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Overview of the Current State of Physical-Mathematical Modelling of Solid Fuel Combustion Processes

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ABSTRACT

This study provides a comprehensive introduction to the combustion of solid propellants. We conduct a thorough review of existing physical-mathematical models related to solid fuel combustion processes. Additionally, we explore the heat propagation within the solid phase, examine the physical chemical processes in the k–phase, and investigate the fundamental solution of the heat conduction equation in a multiphase (k–phase) medium. The heat conduction equation plays a crucial role in governing the temperature distribution within a given material, and a profound understanding of its fundamental solution is essential for various engineering and scientific applications. In this research, we expand our analysis to a multiphase scenario, considering different phases with distinct thermal properties coexisting.

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The List of Abbreviations, Symbols and Notations

Abbreviations: SRE – Solid Rocket Engine, IBC – Intra-Ballistic Characteristics, k–phase, Condensed Phase (Solid Fuel).

Key notations: p – pressure, u – burning rate, t – time, x – distance in the coordinate system related to the combustion surface, T – temperature, f – temperature gradient, α – thermal conductivity coefficient, λ – thermal conductivity coefficient, c – heat capacity, ρ – density, E – activation energy, H – pre-exponential factor, R – universal gas constant, Q – heat of reaction, A – concentration, Z – molar fraction, ε – heat quantity.

Symbols: o – steady-state conditions, s – combustion surface, s_o – steady-state conditions at the combustion surface, g –gas phase, N – initial conditions.

Introduction

Modeling solid fuel combustion processes is a complex task that involves the interaction of various physical and chemical phenomena. Researchers use mathematical models to understand and predict the behavior of solid fuel combustion in different systems, such as industrial boilers, power plants, and furnaces. Here are some key aspects of the modeling process

- **Mass and Energy Balances:** Mathematical models often begin with mass and energy balances to describe the overall combustion process. These balances account for the fuel, oxidizer, and products of combustion, as well as heat transfer mechanisms
- **Chemical Reactions:** Solid fuel combustion involves complex chemical reactions. Models include reaction kinetics to describe how fuel particles decompose, release volatile gases, and react with oxygen
- Detailed reaction mechanisms for different types of solid fuels are essential for accurate modelling
- **Heat and Mass Transfer:** Heat and mass transfer between the solid fuel, gas phase, and surrounding surfaces play a crucial role. Models consider convective and radiative heat transfer, as well as mass transfer of gases within the combustion chamber
- **Particle Dynamics:** In solid fuel combustion, the behavior of individual fuel particles is important. Models may account for particle size distribution, shape, and trajectory
- **Particle dynamics influence combustion efficiency and pollutant formation:** pollutant formation modeling includes the prediction of pollutant formation, such as NOx, SOx, and particulate matter. Understanding the factors influencing pollutant formation helps in designing cleaner and more efficient combustion processes
- **Computational Fluid Dynamics (CFD):** CFD techniques are commonly used for simulating the fluid flow, temperature distribution, and species concentrations within combustion chambers. Advanced CFD models provide insights into the three-dimensional and transient nature of combustion processes

- **Validation and Experimental Data:** models need to be validated against experimental data to ensure their accuracy and reliability. Continuous improvement and refinement of models are ongoing processes based on new experimental findings. The field of solid fuel combustion modeling is dynamic, with ongoing research focused on improving the accuracy and applicability of models to various practical scenarios. Researchers are also exploring sustainable and cleaner combustion technologies, which may involve alternative solid fuels and novel combustion processes.

Success in space research and practical applications hinges largely on advancements in rocket engine development, with a particular emphasis on the successful execution and theoretical understanding of solid fuel combustion processes. This involves refining methods for calculating engine characteristics. Currently, a substantial body of scientific work is dedicated to theoretically describing non-stationary processes occurring during the combustion of solid fuel in rocket engine chambers.

The most extensively studied aspect of non-stationary solid fuel combustion theory involves the investigation of vibrational processes and the rigorous analysis of combustion harshness. Esteemed researchers such as Zeldovich, Novozhilov, Pershnikov, and others, both from Russia and abroad, have delved into this critical area. However, the existing theoretical framework falls short in addressing the imperative for the development of solid fuel rocket engines, primarily due to the lack of practical methods for calculating non-stationary combustion rates.

This limitation arises from the inherent complexity of combustion processes, especially when catalysts are introduced. Catalysts significantly alter the relationship between solid fuel combustion rates and pressure, adding an extra layer of intricacy. Furthermore, the underutilization of findings from related scientific fields compounds this challenge. For instance, the theory of chain-branching reactions, which has proven successful in liquid fuel combustion theory and was developed by Academician Semenov, has not been effectively incorporated into solid fuel combustion theory.

The combustion velocity of solid fuel within the Intraballistic Characteristic (IBC) of a solid fuel rocket motor (RMSF) is determined by the law of burning rate, which establishes its dependence on pressure and initial temperature. This law is derived through experimental burning of fuel samples under stationary conditions. Stationary burning rate laws are deemed appropriate when the crater time of the process is sufficiently large, approximately around 10^{-1} s. However, under non-stationary conditions, such as rapid pressure changes in RMSF occurring within a crater time of approximately 10^{-3} s or less, the burning rate varies. In such instances, the burning rate cannot instantly conform to the value calculated by stationary laws. It requires some time during which complex processes occur, leading to a restructuring of the fuel burning front. These processes occur during the transition to the operating mode, pressure drop at the end of operation, and throughout the entire operational cycle of certain types of RMSF.

It is essential to consider the non-stationary nature of the burning rate of solid fuel when calculating intra-ballistic characteristics. This necessity arises from the prevalent use of rocket engines operating in “impulse” mode, where the engine functions for a duration of $5-50$ milliseconds. Such engines find application in guidance systems for aircraft, ejector seats, and launch engines for diverse purposes.

The theory of Solid Fuel Combustion (SFC) is a standalone and well-developed branch of science. However, the internal ballistic calculations of specific Solid Rocket Motors (SRM), including those with “impulse” characteristics, are currently based solely on dependencies of burning rate on pressure obtained experimentally under stationary conditions.

