

Article

Investigations of Chemical Nonequilibrium Two-Phase Flow in Solid Rocket Motor Nozzles

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Abstract

In this study, a calculation method for two-phase nonequilibrium flow in solid rocket motor nozzles is established, and an in-depth investigation into the nonequilibrium flow within the nozzle is conducted. Based on NEPE high-energy propellant, a simplified reaction mechanism model is established and validated using the full-component sensitivity analysis method for chemical nonequilibrium flow in the nozzle, consisting of 16 components and 22 steps. The nonequilibrium and frozen flow in the nozzle are simulated, and it is found that in nonequilibrium flow, the chemical reactions result in a 22.4% increase in the flow field temperature and an approximate 4.13% improvement in specific impulse. In addition, the impacts of different total pressure conditions on the nonequilibrium flow in the nozzle are studied, in which the increase in pressure enhances the overall temperature, but the change in velocity and Mach number are negligible. Finally, a discrete phase model is adopted in the nonequilibrium flow simulation to predict the evolution of aluminum oxide particles with different sizes within the nozzle. The results indicate that the presence of particles can enhance nozzle total thrust while reducing the specific impulse. As the particle size increases, both the nozzle thrust and specific impulse decrease, with the specific impulse being more significantly affected by particle size variations due to the variation in the gas-phase mass flow rate.

Keywords: solid rocket motor; non-equilibrium flow; simplified mechanism; two-phase flow

1. Introduction

Solid rocket motors (SRMs) are widely used in the propulsion systems of aircraft due to their advantages of simple structure and excellent storage performance. As a key component for energy conversion in solid rocket motors, the performance of the nozzle directly impacts the overall engine efficiency. Within a nozzle, due to the drastic changes in temperature and pressure, a series of chemical reactions occur among the gaseous species (e.g., CO₂, H₂O, CO, H₂, etc.) produced by the combustion of the propellant. As the velocity in the nozzle is extremely high, the characteristic time scale of the flow is comparable to the time scale of the chemical reactions. In addition, the reaction rates among the gaseous species cannot keep pace with the drastic changes in temperature and pressure. As a result, a typical nonequilibrium flow is often encountered in SRM nozzles. To precisely simulate such nonequilibrium flow, a chemical reaction mechanism should serve as the foundation for simulating the non-equilibrium two-phase flow processes in the nozzle, which consists



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of various elementary reactions involving all components in the gas and the Arrhenius equation coefficients included in each elementary reaction, enabling effective prediction of the flow field inside the nozzle and the engine performance. On the other hand, with the presence of the aluminum oxide (Al_2O_3) generated by aluminum-containing composite propellant, a typical two-phase non-equilibrium flow should be precisely simulated to better predict the performance of the SRM nozzle.

Numerous studies have been conducted regarding the transonic chemical nonequilibrium flow [1–11]. Based on the continuum flow assumption, Lee [1] derived conservative governing equations for 11 air components that can describe chemical nonequilibrium flow, incorporating the effects of translational, vibrational, and electronic temperatures. However, Liu et al. [2] pointed out that to effectively solve the governing equations involving chemical components, it is necessary to address the severe “stiffness” problem caused by the coexistence of multiple types of time scales differing by several orders of magnitude in the flow field. Although implicit methods can handle such problems, they still have significant drawbacks [6], consuming substantial computational resources. To resolve this issue, there are currently two main approaches to reducing the number of solution variables. The first is the skeletal reaction mechanism method [4–9], which simplifies detailed mechanisms containing a large number of components and reactions. This has led to the development of various simplification techniques, such as the direct relation graph (DRG) method [7], component-based sensitivity analysis (STSA) [4], and full species sensitivity analysis (FSSA) [6]. The second is the application of decoupling methods [10,11], which decompose complex multi-physics problems into several sub-problems based on their physical meanings.

Since the main components of the primary combustion products generated by the composite propellant in high-performance SRM are CO , H_2 , CO_2 , H_2O , N_2 , AlCl , HCl , and liquid Al_2O_3 , the chemical reactions can be directly constructed using the existing $\text{H}_2/\text{CO}/\text{HCl}$ system or introducing Cl -containing reaction mechanisms into the existing H_2/CO reaction mechanism, on the assumption that no reactions of Al element are considered. Corresponding chemical reaction mechanisms have been established for the AP/HTPB system [12–17]. Felt [12] proposed a combustion model for AP /HTPB composite propellant, in which three types of flames were involved and a 127-reactions mechanism for gas phase was developed. Korobeinichev et al. [13] proposed a chemical reactions mechanism consisting of 35 components and 58 elementary reactions of mixed composition based on ammonium perchlorate and polybutadiene rubber. Jeppson et al. [14] developed a chemical reaction mechanism with 36 components and 72 elementary reactions for the premixed combustion of a fine AP/HTPB composite propellant. Tanner et al. [15] presented a more detailed chemical reaction mechanism for the modeling of RDX/GAP and AP/HTPB propellant. Following Felt [12], Zhao et al. [16] established a combustion model for ammonium perchlorate AP/ HTPB composite propellant, and Liu et al. [18] simplified the mechanism to a 17-component 19-step simplified reaction mechanism and studied the surface roughness effects on non-equilibrium flow in the expansion section of SRM nozzles. Gao et al. [19] applied three chemical reaction mechanisms, i.e., the 37-component 127-step chemical reaction [15], 39-step H_2/CO chemical reaction [20,21], and the 41-step H_2/CO chemical reaction [22], and compared the results with an experimental study using a TDLAS system. Grossi [23] adopted a numerical approach in order to investigate the role of finite-rate kinetics on the predictions of nozzle performance, in which two different chemical mechanisms are employed by George [24] and Troyes et al. [25] of, respectively, 15 and 17 reactions in the expansion part of a nozzle. Recently, Grégoire et al. [26] systematically evaluated existing AP combustion chemical kinetic models, compared their performance

against experimental data on ammonia, perchloric acid, and related intermediates, and pointed out the shortcomings of the current models.

Although the above studies have been conducted on the chemical non-equilibrium flows in SRM nozzles, the simplification chemical reactions for high-energy-based propellant like NEPE and the analysis of the two-phase non-equilibrium flow characteristics in nozzles are limited. Therefore, in this study, we intend to study the nonequilibrium two-phase flow characteristics in SRM nozzles with NEPE propellant, in which the gas components at the nozzle inlet were calculated and then a chemical reaction mechanism simplified from Felt [12] was obtained. The influence of the nonequilibrium flow, the total pressure, and Al_2O_3 particles are thoroughly investigated, revealing the influence of chemical nonequilibrium effects on nozzle performance and providing an effective approach for the accurate prediction of SRM performance.

2. Numerical Methods of Gas Components in SRM Nozzles and the Chemical Reaction Mechanisms

2.1. Numerical Methods of Gas Components

In SRM nozzles, the gas-phase nonequilibrium flow is a multicomponent, compressible, unsteady, and turbulent flow. The multicomponent compressible Navier–Stokes (N–S) equations are as the governing equations, and the eddy dissipation concept model is applied as the species transport model. The conservative forms of the equations are written as follows:

$$\frac{\partial}{\partial t} \int_{\Omega} \vec{W} d\Omega + \oint_{\partial\Omega} (\vec{F} - \vec{G}) \cdot d\vec{S} = \int_{\Omega} \vec{H} d\Omega \quad (1)$$

in which $\vec{W}$ conserved quantity, $\vec{F}$ is the inviscid flux vector, $\vec{G}$ is the term caused by viscosity, thermal diffusion, and species diffusion, and $\vec{H}$ is the chemical reaction source term:

$$\vec{F} = F_x \vec{i} + F_y \vec{j} + F_z \vec{k}, \vec{G} = G_x \vec{i} + G_y \vec{j} + G_z \vec{k}, \vec{H} = (0 \ 0 \ 0 \ 0 \ S_h \ \omega_i) \quad (2)$$

where

$$\vec{W} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho e \\ \rho Y_i \end{pmatrix}, F_x = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uw \\ (\rho e + p)u \\ \rho u Y_i \end{pmatrix}, F_y = \begin{pmatrix} \rho v \\ \rho vu \\ \rho v^2 + p \\ \rho vw \\ (\rho e + p)v \\ \rho v Y_i \end{pmatrix}, F_z = \begin{pmatrix} \rho w \\ \rho wu \\ \rho wv \\ \rho w^2 + p \\ (\rho e + p)w \\ \rho w Y_i \end{pmatrix} \quad (3)$$

$$G_x = \begin{pmatrix} 0 \\ \tau_{xx} \\ \tau_{xy} \\ \tau_{xz} \\ u\tau_{xx} + v\tau_{xy} + w\tau_{xz} - q_x \\ \rho_i D_{im} \partial Y_i / \partial x \end{pmatrix}, G_y = \begin{pmatrix} 0 \\ \tau_{yx} \\ \tau_{yy} \\ \tau_{yz} \\ u\tau_{yx} + v\tau_{yy} + w\tau_{yz} - q_y \\ \rho_i D_{im} \partial Y_i / \partial y \end{pmatrix}, G_z = \begin{pmatrix} 0 \\ \tau_{zx} \\ \tau_{zy} \\ \tau_{zz} \\ u\tau_{zx} + v\tau_{zy} + w\tau_{zz} - q_z \\ \rho_i D_{im} \partial Y_i / \partial z \end{pmatrix} \quad (4)$$

in which i is the number of species, ρ is the density of the mixture, ρ_i is the concentration of each species, u, v, w is the velocity component in the x, y, z direction, e is the total energy per unit mass of the control volume, S_h is the chemical reaction heat source term within the control volume, Y_i is the mass fraction of species i , D_{im} is the mass diffusion coefficient of species i , ω_i is the mass production rate of species i in chemical reactions, and τ_{ij} is the viscous stress component.

