, which complicates the analysis of burning rates, surface temperatures, and gas composition. Additionally, variations in purity and the number of terminal -OH groups in GAP can influence its decomposition behavior. Arisawa and Brill conducted studies on various GAP polymers using flash pyrolysis [1], measuring decomposition products that include N_2, CH_4, HCN, CO, C_2H_4, NH_3, CH_2O, CH_2CO, and H_2O. The surface temperature of GAP during decomposition was assumed to be 700 K, as reported by Kubota and Sonobe [10].

Table 1 summarizes the properties and input parameters used in the simulations. We assumed that the burning rate for both components follow Vieille's law:

$$r = A_0 \left(\frac{p}{p_{ref}} \right)^n \tag{7}$$

To account for the gas phase reactions and their interactions with the combustion products of ADN, we also considered the Gri-Mech mechanism [6].

Table 1 Material properties of ADN and GAP

	ADN	**GAP**
Density [kg/m3]	1411	1300
Burning rate (Vielle’s Law):		
A_0 [mm/s]	16.6	0.76
Pressure exponent n [-]	0.18	0.706
T_s [K]	810 [8]	700K [10]
Composition [w%]	$HN(NO_2)_2$: 86.3; NH_3: 13.7 [8]	N_2: 27.6, CH_4: 15.7, HCN: 18, CO: 13.7, C_2H_4: 13.7, NH_3: 7.5, CH_2O: 3.8, H_2O: 0.2 [1]

In the investigated cases, we fixed the mass fraction of ammonium dinitramide (ADN) at 70 w% using spherical ADN particles with a size of 50 µm [3]. A typical setup for the simulation is illustrated in Figure 1. The investigation was conducted in a two-dimensional perspective, which implies that the spherical particles are represented as cylinders. We adjusted the diameter of the particles to ensure consistency with the mass fraction of the propellant, resulting in a reduction in particle size. The computational domain measures 2000 µm in length and 200 µm in height, with the initial interface positioned in the middle of the domain. The outlet boundary is set to atmospheric pressure, and the simulations were conducted at pressures of 40, 60, and 80 bar.

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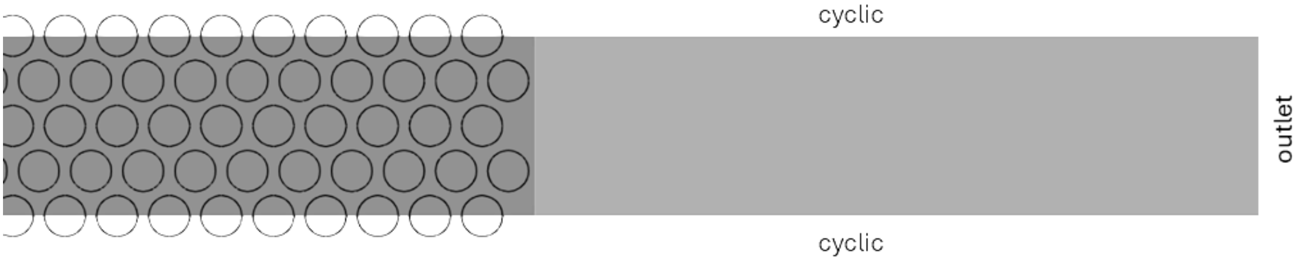

Figure 1 Numerical Setup of a representative part of a composite propellant. Light grey: gas region. Darker grey: solid propellant. Black circles: spherical oxidizer particles.