The current situation arises from a twofold challenge. Firstly, there is uncertainty among developers of solid propellant rocket missiles regarding the necessity of incorporating the non-stationary component of burning rate. Secondly, there is a lack of specific methods designed to calculate non-stationary burning rates, especially tailored for their integration into the system of equations governing the internal ballistics of solid rocket motors.

The objective of this work is to bridge the existing gap between academic theories of combustion and the practical development of specific Rocket Motor Solid Propellants (RMSP). The ultimate goal is to devise a calculation method for the internal ballistics of solid rocket motors that explicitly takes into account the non-stationarity of the burning rate.

Analyzing the outcomes of computations employing this approach in contrast to experimental data will provide insights into the criteria that, once satisfied, permit the exclusion of non-stationarity considerations in calculating internal ballistics. The lack of established calculation dependencies has hitherto hindered the formulation of such criteria.

By the present time, a significant number of scientific works by researchers like I.B. Zeldovich, Novozhilov, Prisnyakov, both from Russia and abroad, have been published, focusing on the theoretical description of the processes occurring during the combustion of solid propellants in the combustion chambers of rocket engines. However, the results of the existing theory of non-stationary combustion have not found widespread application in the development of solid rocket motors (SRMs).

For the calculation of the internal ballistics characteristics (IBC) of SRMs, burning rate laws are used. These laws describe the burning rate of solid propellants as functions of pressure and initial temperature, which have been experimentally obtained under stationary conditions. This approach is entirely justified when the characteristic time of pressure change $\left(\frac{p}{dp/dt}\right)$ is sufficiently large, on the order of 10^{-1} s or more.

However, the real combustion rate may differ from the value calculated using stationary laws if the pressure change process occurs rapidly, i.e., within a characteristic time on the order of 10^{-3} s or less. Such a process occurs during startup, pressure drop at the end of operation, and throughout the operational cycle of some types of SRMs, especially in the case of impulse SRMs with a firing duration of 5-50 milliseconds used in Crew Escape Systems (CES) for aircraft and spacecraft. When CES is engaged, an error of more than 10 percent in the calculations of acceleration or its rate of increase is unacceptable, and, consequently, an error of more than 5 percent in calculating the burning rate of SRPs is also unacceptable.

Calculations for the IBC of such engines, especially during startup, must take into account all possible factors that can influence the internal chamber characteristics and, therefore, the magnitude of acceleration and its rate of increase, to which the human body is particularly sensitive. In this case, for a more accurate IBC calculation, the stationary burning rate law must be replaced with a relationship that links the non-stationary burning rate and non-stationary pressure.

In the existing theory of non-stationary SRP combustion, there was no question of developing specific methods for calculating the dependence of the non-stationary burning rate on pressure. When theoretically studying the combustion processes of solid propellants, either a time interval is considered in which the influence of initial conditions on the course of the process is negligible, or the problem statement is so general that obtaining a specific solution is not feasible.

In the existing theory of non-stationary combustion of solid fuel, the question of developing specific methods for expenditure dependency of non-stationary burning rate on pressure throughout the entire process was not addressed. The theoretical investigation considered the non-stationarity over a time interval where the influence of initial conditions on the process was negligible. Consequently, the curve problem with initial conditions for the heat conduction equation describing heat propagation in the k–phase was not posed in the study of this issue. Thus, creating a theoretical foundation for studying the non-stationary burning rate of solid fuel, grounded on accumulated results in this field and suitable for a more accurate calculation of the internal ballistics characteristics of solid rocket propellants, appears highly relevant.

Thus, the creation of a theoretical foundation for studying the non-stationary burning rate of solid rocket propellants, which, on one hand, would be based on the accumulated results in this field and, on the other hand, would be suitable for a more precise calculation of the IBC of SRMs, appears highly relevant.

The main goal of this work is to develop the theoretical foundations of a physico-mathematical model for the non-stationary combustion of solid fuel, considering typical time processes on the order of 10^{-3} s. This involves accounting for the influence of initial conditions on the course of the non-stationary combustion process, deriving equations to calculate non-stationary combustion velocities from a closed system of equations, and understanding methods to calculate the dependence of solid fuel combustion velocity on pressure in non-stationary conditions.

The work uses methods of mathematical analysis to derive forms for calculating non-stationary combustion, velocity from fundamental laws of classical physics and gas combustion. Specifically, the main equation of Zeldovich-Novozhilov combustion theory is used, relating the propagation of heat and gas condensation in accordance with the law of energy conservation. The relationship between the equation's links combustion velocity and the temperature of the burning surface. The validity and universality of this equation have been proven in works with Zenin and Novozhilov. Additionally, the theory of branched chain reactions in gas combustion is attributed to the Semenov. The gas dynamics equation in molecular genetic theory is compared with experimental data, and in some cases, experimental dependencies are obtained, such as the theoretical derivation of the stepwise law for stationary combustion velocity.

The mathematical model for solid fuel combustion, accounting for the influence of non-stationary combustion velocity on pulse solid rocket engines, has been proposed and justified. This model differs fundamentally from existing ones by incorporating non-stationarity in the initial period, correctly formulating the problem with an initial condition for a simultaneous non-stationary heat conduction equation with a moving boundary containing the burning velocity as an unknown variable. The model is characterized by the axiomatic construction of a rigorous analytical form for all dependencies from the initial positions, allowing for variable assumptions in the theory of non-stationary solid fuel combustion. Current theories of non-stationary combustion are applied for the first time to solid fuel combustion theory, utilizing results from a developed theory of branched chain chemical reactions. This theory derives a formula for calculating perpetual heat flow from the gas phase to condensation. The derived formula for calculating perpetual flow from the gas phase to condensation is obtained.

The results of this work will be utilized in the State Defense Order (SDO) for the development of calculation methods for the internal ballistics of impulse engines used in catapult seats for automatic crew ejection systems in aircraft, helicopters, and spacecraft.