In this paper, numerical simulation is carried out based on the above species transport model. The SST $k-\omega$ model and standard wall function are used as the viscous models, and the 2D axisymmetric steady-state solver is adopted for the calculation process. The reaction mechanism is based on the chemical reaction mechanism presented in this work (Which will be presented in Section 2.3), as well as that in Felt [12] and Liu et al. [23] to simulate the chemical nonequilibrium flow process. The chemical mechanisms are built into the solver in the form of a reaction file, composed of various elementary reactions involving all components in the gas-phase and the Arrhenius equation coefficients in each elementary reaction.

2.2. Calculation of Gas Components in SRM Nozzle

In the SRM combustion chamber, the flow can be regarded as the adiabatic state. Compared with the substantial heat released by propellant combustion, the heat lost from the combustion chamber of SRM can be neglected. In addition, the characteristic time of flow in the system is much longer than that of chemical reactions occurring in the system. Thus, it is assumed that when the gas reaches the end of the combustion chamber, no further chemical reactions take place between the gas components, which indicates that at the end of the combustion chamber, as well as the nozzle inlet, the gas also remains in an equilibrium state. In the current work, the equilibrium gas at the nozzle inlet is produced by the combustion of NEPE high-energy propellant, and the propellant formulation is presented in Table 1.

Table 1. Formulation of NEPE high-energy propellant.

Component	Molecular Formula	Mass Fraction	Molar Enthalpy of Formation/(kJ/mol)
Cyclotetramethylene Tetranitramine (HMX)	$C_4H_8N_8O_8$	40%	+74.9
Polyethylene Glycol (PEG)	$(C_2H_6O_2)_n$	6.5%	−390.3
Nitroglycerin (NG)	$C_3H_5N_3O_9$	9.75%	−372.5
Al	Al	18.0%	0
1,2,4-Butanetriol Trinitrate (BTTN)	$C_4H_7N_3O_9$	9.75%	−406.8
Ammonium Perchlorate (AP)	NH_4ClO_4	16%	−295.77

The thermodynamic calculations of the NEPE high-energy propellant under constant-pressure and adiabatic conditions were performed using the CEA code developed by NASA Lewis research center [27,28]. The combustion chamber pressure was set to 6.5 MPa, and the trial calculation temperature was 3800 K. The calculated adiabatic combustion temperature of the NEPE high-energy propellant is 3746 K, and the obtained mole fractions of the specific equilibrium components of the propellant are presented in Table 2.

Table 2. Mole fractions of each component of the NEPE high-energy propellant at the nozzle inlet.

Component	Mole Fraction	Component	Mole Fraction
CO	0.26277	AlOHCl ₂	0.00006
H ₂	0.19889	HAIO ₂	0.00006
N ₂	0.19661	AlO ₂	-
H ₂ O	0.11671	AlCl ₃	-
Al ₂ O ₃ (L)	0.08142	AlCl ₂	0.00005
H	0.05281	HCO	0.00004
HCl	0.02831	AlO ₂	0.00003
CO ₂	0.01790	N	0.00003

Table 2. Cont.

Component	Mole Fraction	Component	Mole Fraction
OH	0.01725	HAIO	0.00002
AlOH	0.01046	NH	0.00002
Cl	0.00490	NH ₂	0.00002
AlCl	0.00255	AlHCl	0.00001
NO	0.00250	AlHCl ₂	-
O	0.00245	Cl ₂	-
AlO	0.00107	ClO	0.00001
O ₂	0.00055	HOCl	-
Al(OH) ₂	0.00053	HCN	0.00001
Al	0.00049	HNO	0.00001
AlOHCl	0.00035	NH ₃	0.00001
AlOCl	0.00029		
Al ₂ O	0.00029		
Al ₂ O ₂	0.00015		
Al(OH) ₃	0.00014		
AlH	0.00010		
Al(OH) ₂ Cl	0.00010		

Figure 1 presents a chart of the mole fractions of the top ten major compounds, free radicals, and other components in the equilibrium gas produced by the combustion of the NEPE high-energy propellant under constant-pressure and adiabatic conditions. As shown in the figure, CO, H₂, N₂, H₂O, Al₂O₃, H, HCl, CO₂, OH, and Cl are the top ten compounds or free radicals with the highest proportions in this type of propellant. Therefore, the subsequent mechanism simplification work should be carried out around these ten components. In the present work, aluminum-containing components are not considered in the chemical reactions, as they primarily exist in the form of condensed-phase particles (e.g., liquid Al₂O₃) in the nozzle. The discrete phase model is used to model the Al₂O₃ particles in the nozzle, in which the Schiller–Naumann drag model and the random walk model are used, resulting in the velocity and temperature lag between the two phases. The above simplifications, including neglecting the reactions of gaseous Al species, and considering liquid Al₂O₃ as DPM particles regardless of their microscopic behaviors such as coalescence, breakup, and impact on walls [29,30], might introduce potential errors, which can be further investigated in our future work.

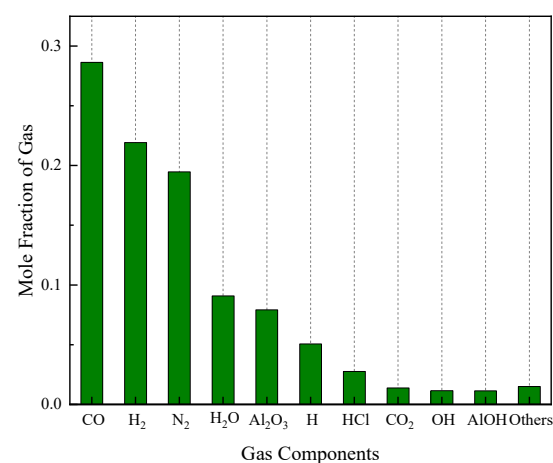


Figure 1. Bar chart of mole fractions of gas components in NEPE high-energy propellant.

2.3. Simplification of the Detailed Mechanism

In this paper, the detailed mechanism proposed by Felt [12] is adopted, which covers 37 gas species and 109 elementary reactions, since the main gas compounds or free radicals

are similar with the present high-energy propellant and Felt's AP/HTPB propellant. The FSSA method [6] is employed to simplify Felt's detailed reaction mechanism. This method calculates the relative induced error of the target parameter caused by the removal of each component and its associated elementary reactions, and ranks the components based on this error. Subsequently, components are removed one by one in order, with the single-step relative induced errors continuously accumulated. The simplification process is terminated once the accumulated error exceeds a preset threshold. The obtained operating conditions and key parameters are presented in Table 3, and the simplified skeletal reaction mechanism is shown in Table 4, in which the exponent Z is the pre-exponential factor, E is the activation energy, and B is the temperature exponent. As shown in the table, the simplified model includes 16 components and 22 elementary reactions, and the simplified species are consistent with the top ones in Table 1.

Table 3. Operating condition of NEPE high-energy propellant.

Condition	Parameters
Ignition time/s	0.0002
Temperature/K	3746
Pressure/MPa	6.5
Key parameters	CO, H ₂ O, N ₂ , H ₂

Table 4. Simplified reaction mechanism of NEPE high-energy propellant.