3. Results and discussion

A critical characteristic of solid composite propellants is the pressure-dependent average burning rate (as described in Equation 7), along with the flame temperature and product composition. These parameters were the focus of our simulations. However, the simulations also provide additional insights into the processes occurring near the combustion surface, as well as how surface morphology and chemical reactions influence flame structure and reaction zones. Figure 2 presents a snapshot of the simulation, illustrating the temperature distribution and the concentrations of key species, including CO_2, O_2, and H_2O. As anticipated, ammonium dinitramide (ADN) generates O_2 and H_2O, which are subsequently distributed and react within the diffusion flame formed by the ADN and gas-absorbing particle (GAP) products. In this diffusion flame, CO_2 is produced while O_2 is consumed. The temperature profile indicates the exothermic nature of the diffusion flame, with this region being the hottest. However, the observed temperature exceeding 3200 K appears to be uncharacteristically high, which contradicts findings in the existing literature (T_f = 2100 K) [8]. Since the heat conductivity between the phases is not accounted in the simulations, this could be one reason of the high temperatures. This observation is further corroborated by the concentration profile at the center of the ADN particle, as illustrated in Figure 3.

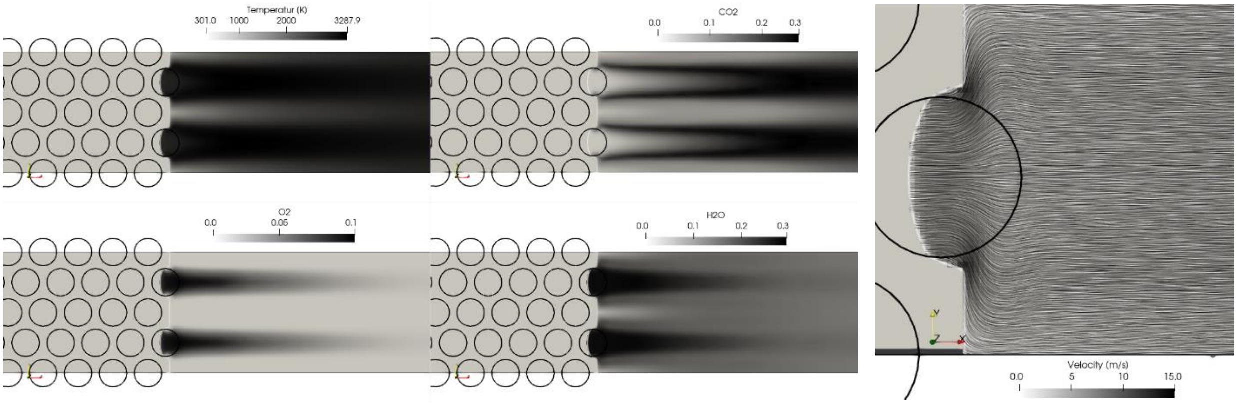

Figure 2 Distribution of temperature (top left), CO2 (top middle), O2 (down left) and H2O (down middle). Right: Velocity distribution with streamlines. ADN particles are indicated as black circles and the burning surface as a white line.

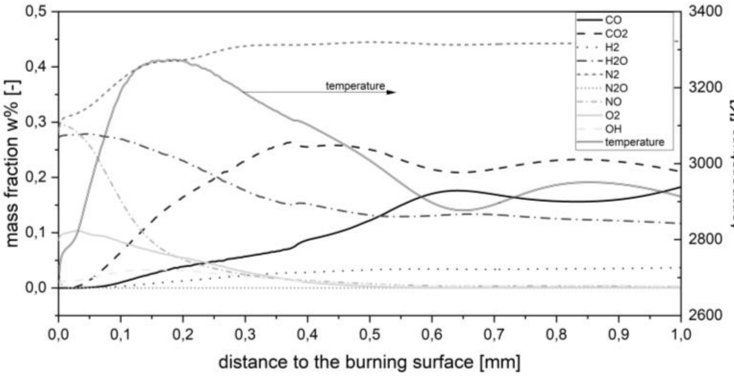

Figure 3 Concentration and temperature above the burning surface (located in the middle of an ADN particle) at the same time as Figure 4.

In addition to analyzing the gas dynamics, including reactions and concentration, an examination of the average combustion characteristics of the propellant was conducted. The results for the pressures investigated (40, 60, and 80 bar) are presented in Figure 4. The left panel of Figure 4 illustrates the burning rate derive by the averaged position of the combustion surface. As anticipated, the burning rate varies due to the heterogeneous nature of the propellant. The average burning rates at the various pressures are provided in Table 2. A significant standard deviation is expected, as there are instances where only GAP is present at the surface, leading to a reduced burning rate.