Physical-Chemical Processes in the *k*–phase

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In [1], it is assumed that the surface combustion temperature is a universal constant for a given type of fuel, independent of pressure and initial temperature. This assumption is equivalent to assuming the absence of chemical reactions in the *k*–phase, reducing the gas formation process during combustion to purely physical processes such as evaporation, distillation, and dispersion. Such an assumption allowed Ya. B. Zeldovich to develop the first physico-mathematical model of combustion. Subsequent studies [10], [19], [21], and others have shown that heat release in the *k*–phase is a significant factor, the consideration of which is necessary for an adequate description of the combustion process.

For example, in [19], the assumption is put forward that the burning rate of solid fuel is completely and unequivocally determined by the surface combustion temperature, i.e., that the combustion rate is governed by an Arrhenius-type equation

$$u = H \exp\left[-\ \frac{E_s}{RT_s}\right] \qquad (2)$$

Thanks to the experimental work of A.A. Zenin and other researchers [10], [11], [12], [24], [25], the validity of this equation has been proven. It has been demonstrated that the surface combustion temperature depends on the initial temperature of the fuel and the pressure, explaining the experimental dependencies of the combustion rate on these factors. The measurements covered a range of initial fuel temperatures from minus 200 to $140^\circ C$ and a pressure range from vacuum to 150 atm.

The dependence $u = u(T_s)$ is presented based on the data from works [11], [12], [21], indicating that, within the experimental errors, it is possible to speak of a unified (universal for all pressure and initial temperature values) dependence of the combustion rate on the surface temperature. This dependence can be described by equation (3). Additionally, in work [21], it is shown that the Jacobian

$$\frac{\partial(u,T_s)}{\partial(p,T_N)} = \left(\frac{\partial u}{\partial p}\right)_{T_N}\left(\frac{\partial T_s}{\partial T_N}\right)_p - \left(\frac{\partial u}{\partial T_N}\right)_p\left(\frac{\partial T_s}{\partial p}\right)_N$$

At the experimentally obtained values of its partial derivatives, the Jacobian is very close to zero. As is known, this indicates the presence of a functional dependence between the quantities $u(p, T_N)$ and $T_s(p, T_N)$, i.e., a connection $u = u(T_s)$. The dependence of the form (3) can be justified by the fact that the chemical decomposition reactions are zero-order reactions, the rate of which does not depend on pressure. Thus, numerous theoretical and experimental studies have shown that the combustion rate can be represented by an equation similar to the Arrhenius equation—an unique dependence of the combustion rate on the surface temperature of the burning fuel. The activation energy E_s entering this equation is apparently the cumulative activation energy of all physico-chemical processes—processes of vaporization, distillation, and decomposition of substances that make up the fuel.

Physico-Chemical Processes in the Gas Phase

The theory of solid fuel combustion was developed by Zeldovich in the assumption that the temperature of the surface in *k*—phase is constantly elevated. In the work [1] the assumption is made that the surface combustion temperature is universal and constant for a given type of fuel, regardless of pressure and ambient temperature.

This assumption is equivalent to assuming the absence of chemical reactions in the condensed phase, reducing the process of gas formation during combustion to an oxygen-dependent process of vaporization and dispersion. This assumption allowed Zeldovich to develop the first physico-mathematical model of combustion. However, subsequent research, for example, in [16], [26] and [41], definitively indicates the presence of chemical reactions in the condensed phase, showing that the heat release in the condensed phase is a crucial factor necessary for an adequate description of the combustion process.

In [19] the assumption was first introduced that the combustion rate of solid fuel is entirely and unambiguously determined by the surface combustion temperature. In other words, the burning rate follows a dependence similar to the Arrhenius-type relationship.

Physico-chemical processes in the gas phase play a pivotal role in understanding and manipulating the behavior of matter under various conditions. This interdisciplinary field encompasses the study of physical and chemical transformations that occur in gaseous substances, shedding light on fundamental principles governing molecular interactions and reactivity. This comprehensive exploration delves into the intricacies of gas-phase phenomena, examining their significance across diverse scientific disciplines

- **Gas Phase Kinetics:** gas phase kinetics elucidates the rates at which chemical reactions occur in the gaseous state. The study involves understanding reaction mechanisms, collision theory, and factors influencing reaction rates, such as temperature, pressure, and concentration. This knowledge is indispensable for designing efficient industrial processes, optimizing reaction conditions, and predicting reaction outcomes
- **Thermodynamics of Gases:** the thermodynamics of gases explores the relationship between heat, energy, and the spontaneous direction of gas-phase reactions. Key concepts, such as enthalpy, entropy, and Gibbs free energy, provide insights into the feasibility and spontaneity of reactions. The understanding of thermodynamics in the gas phase is crucial for assessing the energy changes associated with chemical processes
- **Gas–Phase Spectroscopy:** gas–phase spectroscopy involves the study of the interaction between electromagnetic radiation and gaseous molecules. Techniques like infrared spectroscopy and mass spectrometry enable researchers to analyze molecular structures, study vibrational and rotational transitions, and investigate electronic states. This information is vital for identifying and characterizing gas-phase species in various applications, from environmental monitoring to astrophysics
- **Molecular Dynamics in Gases:** molecular dynamics simulations offer a powerful tool for exploring the behavior of gas-phase molecules at the molecular level. This computational approach allows researchers to simulate the

trajectories and interactions of individual particles over time, providing valuable insights into gas-phase phenomena that are challenging to observe experimentally. Applications range from understanding gas-phase reactions to predicting the properties of novel materials

- **Atmospheric Chemistry:** the study of physico–chemical processes in the gas phase is particularly relevant in understanding atmospheric chemistry. Reactions occurring in the Earth's atmosphere, such as the formation of ozone and reactions leading to air pollution, have profound implications for climate, air quality, and human health. Investigating these processes is crucial for developing strategies to mitigate environmental challenges.

Physico–chemical processes in the gas phase represent a rich and diverse area of scientific inquiry, with implications spanning chemistry, physics, environmental science, and beyond. As researchers continue to unravel the complexities of gas-phase phenomena, their findings contribute not only to fundamental scientific knowledge but also to the development of innovative technologies and solutions addressing contemporary challenges.

Experimental studies show that the combustion rate of solid fuel is significantly influenced by the pressure in the combustion chambers, highlighting the substantial role of the gas phase in the combustion process. To rigorously mathematically represent the combustion process in the gas phase, it is necessary to develop an adequate physical model that takes into account the real physics of chemical processes occurring.