Component	Numbers	Elementary Reaction	Z	B	E
HNO	R1	$HCl + OH = Cl + H_2O$	5.0×10^{11}	0	7.5×10^2
H ₂ O	R2	$HNO + OH = NO + H_2O$	1.3×10^7	1.9	-9.5×10^2
HCO	R3	$HNO + H = H_2 + NO$	4.5×10^{11}	0.7	6.6×10^2
HCl	R4	$NO + H + M = HNO + M$	8.9×10^{19}	−1.3	7.4×10^2
H	R5	$H_2 + OH = H_2O + H$	2.16×10^8	1.5	3.43×10^3
H ₂	R6	$HCO + M = CO + H + M$	1.87×10^{17}	−1.0	1.7×10^{14}
CO	R7	$CO + OH = CO_2 + H$	4.76×10^7	1.2	7.0×10^1
CO ₂	R8	$CO + ClO = CO_2 + Cl$	3.0×10^{12}	0	1.0×10^3
ClO	R9	$H + O_2 = O + OH$	8.3×10^{13}	0	1.4413×10^4
Cl	R10	$H + Cl + M = HCl + M$	5.3×10^{21}	−2.0	-2.0×10^3
OH	R11	$ClO + O = Cl + O_2$	6.6×10^{13}	0	4.4×10^2
O ₂	R12	$H + HCl = Cl + H_2$	7.94×10^{12}	0	3.4×10^3
O	R13	$HCl + O = Cl + OH$	2.3×10^{11}	0	9.0×10^2
NO	R14	$2H + M = H_2 + M$	1.0×10^{18}	−1.0	0
N ₂	R15	$2H + H_2 = 2H_2$	9.0×10^{16}	−0.6	0
NH	R16	$2H + H_2O = H_2 + H_2O$	6.0×10^{19}	−1.3	0
	R17	$2H + CO_2 = H_2 + CO_2$	5.5×10^{20}	−2.0	0
	R18	$H + HCO = H_2 + CO$	7.34×10^{13}	0	0
	R19	$2OH = H_2O + O$	6.0×10^8	1.3	0
	R20	$NH + NO = N_2 + OH$	1.0×10^{13}	0	0
	R21	$NH + NO = H + N_2 + O$	2.3×10^{13}	0	0
	R22	$NH + OH = H_2 + NO$	1.6×10^{12}	0.6	1.5×10^3

2.4. Validation of the Simplified Mechanism and Boundary Conditions

In this paper, a two-dimensional axisymmetric nozzle model is adopted for numerical simulation validation. A virtual combustion chamber with a length of 20 mm is added in front of the convergent section of the nozzle. The total length of the nozzle section is 132.6 mm, including a convergent section of 21.6 mm and a divergent section of 111 mm. The throat diameter is 39.5 mm, the outlet diameter is 125 mm, the inlet expansion half-

angle is 14° , and exit expansion half-angle is 26° . The nozzle is meshed with a structured grid, consisting of approximately 20,000 grid cells, and grid refinement is performed in the boundary layer region. The range of y^+ in this case is from 1.84 to 40.34, which is enough to meet the requirement of current simulations. The applied two-dimensional axisymmetric nozzle grid model is shown in Figure 2, the boundary conditions of the computational domain are listed in Table 5, and the boundary conditions of the components at the inlet are shown in Table 2.

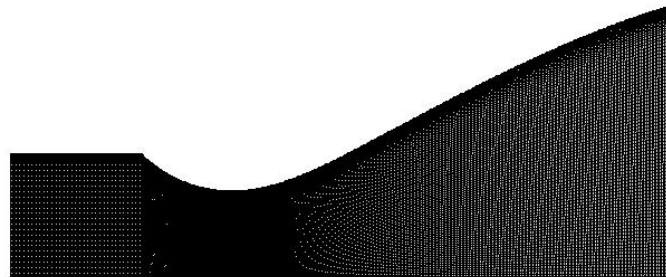


Figure 2. Two-dimensional axisymmetric grid model.

Table 5. Boundary conditions of the computational domain.

Boundary	Boundary Condition	Value
Inlet	Pressure inlet	6.5 MPa
	Temperature	3746 K
Outlet	Pressure outlet	0.1 Mpa
	Temperature	300 K
Wall	No-Slip boundary, adiabatic	

To verify the accuracy of the presented simplified model, we compare our simulation results with those obtained by the detailed mechanism of Felt [12] and another simplified mechanism of Liu et al. [18] in this section. It should be noted that the simulations with the two mechanisms are performed by us with the chemical reaction mechanisms of Felt [12] and Liu et al. [18] under the simulation parameters in Table 5. Figure 3 shows the CO mole fraction, H₂ mole fraction, and Mach number along the axis for three mechanisms. CO and H₂ are chosen as the representative components since they are components with the highest mole fractions for the present propellant, as shown in Table 1. As shown in the figure, the predictions of the three mechanisms for Mach number are basically consistent, and the maximum relative error between the results of the two mechanisms and Felt's detailed mechanism is 0.014%. For CO and H₂, there are slight differences among the three mechanisms, and the simplified mechanism by the present method shows better agreement with Felt's detailed mechanism. The maximum relative error of the CO mole fraction is 0.026% (the present simplified mechanism) and 0.272% (simplified mechanism of Liu et al. [18]), respectively; while the maximum relative errors of the H₂ mole fraction are 0.028% and 0.44%. Therefore, the simplified mechanism obtained by the present FSSA method shows better agreement with the detailed mechanism [12] and can effectively represent the detailed chemical reaction mechanism.

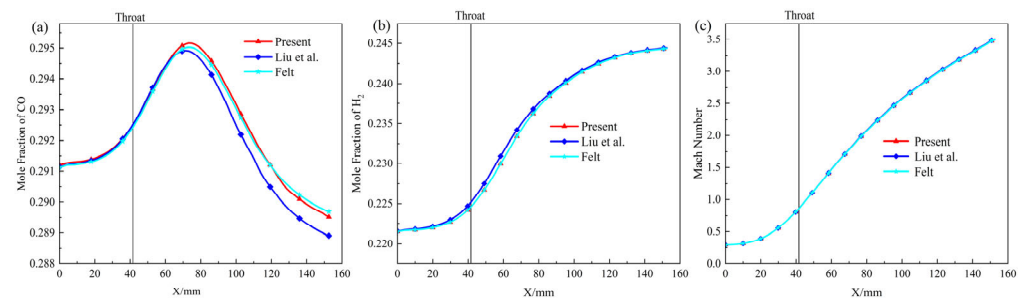


Figure 3. (a) CO mole fraction, (b) H₂ mole fraction, and (c) Mach number along the axis for mechanisms obtained by the present work, Liu et al. [22] and Felt [12].

3. Flow Field Analysis of Frozen Flow and Non-Equilibrium Flow

3.1. Grid Independence Analysis

First, we perform a grid independence test with grid cells of 10,000, 20,000, and 40,000. The CO mole fraction, H₂ mole fraction, Mach number, temperature along the nozzle axis and H₂ mole fraction, and temperature along the wall for the three grids are presented in Figure 4, and the average data at the nozzle outlet is shown in Table 6. As shown in the figure and table, the difference of variables between the 10,000 and 20,000 grids and the grid of 40,000 are all acceptable, with the maximum relative error of 0.808% along the axis and 1.53% along the wall. Considering the accuracy and computational efficiency, the grid size with 20,000 cells is enough and adopted for all subsequent simulations.

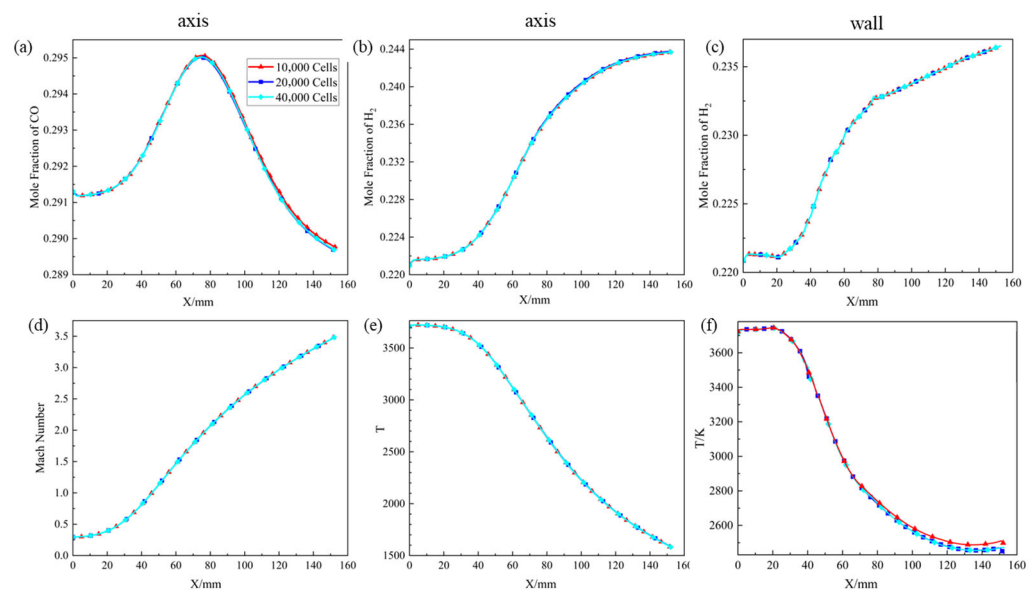


Figure 4. (a) CO mole fraction, (b) H₂ fraction, (d) Mach number, (e) temperature along the axis and (c) H₂ fraction, (f) temperature along the wall under different grid numbers.