Table 2 Average burning rates of a composite solid propellant with the particle size of 50 µm at 40, 60 and 80 bar.

	40 bar	**60 bar**	**80 bar**
Average burning rate [mm/s]	20.5±5.2	23.2±4.9	25.5±4.3

The simulations yield valuable insights regarding the local pressure at the combustion surface. The average and maximum pressures recorded during the simulations are illustrated in Figure 4 (right). It is anticipated that the maximum pressure occurs at the combustion surface. Notably, the increase in maximum pressure is more pronounced at lower ambient pressures compared to higher pressures. Various factors influence the pressure dynamics, including combustion rates and amount production gas, which result in elevated pressure. Furthermore, the chemical reactions taking place near the surface induce volumetric expansion, which accelerates the gases toward the atmosphere and increase the local pressure. Additionally, the morphology of the combustion surface plays a significant role in pressure development. Specifically, when the generated gases are introduced perpendicularly to the surface within the gas volume, concave geometries can lead to increased pressure. This phenomenon is evidenced by the maximum pressures depicted in Figure 4 (right).

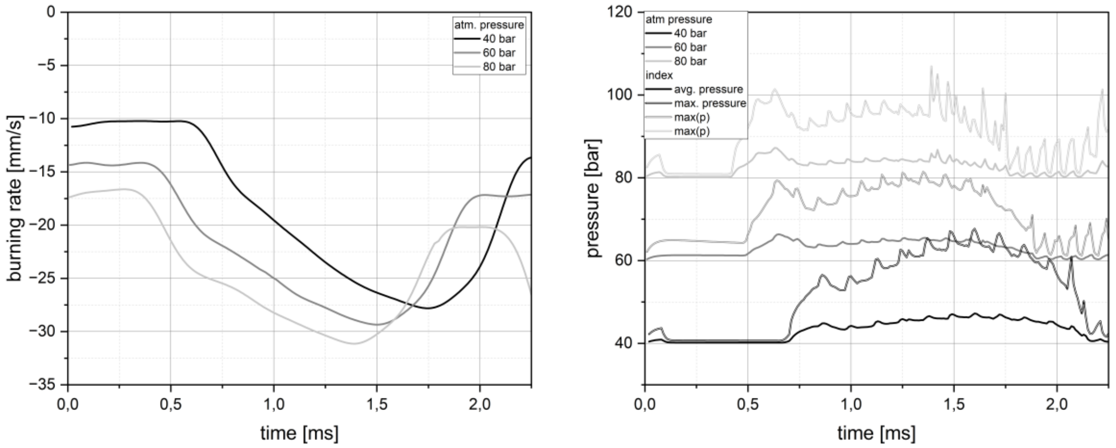

Figure 4 Left: Burning rates calculated from the average position of the burning surface. Right: Average and maximum pressure. The results are color-coded according to their atmospheric pressure for 40, 60 and 80 bar.

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4. Conclusion

In this work we present our recent advancements in the numerical simulation of microscale combustion of solid composite rocket propellants. We employed an in-house developed CLSMVOF solver to examine processes at the microscale, including surface regression, dynamic behavior, and chemical reactions within the gas phase. The study focused on an ammonium dinitramide (ADN)-based composite propellant with a particle size of 50 µm, evaluated at three different pressures. The simulations yielded essential combustion parameters, including the average burning rate, flame temperatures, and product composition. The results successfully illustrated all investigated processes and provided valuable insights into the flame structure of composite solid propellants. Furthermore, novel observations regarding the interaction between the flame structure and the combustion surface were made. However, discrepancies with existing literature were noted, which will be a focal point for future research. Moving forward, we aim to integrate the energy equation for the solid phase to account for heat loss due to conductivity, as well as address radiative effects in the gas phase. In summary, our methodology demonstrates promising results for further exploration of various composite solid propellants, facilitating a deeper understanding of their behavior and contributing to the development of new, optimized, and tailored propellants.

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