For a rigorous mathematical representation of combustion processes in the gas phase, it is necessary to create an adequate physical model that considers the real physicochemical processes occurring near the burning surface.

Yakov B. and Zeldovich's combustion model [1], [2], methods based on flame propagation theory in gases were used to calculate the combustion rate. The equations of mass conservation, conservation of the number of each type of atom, conservation of energy (enthalpy constancy), and diffusion equations were considered. These works introduced the spatial division of the combustion zone into zones, and the processes were examined separately for each zone. Assuming equal diffusion coefficients and thermal conductivity, the similarity of concentration and temperature fields throughout the gas phase was established. The integration of equations for the "dark" zone was performed, neglecting heat release, and the equations for the reaction zone were integrated with the assumption of temperature constancy.

Effectively, the concept of the "flame front" was justified in [1], the representation of an infinitely thin reaction zone where heat release occurs.

The processes occurring in the gas phase during the combustion of solid fuel are most comprehensively described in [19], [22]. However, the fundamental equations derived in these works do not differ significantly from the equations in [1].

To calculate the combustion rate of solid fuel, a crucial aspect is the description of heat transfer from the gas phase to the condensed phase. To determine the heat flux entering the condensed phase, second-order boundary conditions [1], [19], or third-order boundary conditions [16], [18], with a pressuredependent heat exchange coefficient, are used. Models that account for thermal radiation from the flame are also available [26]. In [19], [22], it is assumed that the heat flux into the condensed phase may depend on the combustion rate (either directly proportional or proportional to the magnitude. It can be noted that there is the greatest divergence of opinions among various researchers on this issue. In fact, each study uses its own model for calculating the heat flux.

It is necessary to emphasize that in all physical-mathematical models of processes occurring in the gas phase, specific chemical reactions constituting the combustion process itself are not considered. However, despite the complexity of the processes occurring in the flame, which strongly depend on the type of fuel used, some general regularities can be established. For example, it can be asserted that in the decomposition products of the condensed phase of all solid fuels, free hydrogen and free oxygen are necessarily present. The mechanism of hydrogen combustion is well-known thanks to the works of Academician N.N. Semenov [27], [28], who was awarded the Nobel Prize. According to these works, hydrogen combustion occurs as a result of branched chain reactions involving free radicals (active centers). The derivations of equations and dependencies required for the construction of a physical-mathematical model for nonstationary solid fuel combustion. It presents the main equation for calculating non-stationary combustion velocity as the solution to a system of equations, which includes the heat conduction equation in the k– phase with boundary and initial conditions, the heat balance equation at the combustion surface, and an additional boundary condition. The project formulates the initial and boundary value problem for the heat conduction equation in a one-dimensional formulation, introducing a coordinate system connected to the combustion surface. The key equations and conditions are derived in this part, and the project elaborates on the physical meaning and significance of these equations.

Overall, the work delves into the complex process of non-stationary solid fuel combustion, providing a theoretical foundation for understanding the interplay of factors such as temperature, pressure, and reaction kinetics in the combustion process. The use of mathematical models and physical principles enables the analysis and prediction of non-stationary combustion behavior.

0. $H_2 + O_2 \rightleftarrows 2OH$ – chain initiation reaction;
1. $H_2 + OH \rightleftarrows H_2O + H$ – chain propagation reaction;
2. $O_2 + H \rightleftarrows OH + O$
3. $H_2 + \mathrm{O} \rightleftarrows OH + H$ – chain branching reactions;
4. $H + H + M \rightleftarrows H_2 + M$
5. $H + OH + M \rightleftarrows H_2\mathrm{O} + M$ – chain breakdown in the volume;
6. H + parede – chain de breakdown in the surface. (3)

Here, *M* stands for any molecule or radical. Reaction 6 refers to chain breaking when a free radical collides with the surface of a condensed particle present in the fuel decomposition products. According to the theory of branched chain reactions developed by the academic Semyonov, after reaching the necessary conditions due to the mixture of hydrogen and oxygen that promote chain reactions, the ignition of hydrogen combustion occurs with a delay. This delay, or the induction period, is caused by the need to accumulate a sufficient quantity of free radicals responsible for the continuation and branching of the chains. For the same reason, there is a delay in ignition in the case of solid fuel combustion mixtures (CSM) during the passage of the "dark zone" through the gases [27], [28], are

1. The presence of a clearly defined pressure threshold below which the reaction practically does not occur, and above which the reaction proceeds at a high speed. The pressure values considered in the theory of combustion are deliberately

higher than the limiting ones.

2. The presence of an induction period, i.e., the time from the moment the initial fuel mixture reaches the conditions necessary for spontaneous ignition (specific values of temperature and pressure) until the onset of the rapid reaction. The magnitude of the induction period is inversely proportional to the rate of the chain-branching reaction (reaction 2 of mechanism 3). In other words, the induction period is the time required to accumulate a sufficient number of active centers for the oxidation reaction of hydrogen to proceed.
3. A very high reaction rate after the completion of the induction period - the reaction is perceived as an explosion or flash.

In the works of N.N. Semenov, theoretical dependencies for the rate of branching chain reactions have been obtained. These dependencies do not involve the concepts of "activation energy" and "reaction order", i.e., branching chain reactions are not described by Arrhenius-type equations. A theoretical dependence for the induction period was also derived, which was subsequently experimentally verified [31], [32] and applied to the combustion of hydrocarbons [33]. It is worth noting that the formula for calculating the induction period was known earlier [34], but only in the works of N.N. Semenov and his students did it receive sufficient theoretical and experimental justification. Subsequently, the concept of the induction period has been used in the theory of liquid fuel combustion [35], while in the theory of solid fuel combustion, this concept has not been utilized up to the present.

It is necessary to note that the approximate formula for calculating induction periods was known before. However, it was only in the work of Semenov and his students that it received theoretical and experimental justification. Subsequently, the concept of the induction period was used in the theory of combustion of liquid fuels [33]. In the theory of solid fuel combustion, this concept was not utilized. In this study, the results of the theory of exploratory chain chemical reactions are adopted as the theoretical basis for calculating the heat flux from the gas phase to the k–phase.