Table 6. Average data at the nozzle outlet.

Grid Number	Temperature/K	Axial Velocity/(m/s)	Mach Number	H ₂ Mole Fraction	CO Mole Fraction
10,000	1701.842	3001.852	3.302	24.464%	28.893%
20,000	1703.359	3001.526	3.300	24.474%	28.898%
40,000	1704.439	3000.241	3.298	24.473%	28.896%

3.2. Comparison of the Frozen Flow and Non-Equilibrium Flow

Now we investigate the difference between the non-equilibrium flow and the frozen flow without the consideration of chemical reactions. Figure 5 presents the temperature field and Mach number field for frozen and nonequilibrium flow with NEPE propellant. As shown in Figure 5a, in the combustion chamber, the flow velocity is small and the temperature is close to the inlet temperature of 3710 K. In the convergent section of the nozzle, the temperature variation of the frozen and nonequilibrium flow is slightly different, and the temperature of frozen flow decreases a little faster than that of the nonequilibrium flow, indicating that chemical reactions in nonequilibrium flow proceed in the exothermic direction, delaying the temperature decrease. In the divergent section of the nozzle, the exothermic phenomenon of nonequilibrium flow is more pronounced, with a temperature difference exceeding 250 K compared to frozen flow at the same position. Additionally, at the same cross-section, both frozen flow and nonequilibrium flow exhibit the similar trend, i.e., the temperature is the highest in the wall boundary layer, decreases rapidly after leaving the boundary layer, and then increases as it approaches the axis. It should be noted that for the nonequilibrium flow, the chemical reactions are promoted by the temperature boundary layer, which in turn results in a higher temperature increase. In Figure 5b, the difference in Mach number between frozen flow and nonequilibrium flow is relatively small in the convergent section and the start of the divergent section. However, in the late stage of the divergent section, especially near the nozzle exit, the Mach number of frozen flow is higher than that of nonequilibrium flow. This may be caused by the fact that the local effect of equilibrium shift on temperature outweighs its effect on velocity, leading to a lower Mach number for nonequilibrium flow compared to frozen flow.

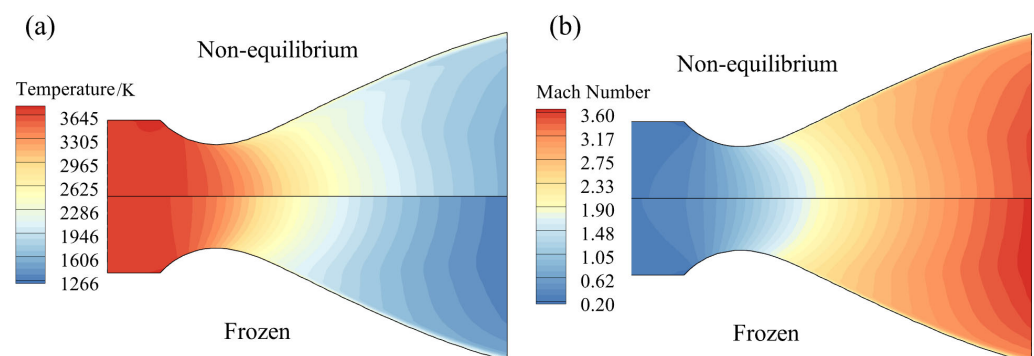


Figure 5. Contour of (a) the temperature and (b) Mach number for frozen and nonequilibrium flow.

Figure 6 presents the curves of temperature and axial velocity of frozen flow and nonequilibrium flow along the axis. In Figure 6a, the axial velocity of nonequilibrium flow is similar to the frozen flow in the convergent section and the early stage of the divergent section; but in the middle-late stage of the divergent section, the nonequilibrium flow grows faster than the frozen flow, with the maximum difference (3.47%) at the nozzle exit. Also, we can see that the temperature difference between nonequilibrium flow and frozen flow is much larger. The temperature difference begins to expand in the convergent section and becomes more pronounced in the divergent section. At an axial distance of 86 mm, the temperature difference reaches its maximum value of 348 K, where the temperature of the nonequilibrium flow is 16.1% higher than that of the frozen flow. Subsequently, the temperature difference gradually decreases, dropping to 294 K at the exit, with the nonequilibrium flow temperature increasing by 22.9% compared to the frozen flow. Figure 6b shows the variation curves of the Mach number of frozen flow and nonequilibrium flow at the nozzle axis. In the divergent section, the maximum difference reaches 0.15 Mach, with the nonequilibrium flow Mach number being 4.12%

lower than that of the frozen flow. The reason for this difference is that although both velocity and temperature increase in the nonequilibrium flow compared to the frozen flow, the magnitude of velocity increase is much smaller than that of temperature increase. As a result, the Mach number of the nonequilibrium flow in the divergent section is lower than that of the frozen flow.

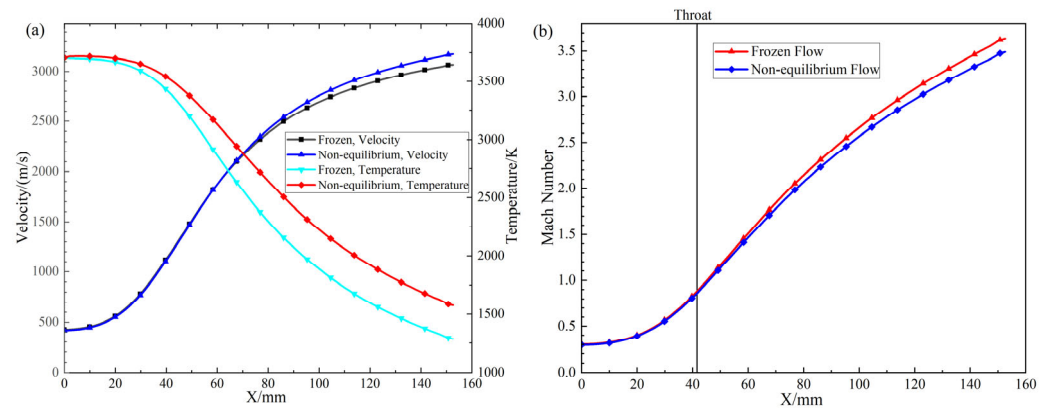


Figure 6. (a) Velocity/temperature and (b) Mach number along the axis for frozen flow and nonequilibrium flow.

Figure 7 presents the mole fractions of the main gas components for the non-equilibrium flow in the nozzle, which includes eight compounds and free radicals—CO, H₂, N₂, H₂O, H, HCl, CO₂, and OH—ranked by mole fraction from highest to lowest, accounting for 98.8% of all gas components. As shown in the figures, the distributions of the components are greatly influenced by the temperature field. Among the components, H₂, N₂, HCl, and CO₂ are on the product side of the chemical reaction system. Their mole fractions gradually increase with the increase in the temperature. In contrast, the two free radicals H and OH are on the reactant side, and their mole fractions gradually decrease as the temperature increases. Differently, CO acts as a product in the reaction system in the convergent section of the nozzle, with its mole fraction gradually increasing and forming a local high-concentration region near the throat; while in the divergent section of the nozzle, CO acts as a reactant and gradually decreases, eventually falling below the value at the inlet. Similar to CO, H₂O also exhibits a trend of first decreasing and then increasing in mole fraction, but its high-concentration region is located in the middle of the divergent section.

Figure 8 presents the mole fractions of each gas component at the axis and wall of the nozzle. In the figure, solid dots represent data on the axis. Overall, the distribution of each component on the wall is similar to that on the axis, but there are differences among the components. Specifically, the mole fractions of six compounds (CO, H₂, N₂, H₂O, HCl, and CO₂) on the axis are higher than those on the wall. In contrast, the mole fractions of the two free radicals (H and OH) on the axis are lower than those on the wall, indicating that the consumption of free radicals on the axis is more severe than that on the wall, and the decreasing amplitude of H is greater than that of OH. The growth rates of each propellant component at the outlet compared with those at the inlet (negative values indicate that the component is consumed during the flow process) are presented in Table 7, and the data in the table also confirm the conclusions of the previous analysis.