Methods for Calculating the Burning Rate of Solid Propellant

The task of calculating the combustion speed of solid fuel was first addressed in the article of Zeldovich [21]. Methods based on flame propagation theory in gases were used to compute the steady-state combustion speed. This involved considering mass conservation equations, where ug is the flame propagation speed in the gas phase, equations for conserving the number of atoms of each species, energy conservation equations, enthalpy constancy, and diffusion equations. Assuming equal diffusion coefficients and temperature conductivity in established similarity fields of concentration and temperature throughout the gas phase, integration of equations was performed for the "dark zone", anticipating heat release.

Calculating the burning rate of solid propellant is a crucial aspect of designing solid rocket motors and propellant-driven rockets. The burning rate refers to the speed at which the solid propellant burns over time. This measure is essential for understanding engine performance and ensuring safe and efficient operation. There are various approaches to calculating the burning rate of solid propellant, and they can be categorized into analytical, empirical, and numerical methods. Analytical methods BATES–GRUNEISEN Law is based on the Bates-Gruneisen law, which relates the burning rate to gas pressure and propellant density. Internal ballistics Mmdels utilizes mass and energy conservation equations to describe the burning of solid propellant inside the motor. Includes considerations for motor geometry, propellant characteristics, and thermal effects. Empirical Methods proposed by Crawford, it relates the burning rate to gas pressure. Correlation methods from experimental data relies on experimental data, such as laboratory burning tests. Uses statistical techniques to correlate the data and derive empirical equations for the burning rate. Computational Fluid Dynamics (CFD) modelling uses computational simulations to model fluid dynamics inside the motor. Considers the interaction between gas and solid, including factors like heat transfer and changes in surface area. Finite element models divide the motor into finite elements to analyse the mechanical and thermal behaviour of solid propellant during burning. May include thermo-structural coupling to capture thermo-mechanical interactions. Key Considerations: propellant properties, understanding propellant properties such as chemical composition, grain size, and additives is crucial for accurate modelling. Environmental Conditions like temperature and atmospheric pressure influence the burning rate and should be considered in calculations. Experimental validation results from analytical and numerical methods should be validated through practical experiments to ensure accuracy and reliability. The development and application of these methods require advanced knowledge in thermodynamics, fluid mechanics, and computational modelling, reflecting the multidisciplinary nature of solid propellant rocket motor design.

In the works [1], [2], the calculation of the steady-state burning rate of solid fuel was carried out using the mass conservation equation $\rho u = \rho_g u_g$ where u_g - the flame propagation velocity in the gas phase. Another method for calculating the steady-state burning rate, also proposed by Ya.B. Zeldovich [1], [2], involves the use of the heat balance equation in the *k*–phase, which is expressed as: $\lambda f_o = \rho c u_o (T_{so} - T_N)$. In this case, to calculate u_o, it is necessary to know the analytical expressions for T_{so} and f_o. In works [1], [2], it was assumed that T_{so} = const, and the heat balance equation was considered valid even for non-stationary combustion regimes.

The calculations for the steady combustion velocity are reduced to solving the heat balance equation in the *k*–phase. To solve this equation, one needs to know the dependence of the steady combustion velocity on pressure and initial temperature, obtained either from experiments or the theory of steady combustion. This approach to calculating the steady combustion velocity is justified because the combustion rate, considered in quasisteady state conditions, behaves similarly to the steady-state conditions, with the same temperature gradient at the surface of the condensed phase. In other words, the quasi-steady combustion velocity is determined solely by the instantaneous values of pressure and temperature gradient and is currently not linked to the temperature distribution throughout the volumes of the condensed phase.

Thus, for the stationary case, the heat balance equation was considered valid, extending to the nonstationary combustion regime. Novozhilov generalized Zeldovich's theory of non-stationary combustion to the case of variable temperature of the hot surface, fundamentally preserving the main idea of accounting for the quasi-stationarity of the process and using it as a link for the stationary dependence of the combustion rate on pressure.

The approach to calculating non-stationary combustion velocity is justified by considering the combustion rate at the moment in a quasi-stationary regime, which equals the rate in a stationary regime with the same temperature gradient at the condensed phase surface. In this way, the quasi-stationary combustion velocity is solely determined by the instantaneous pressure and temperature gradient and is not currently linked to the temperature distribution throughout the condensed phase volume. Therefore, the heat balance equation valid for the stationary case is adopted for non-stationary combustion. Novozhilov extended Zeldovich's theory of non-stationary combustion to cases with changing temperatures on the burning surface. He utilized the stationary combustion law and the dependency of combustion velocity on surface temperature, coupled with vitamin equations for heat flow. Vozhilov introduced an integral equation for calculating non-stationary combustion velocity, applied to processes far from the influence of initial conditions. However, its use in developing a calculation method for non-stationary combustion velocity is significantly challenging, requiring a specific dependency for surface temperature and heat flow.

In Novozhilov's work [42], an integral equation is introduced for calculating the non-stationary combustion velocity, applied to processes occurring far from the influence of initial conditions. The use of this equation in developing methods for calculating non-stationary combustion velocity faces significant challenges, both due to its need for a specific dependency for the surface temperature of combustion and heat flux into the *k*–phase. Romanov's articles at [47]–[49] provide a calculation for non-stationary combustion velocity formulae.

In works [19], [21], [22], equations (1) and (2) were used to calculate the combustion rate in combination with various equations for heat flux. Analytical expressions for some specific cases of pressure variation over time were first obtained in work [19]. However, the practical use of these expressions, even for specific cases, is quite limited primarily because they contain functions of a complex argument, requiring the development of sufficiently complex calculation methods. In the works of B.V. Novozhilov [21], [36], a general integral equation for calculating non-stationary combustion velocity has been derived, which needs to be complemented with specific dependencies for the surface temperature of combustion and heat flux into the combustion phase.