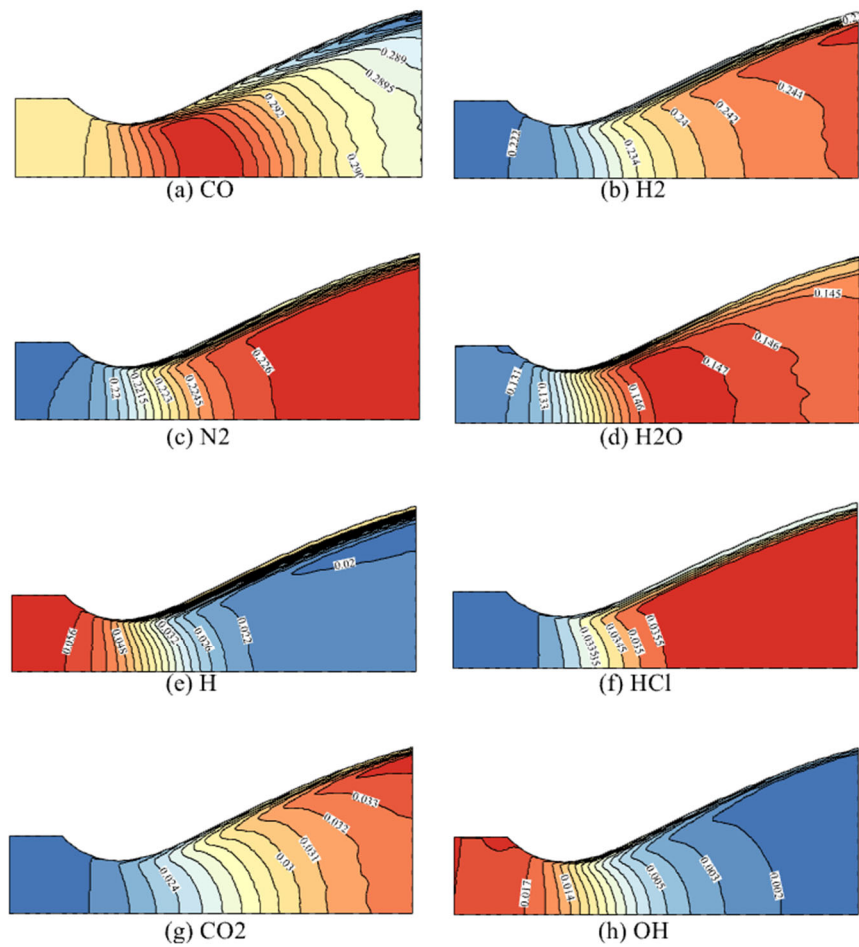


Figure 7. The mole fractions of the main gas components in non-equilibrium flow.

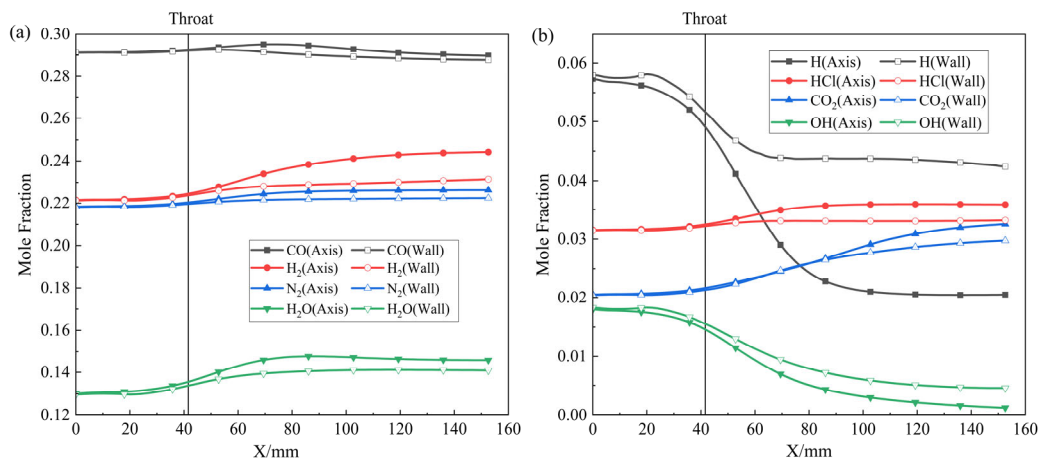


Figure 8. Variation of component mole fractions of (a) CO, H₂, N₂ and H₂O (b) H, HCl, CO₂ and OH at the axis and wall.

Table 7. The growth rates of each component at the outlet relative to those at the inlet.

Position	Component	Growth Rate	Component	Growth Rate
Axis	CO	−0.51%	H	−64.3%
	H ₂	10.2%	HCl	13.72%
	N ₂	3.70%	CO ₂	58.51%
	H ₂ O	12.06%	OH	−93.12%

Table 7. Cont.

Position	Component	Growth Rate	Component	Growth Rate
Wall	CO	−1.16%	H	−26.9%
	H ₂	4.62%	HCl	5.51%
	N ₂	2.01%	CO ₂	45.5%
	H ₂ O	8.67%	OH	−75.1%

Then, we evaluate the performance of the SRM for the frozen and non-equilibrium flows. Usually, the performance of SRM is evaluated by thrust and specific impulse, and for pure gas, they are calculated as follows:

$$F = \iint_S (\rho \cdot u_{ex}^2 + p_e - p_a) dS, \quad I_s = \frac{F}{\dot{m}g} \quad (5)$$

in which F is the thrust, ρ is the gas density, u_{ex} is the axial component of the gas outlet velocity, p_e is the pressure at the outlet section, p_a is the atmospheric pressure at the altitude where the nozzle is located (the sea-level atmospheric pressure of 101,325 Pa is used for calculation), $\dot{m}$ is the mass flow rate of the gas, and I_s is the specific impulse. For two-phase flows (the simulations in Section 3.4), the thrust is divided into gas-phase thrust F_g and solid-phase thrust F_p , which are calculated as follows:

$$F_g = \iint_S (\rho \cdot u_{ex}^2 + p_e - p_a) dS, \quad F_p = \sum \dot{m}_p u_{pe} \quad (6)$$

where $\dot{m}_p$ is the particle mass flow rate and u_{pe} is the particle velocity at the outlet.

Table 8 lists the main data of the nozzle, including the mass flow rate, axial velocity, thrust, specific impulse, and temperature of frozen flow and nonequilibrium flow at the nozzle exit, where the thrust and specific impulse are sea-level data. As shown in the table, compared with frozen flow, chemical reactions in nonequilibrium flow proceed in the exothermic direction but most of the released heat is used to increase the internal energy of the gas itself, increasing the exit temperature by 22.4%. The mass flow rate is slightly decreased due to the chemical reactions by 1.99%, while the axial velocity increases by 3.13% and thrust by 2.02%, making a nearly 4.13% contribution to the specific impulse.

Table 8. Nozzle performance data at the nozzle outlet.

Flow Type	Mass Flow Rate/(kg/s)	Axial Velocity/(m/s)	Thrust/N	Specific Impulse/s	Exit Temperature/K
Frozen flow	4.165	2909	11,687.76	286.32	1381.6
Non-equilibrium flow	4.082	3000	11,928.19	298.14	1691
Variation	1.99%	3.13%	2.02%	4.13%	22.4%

3.3. Study on Nonequilibrium Flows Under Different Pressure

In this subsection we study the effect of total pressure variation on nonequilibrium flow. For a chemical system in equilibrium, changes in pressure will cause the originally stable system to undergo an equilibrium shift until a new equilibrium temperature and equilibrium composition are achieved. In Table 9, we list the total pressure and temperature conditions in our simulations, in which the total pressure varies in a wide range from 6.5 to 13.5 MPa, and the corresponding temperature is calculated by the minimum Gibbs free energy method by the total pressure with the NEPE high-energy propellant. Table 10 lists the mole fractions of the equilibrium gas components at the inlet after combustion under the operating conditions of 10 MPa and 13.5 MPa.