Let's consider various existing descriptions of the physical-mathematical aspects of the combustion process of solid fuel based on the results of theoretical and experimental studies outlined in the works of both domestic and foreign researchers. This review of works dedicated to the study of heat transfer from the gas phase to condensation reveals a significant divergence of opinions among different researchers. Each work essentially employs its own model for calculating heat flux. The fundamental principles of the theory of chain branching combustion reactions, including those introduced by Academician Semenov, are presented. Currently, these principles serve as the theoretical basis for calculating the heat flux from the gas phase to the condensed phase. The review also covers existing methods for calculating the burning rate of solid fuel, demonstrating that these methods may only apply to specific cases of pressure variation over time or possess such a general nature that additional research is required for their application in specific calculation.

Physico-Mathematical Model of Non-Stationary Combustion of Solid Fuel

The physico-mathematical model of non-stationary solid fuel combustion adopted in this study is based on the findings of works [19], [21], [22], with certain refinements and additions. The assumptions made during the model construction are primarily formulated in work [21]

1. The solid fuel is homogeneous and isotropic
2. The combustion surface is a plane; heat release in the combustion phase occurs only on the combustion surface
3. The flame front is a plane parallel to the combustion surface; heat release in the "dark" zone does not occur
4. Processes occurring behind the flame front (secondary reactions, combustion of dispersed particles) do not affect the combustion rate
5. The processes of solid-phase decomposition and combustion in the gas phase occur much faster than the heating of the combustion phase, i.e., the gas phase is considered non-inertial.

All processes are considered in a one-dimensional setup in a coordinate system attached to the combustion surface. The positive direction of the longitudinal coordinate is considered as the direction into the solid fuel.

The accepted assumptions have been confirmed by experimental publications [1], [19], [21], [26] and [27]. The proposed physical model allows for the mathematical formulation of the problem of nonstationary combustion velocity of solid fuel and the introduction of a linear integral equation. In such a problem formulation, the non-stationary combustion velocity depends not only on the instantaneous temperature gradient, as is the case in a quasi-stationary regime but is determined by the entire history of the combustion process. To convert the calculation of the non-stationary combustion velocity into an integral equation and find the solution to this equation, subsequent paragraphs will address the processes occurring in the gas phase and at the combustion surface. Additionally, the combustion problem will be formulated and solved with an initial condition for the non-stationary equation, involving heat and *k*–phase.

The Equation for Heat Propagation in the *k*–phase

Experimental studies of the solid fuel combustion process indicate that the expanding contribution to the non-stationarity of this process is associated with the condensed phase. In existing physics-mathematical models, the inertia in the *k*–phase is taken into account by the heat conduction equation. According to the work of researchers [16], [21] and [40], and others, the heat propagation equation in the *k*–phase has the following form:

$$\frac{\partial T}{\partial t} = æ\frac{\partial^2 T}{\partial x^2} + u(t)\frac{\partial T}{\partial x}. \qquad (4)$$

The boundary conditions for equation (4) in a general form are given by

$$T(0,t) = T_s(t), \qquad (5)$$

$$\frac{dT}{dx}(0,t) = f(t), \qquad (6)$$

$$\lim_{x\to\infty} T(x,t) = T_N, \qquad \lim_{x\to\infty} \frac{dT}{dx}(x,t) = 0. \qquad (7)$$

The initial condition in a general form is given by

$$T(x,0) = T_N + \varphi(x). \qquad (8)$$

The heat release in the *k*–phase is accounted for by the heat balance equation on the combustion surface

$$\lambda_g f_g(t) = \lambda f(t) + \rho u(t) Q_s. \qquad (9)$$

Here, f_g - the temperature gradient at the combustion surface from the gas phase side. In the cited works, particularly in works [15], [20], [29] and [40], it is demonstrated that the depth of the heated *k*–phase layer is very small, and the temperature changes in the *k*–phase reaction layer are always very small compared to the temperature difference $T_S - T_N$. This fact allows us to conclude that, with good approximation, the extent of the reaction zone can be considered equal to zero. Thus, the chemical reaction of *k*–phase decomposition practically occurs only on the combustion surface where the temperature of the *k*–phase is maximally different from T_S. To fulfill this assumption, it is necessary to assume that the function W tends to 0 at low temperatures. Despite the fact that according to Arrhenius levels, at sufficiently low T values, the function W becomes negligibly small for the precise mathematical formulation of this condition.

Specification of the Initial Condition

Clearly state the objective of the goal or purpose of defining the initial conditions. Provide a brief description of the system or process under consideration. Identify the relevant variables that define the state of the system at the initial time. Clearly list any assumptions made regarding the initial condition. Express the initial condition mathematically, using appropriate symbols and equations. For example, the initial conditions. If applicable, include any boundary conditions that might affect the initial state of the system. Identify any dependencies between variables or parameters that influence the initial condition.

To specify the initial condition (8), we assume that the beginning of the process is the moment when combustion of the fuel started at a rate of u_o and at a pressure of p_o after the igniter is triggered. Thus, we consider that in the combustion phase at the initial moment, a stationary temperature distribution (Michelson distribution) has formed, which can be obtained from (4), (5), (7) under

$\frac{\partial T}{\partial t} = 0,\ u(t) = u_o =$ const, $T_s = T_{s_o} =$ const:

$$\varphi(x) = (T_{s_o} - T_N)\exp\left(-\frac{u_o x}{\text{æ}}\right). \qquad (10)$$

Specification of the Boundary Conditions

When developing a specification for boundary conditions, it's crucial to provide clear and comprehensive information about the constraints or requirements at the system's boundaries. Here's a generic example of how you might outline the specification of boundary conditions. Clearly state the goal or purpose of defining the boundary conditions. Provide a concise description of the system or process under consideration. Identify the different boundaries or interfaces within the system. List the variables that are relevant to the boundary conditions. Express the boundary conditions mathematically, using appropriate symbols and equations. For example, boundary condition: $f(x, y, t) = g(x, y, t)$ at $x = xb$ and $y = yb$. Provide a physical interpretation of the boundary conditions. Explain what each condition represents in the context of the system. Specify the types of boundary conditions (e.g., Dirichlet, Neumann, mixed) and their significance.