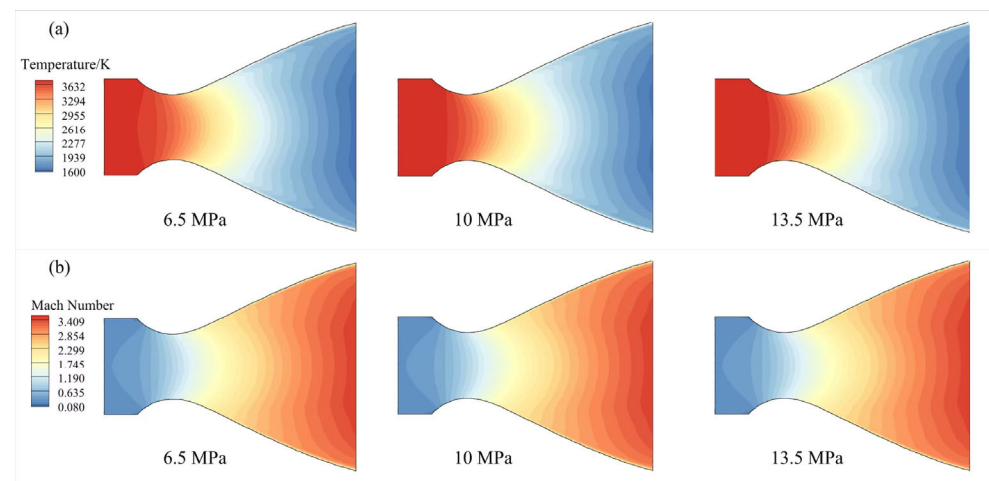
Table 9. Conditions of total pressure and temperature.

Conditions	Total Pressure/MPa	Temperature/K
1	6.5	3746
2	10	3796
3	13.5	3831

Table 10. Mole fractions of equilibrium components at the nozzle inlet after combustion of NEPE propellant.

Components	Mole Fraction (10 MPa)	Mole Fraction (13.5 MPa)	Components	Mole Fraction (10 MPa)	Mole Fraction (13.5 MPa)
CO	0.2924216	0.2934090	Cl	0.004899756	0.004542622
H ₂	0.2241826	0.2262701	NO	0.002754311	0.002623229
N ₂	0.2191698	0.2199480	O ₂	0.0005117850	0.001919341
H ₂ O	0.1317290	0.1332403	HCO	0.00006108134	0.0004398245
H	0.05231282	0.04830115	NH	0.00003117307	0.00007475312
HCl	0.03212593	0.03259651	ClO	0.000002258065	0.00003472749
CO ₂	0.02044696	0.02047567	HNO	0.000006376267	0.000007103056
OH	0.01698836	0.01597343	O	0.002236109	0.000002247944

Figure 9 presents the temperature and Mach number under different pressures. It can be seen that the total pressure mainly influences the temperature field by changing the inlet temperature boundary condition: the higher the total pressure, the higher the initial temperature at the inlet and the entire flow field. In addition, the temperature variations from the inlet to outlet along the axis under different pressure conditions are almost consistent (see in Table 11). On the other hand, it can be seen in Figures 9b and 10 that the influence of total pressure variation on the velocity and Mach number can be neglected.

**Figure 9.** (a) Temperature and (b) Mach number contours under different pressures.

Similar to the previous subsection, the variation characteristics of components can be divided into three types: increasing with flow, decreasing with flow, and high-concentration region type. Correspondingly, three representative components are chosen, namely H₂, H, and CO. Figure 11 presents the mole fraction of H₂, H, and CO under different pressures. As the pressure increases, the initial mole fractions of H₂ and CO increase, while the initial mole fraction of H decreases, which leads to an overall change in component distributions. To quantitatively analyze the results, Table 11 lists the changing rates of the mole fractions of the temperature and three components along the axis between the outlet and the inlet

under different pressure. As shown in the table, the changing rates of H_2 and CO are not significantly affected by the total pressure, generally hovering around 10.5% and -0.46% , respectively, consistent with the temperature. For the H free radical, however, the increase in pressure leads to a growth in its consumption rate. This might be because of the fact that the reaction rate of H decreases when the mole fraction of H reduces below a limiting value, which decreases with the pressure.

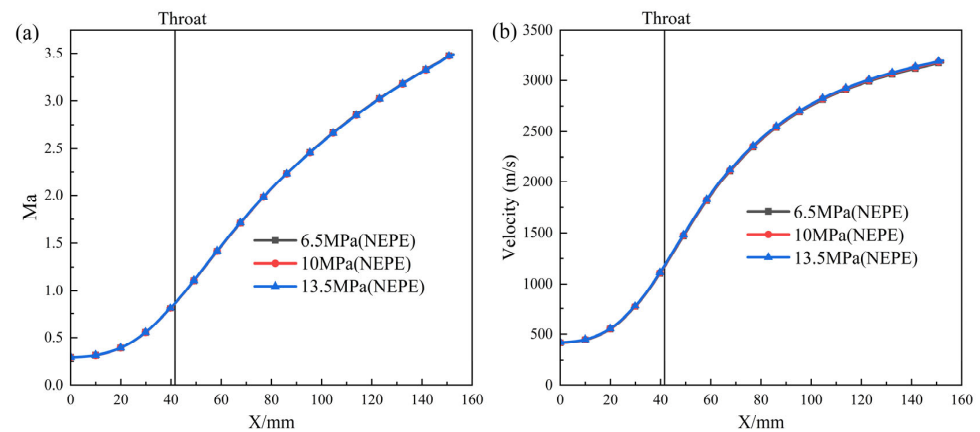


Figure 10. (a) Mach number and (b) axial velocity along the axis under different pressures.

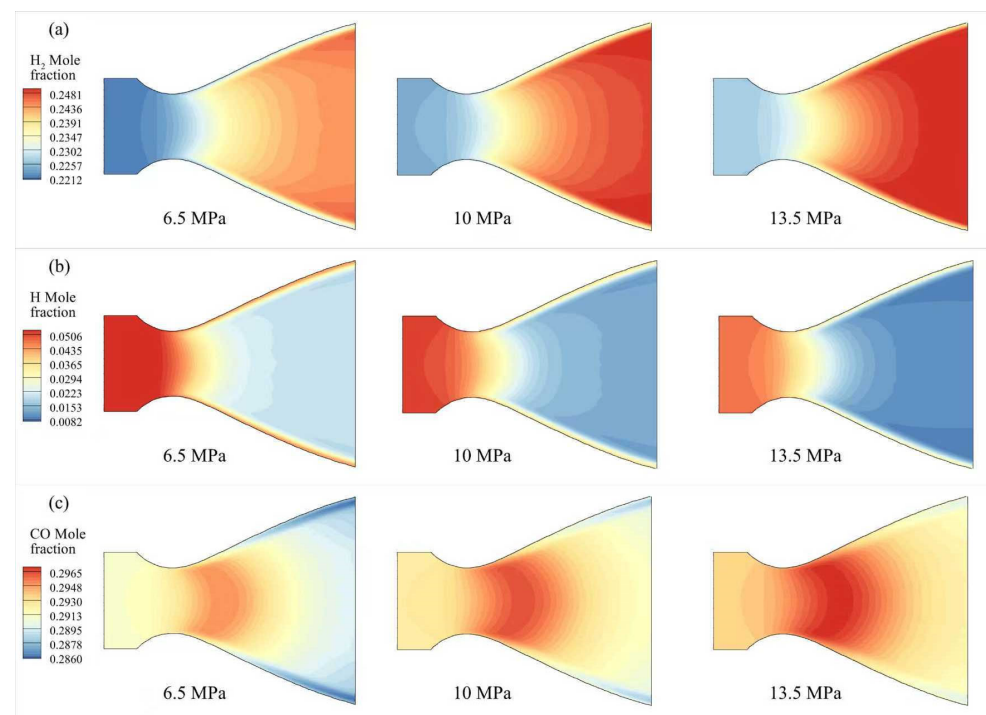


Figure 11. The mole fraction of (a) H_2 , (b) H, and (c) CO under different operating conditions.

Table 11. The growth rates of temperature and the mole fractions of three components at the outlet relative to those at the inlet along the axis.