We will obtain an analytical expression for $T_s(t)$ from the Arrhenius equation (2), writing it for the current moment as well as for the moment t = 0:

$$T_s(t) = T_N + (T_{s_o} - T_N)\frac{1 + \gamma\theta \ln U}{1 - \gamma \ln U}, \qquad (11)$$

or

$$T_s(t) - T_N = (T_{s_o} - T_N)V(U).$$

Here,

$$U(t) = u(t)/u_o, \qquad \gamma = RT_{s_o}/E_s,$$
$$\theta = T_N/(T_{s_o} - T_N), \quad V(U) = \frac{1 + \gamma\theta \ln U}{1 - \gamma \ln U}\ .$$

Equation (11) establishes a unique relationship between the surface temperature and the combustion rate.

We will obtain an analytical expression for $f(t)$ from the definition of the heat flux transmitted by thermal conductivity

$$\lambda_g f_g(t) = -\lambda_g [T_g(t) - T_s(t)]/h(t). \qquad (12)$$

Here, $T_g(t)$ - the temperature of the flame front, $h(t)$ - the width of the "dark" zone. In accordance with the concept of the nature of the hydrogen oxidation reaction progression outlined in *k*–phase and the dependencies obtained from experimental studies of the induction period of chain-branching reactions [32], [33], let's adopt the formula for the induction period.

$$\tau_g = \tau_* \frac{\exp\left(\frac{E_g}{RT_g}\right)}{A_1^{\nu_1} A_2^{\nu_2}}. \qquad (13)$$

Here, $\tau g(t)$ is the induction period, A_1 and A_2 are the concentrations of hydrogen and oxygen in the products of fuel gasification, τ_*, Eg, v_1, v_2 are constants specific to the particular type of fuel. Since, according to the mass conservation equation, $v_g = \rho u(t)/\rho g$ (v_g - gas outflow velocity from the burning surface), and $h(t) = v_g \tau_g$, then from (12) and (13), considering the equation of state and the equations determining the concentrations of gas mixture components before combustion, we obtain

$$\lambda_g f_g = -\lambda_g \frac{[T_g - T_s]p^{2\nu}}{Ku(t)}. \qquad (14)$$

Here, $K = \tau_* \rho (RT_g)^{2\nu} \exp\left(\frac{E_g}{RT_g}\right)/(z_1^{\nu_1} z_2^{\nu_2}), \quad 2\nu = 1 + \nu_1 + \nu_2,\ z_1,\ z_2$

- molar fractions of hydrogen and oxygen in the products of fuel gasification. The quantities K and ν depend only on the type of fuel. Writing equations (9) and (14) for the current moment in time and for the moment t = 0, after transformations, we obtain

$$f(t) = -\frac{Uu_o}{\text{æ}}(T_{s_o} - T_N)[(1 - \sigma)W(t)\frac{P^{2\nu}}{U^2} + \sigma] \qquad (15)$$

or

$$f(t) = -\frac{u_o}{\text{æ}}(T_{s_o} - T_N)UQ.$$

$$P(t) = \tfrac{p(t)}{p_o},\ Q(t, U) = (1 - \sigma)\tfrac{P^{2\nu}}{U^2}W(U) + \sigma,\ W(U) = \frac{1 - \gamma\eta \ln U}{1 - \gamma \ln U},$$
$$,\ \eta = \frac{T_g}{(T_g - T_{s_o})},\ \sigma = \frac{Q_s}{c(T_{s_o} - T_N)}.$$

Dependencies (11) and (15) specify the functions $T_s(t)$ and $f(t)$, i.e., the boundary conditions (5) and (6). Boundary conditions (7) do not require specification.

The Fundamental Solution of the Heat Conduction Equation in the *k*–phase

The heat conduction equation, also known as the heat equation, is a partial differential equation that describes the distribution of heat in a given region over time. The fundamental solution of the heat conduction equation in the *k*–phase refers to the solution that represents the temperature distribution for a point source of heat at a given instant in a medium characterized by a thermal conductivity parameter. The fundamental solution for this equation is often associated with the Green's function.

In more complex situations or in multiple dimensions, the heat conduction equation and its fundamental solution involve additional variables and terms. The solution methodology may also vary depending on the specific boundary and initial conditions of the problem. The solution typically takes the form of an integral or series, and its specific expression depends on the boundary and initial conditions of the problem. The fundamental solution is a Green's function for the heat conduction equation and plays a crucial role in solving more complex heat conduction problems by convolving it with the initial conditions.

Understanding the fundamental solution is crucial in analyzing heat conduction problems, as it provides insights into how temperature evolves over time in response to localized heat sources, and it forms the basis for solving more general heat conduction problems through convolution integrals.

Using the methods developed by the authors in [37], [38], applied to the classical heat conduction equation, the fundamental solution (containing arbitrary functions) of equation (4) has been found

$$\begin{aligned} &T(x,t) = T_1(x,t) + T_2(x,t) + C, \\ &T_1(x,t) = \frac{1}{\sqrt{\pi}} \int\limits_{-\infty}^{\infty} F(z) e^{-s^2}\, ds, \\ &T_2(x,t) = \sqrt{\frac{\text{æ}}{\pi}} \int\limits_0^t \Phi(\tau) e^{-\Psi_*^2} \frac{d\tau}{\sqrt{t-\tau}}. \end{aligned} \tag{16}$$

Here, *F* and *Φ* are arbitrary functions of their arguments, *C* is an arbitrary constant, s and τ are integration variables,

$$z(x,t,s) = x + \xi(t) - 2s\sqrt{\text{æ}t}, \quad \xi(t) = \int\limits_0^t u(t) dt,$$

$$\Psi_* = \frac{x + \xi(t) - \mu(\tau)}{2\sqrt{\text{æ}(t-\tau)}}, \qquad \mu(\tau) = \int\limits_0^\tau u(\tau) d\tau.$$