Item	6.5 MPa	10 MPa	13.5 MPa
Temperature	-55.3%	-55.3%	-55.1%
H_2	10.2%	10.5%	10.5%
H	-64.3%	-73.6%	-79.0%
CO	-0.51%	-0.43%	-0.44%

3.4. Study on Nonequilibrium Flow Under Two-Phase Conditions

Finally, we investigate the nonequilibrium two-phase flows in the SRM nozzle with the presence of condensed-phase Al_2O_3 particles at different sizes, which covers a large range from 1 to 150 μm . The discrete phase model is used to simulate the two-phase flows. The inlet boundary conditions are set as follows: the total temperature of the combustion chamber is 3746 K, the pressure is 6.5 MPa, the inlet velocity of the condensed-phase Al_2O_3 particles is 20 m/s, and the mass flow rate of the particle phase is 1.65 kg/s. An unsteady particle tracking with time step of 10^{-6} s is adopted

Figure 12 presents the distributions of particles colored by particle residence time, particle temperature, and particle velocity in nonequilibrium flow. It can be observed that the particles can reach the wall at the convergent section of the nozzle, but due to the inertia of the particles, after the throat, the particles are unable to promptly follow the gas phase to move toward the wall. Consequently, the particles are distributed in an aggregation zone centered on the axis, and particle-free zones are formed near the wall at the nozzle throat and divergent section. As the particles move downstream of the nozzle, the residence time continuously increases, their velocity rises steadily accelerated by the gas flow, and the temperature gradually decreases through heat exchange with the gas phase. For different particle diameters, the particle aggregation zone shrinks, the particle-free zone expands, and the maximum particle residence time increases with the diameter (see Figure 12a), which can be attributed to the decreased followability of the particles with the diameter. In addition, it can be seen that as the particle diameter increases, the variation of the velocity decrease significantly (Figure 12b), which is also caused by the reduced particle followability with the increase in particle size. The change in particle temperature is also decreased with the diameter because as diameter increases, the specific surface area decreases, leading to significant decrease in the heat exchange between particles and the gas phase.

Figure 13 presents the gas phase temperature field, velocity field, and particle concentration under different particle sizes. As shown in the figures, with the presence of the particles, a hysteresis zone appears in the gas phase temperature and velocity fields (see Figure 13a,b), which are highly consistent with the particle high-concentration region in Figure 13c. At small particle sizes, the particle aggregation zone expands, leading to a larger high-temperature and low-velocity of the gas phase. In addition, as the particle size decreases, the particle followability is stronger at smaller particle sizes, more momentum is transferred to the particle phase, and overall gas velocity is higher. Meanwhile, the specific surface area of particles increases, leading to more heat transfer of energy to the gas phase, resulting in a higher average temperature at the outlet from the particles to the gas phase.

Figure 14 presents the mole fraction of CO, H_2 , and H free radicals containing condensed-phase particles under different operating conditions, respectively. It can be observed that within the particle aggregation zone, the reactions are highly affected by the particles and exhibit a variation trend similar to the distribution of particle concentration and temperature. Through the hysteresis zone induced on the temperature and velocity fields, the presence of particles promotes equilibrium shifts in the chemical reaction system within the particle aggregation zone. When the local temperature increases, the reaction system shifts toward the direction of H generation, while the formation of CO and H_2 compounds decreases.

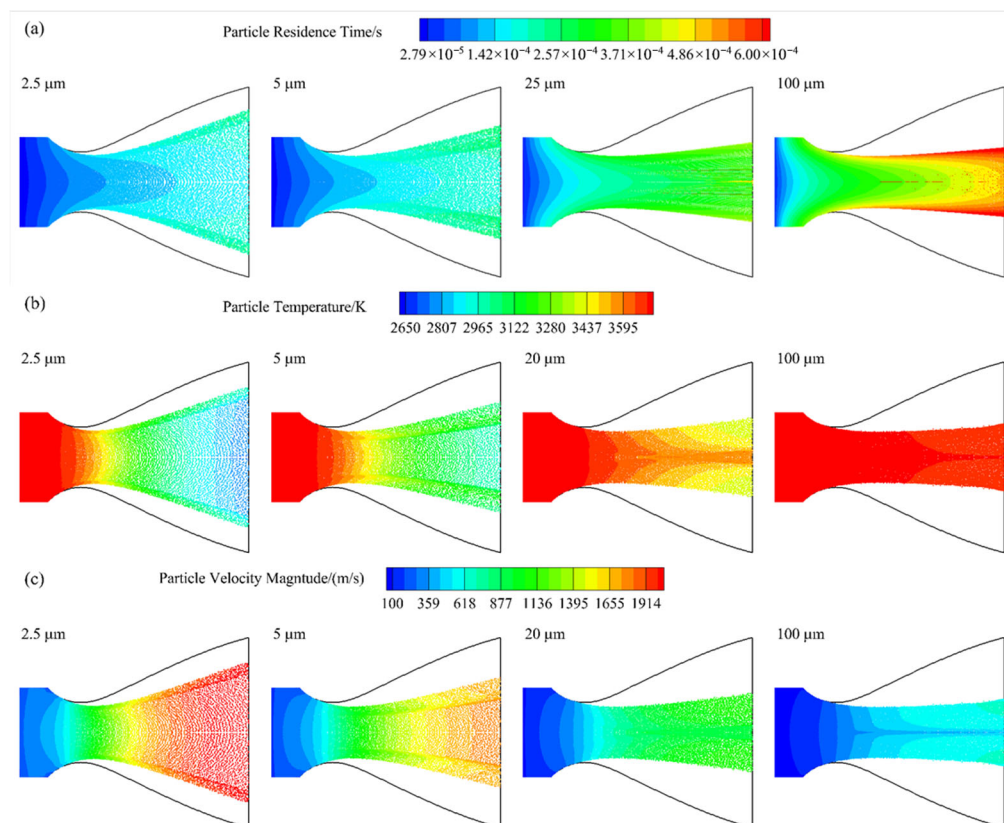


Figure 12. Distribution of particles in the nozzle nonequilibrium flow field colored by (a) particle residence time, (b) particle temperature, and (c) particle velocity.

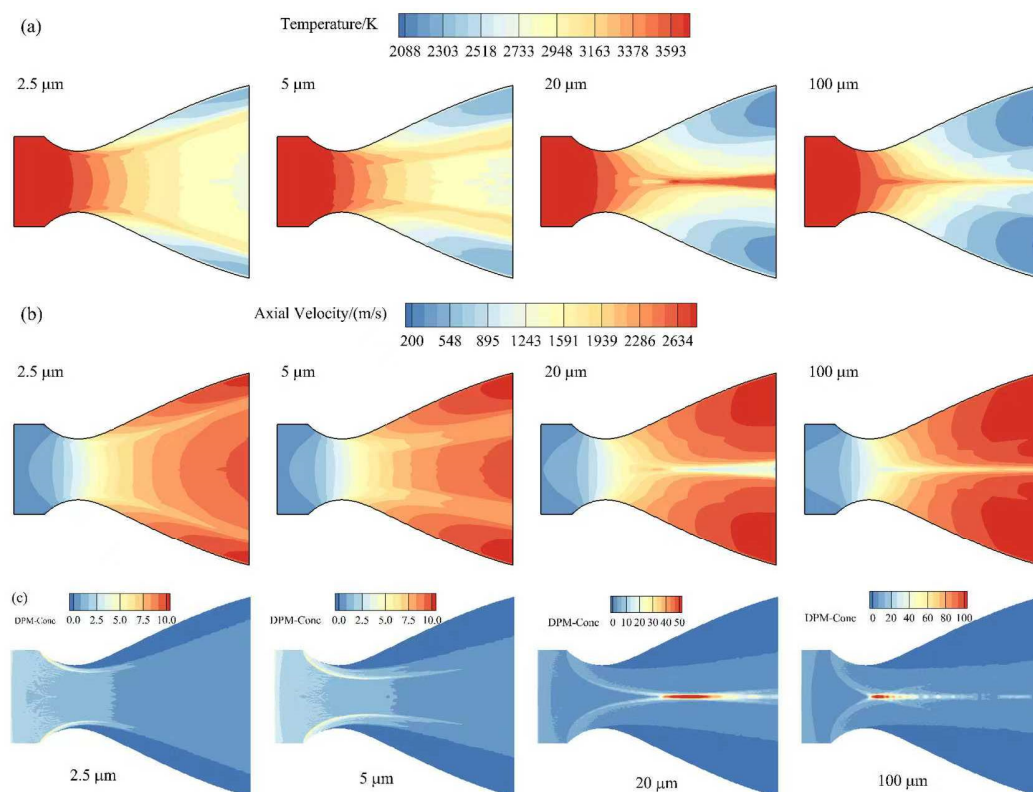


Figure 13. The (a) temperature field, (b) axial velocity and (c) DPM-cone inside the nozzle under different operating conditions.

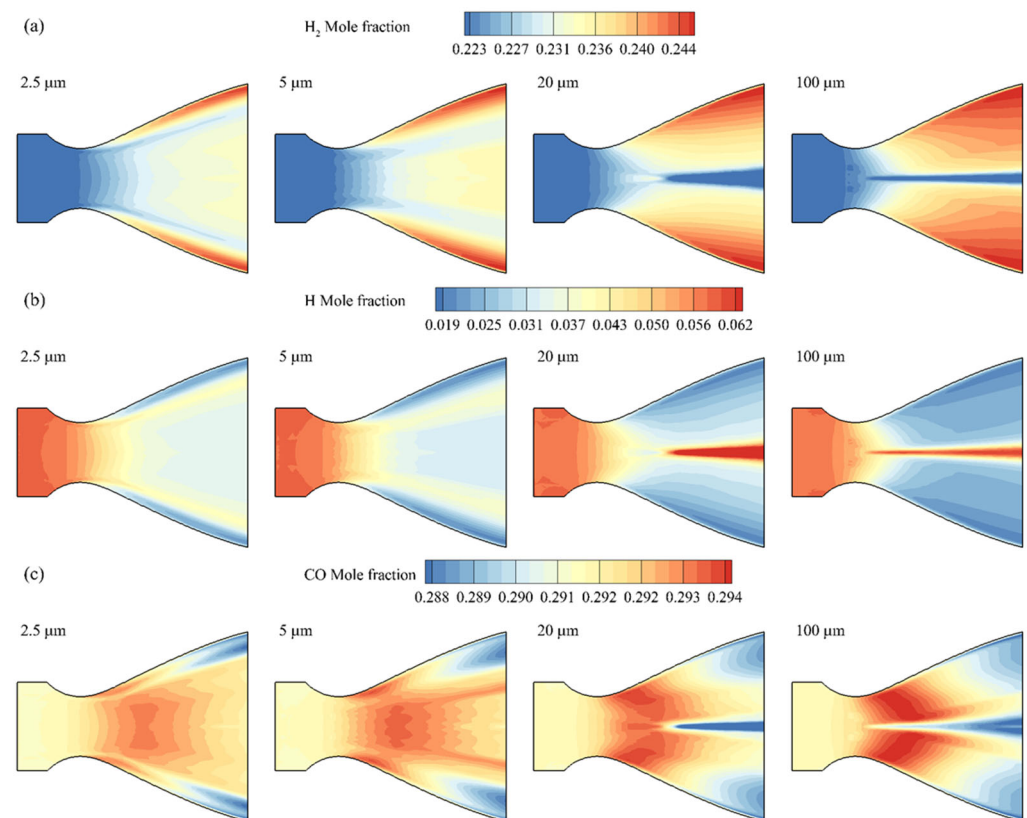
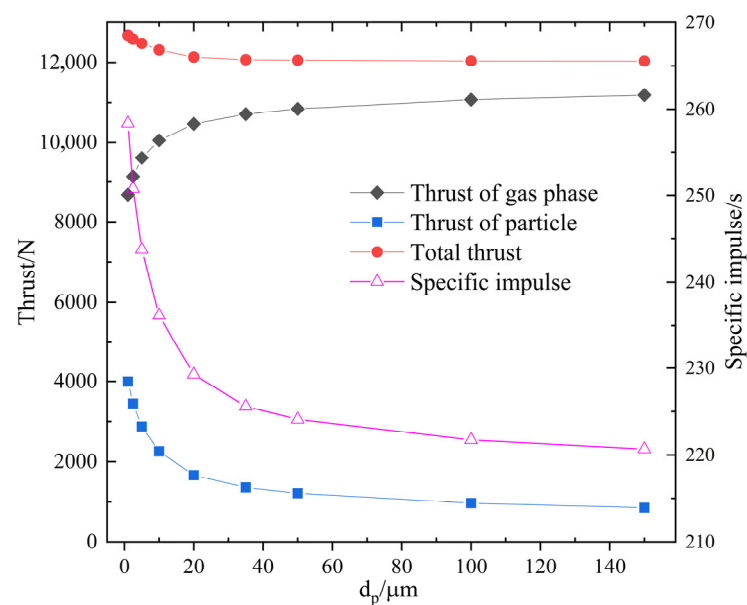


Figure 14. The mole fractions of (a) H_2 , (b) H , and (c) CO inside the nozzle under different operating conditions.

Table 12 and Figure 15 present the performance data of the nozzle, including the mass flow rate, gas phase thrust (including the momentum and pressure thrust), and particle thrust, as well as the total thrust and the specific impulse under different particle sizes, where the diameter of 0 corresponds to the particle-free case. As seen in the table, with the constant inlet pressure, the mass flow rate of the gas-phase is generally smaller with the particle-free case, and increases with the particle diameter. Compared with the particle-free nonequilibrium flow, the gas thrust (mainly contributed by the momentum thrust) is significantly decreased, caused by the reduction of gas mass flow rate, while the particle thrust is enhanced due to the transformed momentum from the gas to the particles, resulting in an overall smaller specific impulse but a larger total thrust. In addition, the gas thrust and momentum thrust increase with the particle diameter while the particle thrust decreases with the diameter, since more momentum is transformed to the particle phase with smaller diameters with better followability. Also, the outlet pressure decreases with the increase in the particle diameter, causing a decrease in pressure thrust and thus a lag of the increase in the gas thrust. As a result, the total thrust and specific impulse both decrease with increasing the diameter, and with the additional influence of the gas-phase mass flow rate, the specific impulse is more significantly affected by the change in particle size. Specifically, the total thrust is enhanced by 6.28% and 0.92% due to the presence of particles with the diameter of 1 μm and 150 μm , while the specific impulse is reduced from 298.14 s for the particle-free case to 258.38 s and 220.68 s for a particle diameter of 1 and 150 μm , representing a maximum decrease of 25.98%.

Table 12. Thrust and specific impulse of the particles under different particle size.

Particle Diameter/ μm	Mass Flow Rate/(kg/s)	Gas Thrust/N	Momentum Thrust/N	Pressure Thrust/N	Particle Thrust/N	Total Thrust/N	Specific Impulse/s
0	4.083	11,928.2	12,218.5	−290.31	0.00	11,928.2	298.14
1	3.357	8682.8	8589.7	93.06	3994.6	12,677.4	258.38
2.5	3.469	9133.4	9082.3	51.09	3446.3	12,579.7	250.77
5	3.573	9602.1	9627.2	−25.15	2874.7	12,476.8	243.75
10	3.669	10,053.5	10,158.7	−105.23	2258.0	12,311.5	236.18
20	3.751	10,471.7	10,648.2	−176.46	1662.2	12,133.9	229.26
35	3.810	10,714.3	10,915.8	−201.55	1356.5	12,070.7	225.59
50	3.839	10,843.1	11,058.6	−215.46	1212.0	12,055.2	224.09
100	3.891	11,073.3	11,309.6	−236.29	966.6	12,039.9	221.73
150	3.916	11,186.7	11,431.1	−244.39	851.5	12,038.2	220.68

**Figure 15.** Variation of thrust and specific impulse with particle size.

4. Conclusions

In this study, a calculation method for two-phase nonequilibrium flow in solid rocket motor nozzles is established, and an in-depth investigation into the laws of nonequilibrium flow within the nozzle is conducted. Firstly, based on NEPE propellant, a simplified chemical nonequilibrium flow reaction mechanism model consisting of 16 components and 22 steps is established and validated using the full-component sensitivity analysis method. Secondly, chemical nonequilibrium flow and frozen flow in the nozzle are simulated. The effects of chemical equilibrium shifts on the temperature, velocity, and component field inside the nozzle are obtained, and the influence of nonequilibrium chemical reactions on nozzle performance is revealed. It is found that in nonequilibrium flow, chemical reactions result in a 22.4% increase in the flow field temperature and an approximate 4.13% improvement in specific impulse. Finally, the effects of different total pressure/total temperature conditions on the nonequilibrium flow in the nozzle are studied. Additionally, a discrete phase model is adopted in the nonequilibrium flow simulation to predict the evolution of Al_2O_3 particles in the nozzle, and the impacts of particle size on the temperature, velocity, component field, and nozzle performance are analyzed. Results show that the particles not only impact the temperature and velocity, but also influence the component fields. As the particle size increases, both the nozzle thrust and specific impulse decrease, with the

specific impulse being more significantly affected by particle size variations due to the variation of the gas-phase mass flow rate. Specifically, the total thrust is enhanced by 6.28% and 0.92% due to the presence of particles with the diameter of 1 μm and 150 μm , while the specific impulse is reduced from 298.14 s for the particle-free case to 258.38 s and 220.68 s for a particle diameter of 1 and 150 μm , representing a maximum decrease of 25.98%.

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