Let's verify that the functions $T_1(x, t)$ and $T_2(x, t)$ (each separately) satisfy equation (4). Find the partial derivatives of the function $T_1(x, t)$

$$\begin{aligned} &\frac{\partial T_1}{\partial t} = \frac{1}{\sqrt{\pi}} \int\limits_{-\infty}^{\infty} \frac{dF}{dz}(z) \left(u - s\sqrt{\frac{\text{æ}}{t}} \right) e^{-s^2}\, ds, \\ &\frac{\partial T_1}{\partial x} = \frac{1}{\sqrt{\pi}} \int\limits_{-\infty}^{\infty} \frac{dF(z)}{dz} e^{-s^2}\, ds, \\ &\frac{\partial^2 T_1}{\partial x^2} = \frac{1}{\sqrt{\pi}} \int\limits_{-\infty}^{\infty} \frac{d^2F}{dz^2}(z) e^{-s^2}\, ds \end{aligned} \tag{17}$$

or after integrating the last expression by parts

$$\frac{\partial^2 T_1}{\partial x^2} = -\frac{1}{\sqrt{\pi \text{æ} t}} \int\limits_{-\infty}^{\infty} \frac{dF}{dz}(z) e^{-s^2} s\, ds.$$

Similarly for the function $T_2(x, t)$

$$\begin{aligned} &\frac{\partial T_2}{\partial t} = -\frac{1}{2}\sqrt{\frac{\text{æ}}{\pi}} \int\limits_0^t \frac{\Phi(\tau) e^{-\Psi_*^2}}{(t-\tau)^{3/2}} (1 - 2\Psi_*^2) d\tau - \frac{u(t)}{\sqrt{\pi}} \int\limits_0^t \frac{\Phi(\tau) e^{-\Psi_*^2} \Psi_*}{(t-\tau)} d\tau, \\ &\frac{\partial T_2}{\partial x} = -\frac{1}{\sqrt{\pi}} \int\limits_0^t \frac{\Phi(\tau) e^{-\Psi_*^2} \Psi_*}{(t-\tau)}\, d\tau, \\ &\frac{\partial^2 T_2}{\partial x^2} = -\frac{1}{2\sqrt{\pi \text{æ}}} \int\limits_0^t \frac{\Phi(\tau) e^{-\Psi_*^2}}{(t-\tau)^{3/2}} (1 - 2\Psi_*^2)\, d\tau. \end{aligned} \tag{18}$$

Substitute the values of the partial derivatives (17) or (18) into equation (4), i.e., the dependence (16) is indeed a fundamental solution to the heat conduction equation in a multiphase medium, containing two arbitrary functions. Choose these arbitrary functions to satisfy the initial and boundary conditions. To satisfy the initial condition (8), it is sufficient to take *F*(*z*) = *φ*(*z*) and C_0 = *TN* . Indeed, since

$z(x, 0, s) = x$ and $T_2(x, 0) = 0$, then $T(x, 0) =$

$$\frac{1}{\sqrt{\pi}} \int\limits_{-\infty}^{\infty} \varphi(x) e^{-s^2}\, ds + T_N = \varphi(x) + T_N.$$ So,

$$T_1(x,t) = \frac{1}{\pi} \int\limits_{-\infty}^{\infty} \varphi(x + \xi - 2s\sqrt{\text{æ}t}) e^{-s^2}\, ds. \tag{19}$$

Let's choose the second arbitrary function *Φ*(*τ*) in such a way that the boundary condition (6) is satisfied. From (16), (19), and (6) it follows

$$\frac{\partial T_2}{\partial x}(0,t) = \frac{\partial T}{\partial x}(0,t) - \frac{\partial T_1}{\partial x}(0,t) =$$

$$f(t) - \frac{1}{\sqrt{\pi}} \int\limits_{-\infty}^{\infty} \frac{d\varphi}{dz} (\xi - 2s\sqrt{\text{æ}t}) e^{-s^2} ds.$$

The change of integration variable $\tau = t - \dfrac{x^2}{4\text{æ}s^2}$

(s - the new integration variable) in the expression (18) yields:

$$\frac{\partial T_2}{\partial x}(x,t) = -\frac{2}{\sqrt{\pi}} \int\limits_{x/2\sqrt{\text{æ}t}}^{\infty} \Phi(t - \frac{x^2}{4\text{æ}s^2})(1 + \frac{\Psi}{s}) e^{-(s+\Psi)^2}\, ds, \tag{20}$$

where

$$\Psi = \Psi_*|_{x=0} = \begin{cases} \dfrac{\xi(t) - \mu(\tau)}{2\sqrt{\text{æ}(t-\tau)}} & , \tau \neq t, \\ 0 & , \tau = t. \end{cases} \tag{21}$$

From (20) follows that $\lim\limits_{x\to 0}\dfrac{\partial T_2}{\partial x}(x,t) = -\Phi(t)$ and, consequently:

$$\Phi(t) = \frac{1}{\sqrt{\pi}}\int\limits_{-\infty}^{\infty}\frac{d\varphi}{dz}(\xi - 2s\sqrt{æt})e^{-s^2}ds - f(t).$$

Finally, the general solution of equation (4) with boundary conditions (6), (7), and initial condition (8) is given by

$$T(x,t) \quad = T_N + \frac{1}{\sqrt{\pi}}\int\limits_{-\infty}^{\infty}\varphi(x+\xi-2s\sqrt{æt})e^{-s^2}\,ds +$$

$$+\sqrt{\frac{æ}{\pi}}\int\limits_{0}^{t}\left[\frac{1}{\sqrt{\pi}}\int\limits_{-\infty}^{\infty}\frac{d\varphi}{dz}(\mu-2s\sqrt{æ\tau})e^{-s^2}\,ds - f(\tau)\right]\frac{e^{-\Psi^2}}{\sqrt{t-\tau}}d\tau \tag{22}$$

Substituting functions (10) and (15), which specify the initial condition and boundary condition (6), into (22), we obtain

$$T(x,t) = T_N + (T_{s_o} - T_N)$$

$$\left(E(t)e^{-\frac{u_o}{æ}x} + \frac{\sqrt{n}}{\sqrt{\pi}}\int\limits_{0}^{t}\left(UQ(\tau) - E(\tau)\right)e^{-\Psi^2}\frac{d\tau}{\sqrt{t-\tau}}\right). \tag{23}$$

where $E(t) = \exp[-n(Y-t)]$, $Y(t) = \int\limits_{0}^{t}U(\tau)\,d\tau$,

$n = \dfrac{u_0^2}{æ} = \dfrac{1}{t_*}$, t_* – the quantity known as the relaxation time of the *k*–phase or the characteristic time of the *k*–phase.

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