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Simulation of underexpanded supersonic jet flows with chemical reactions

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Abstract To achieve a detailed understanding of underexpanded supersonic jet structures influenced by afterburning and other flow conditions, the underexpanded turbulent supersonic jet with and without combustions are investigated by computational fluid dynamics (CFD) method. A program based on a total variation diminishing (TVD) methodology capable of predicting complex shocks is created to solve the axisymmetric expanded Navier–Stokes equations containing transport equations of species. The finite-rate ratio model is employed to handle species sources in chemical reactions. CFD solutions indicate that the structure of underexpanded jet is typically influenced by the pressure ratio and afterburning. The shock reflection distance and maximum value of Mach number in the first shock cell increase with pressure ratio. Chemical reactions for the rocket exhaust mostly exist in the mixing layer of supersonic jet flows. This tends to reduce the intensity of shocks existing in the jet, responding to the variation of thermal parameters.

1. Introduction

Underexpanded jet flows typically exist in the vicinity of the nozzle outlets of launcher vehicles. Due to the complex physical phenomena such as shock interaction, heat transfer, afterburning, etc., the accurate prediction of flow features is important to designers. In the past decades extensive experimental and theoretical studies have been undertaken to predict underexpanded jet structure.[1,2] Although significant progress has been achieved in understanding the phenomenology of the jet interactions with the ambient atmosphere, several important problems still need to be resolved, particularly with regard to chemical reactions in the turbulent mixing region.

Due to the difficulty of measurements for supersonic flows, intrusive pressure probe measurements[3] were initially utilized to obtain the flow properties of underexpanded jets and the measurements were of the far-field flow only.[4] Recently more measurements have been taken via optical techniques such as particle image velocimetry (PIV), laser Doppler velocimetry, and spectrally resolved Rayleigh scattering.[5,6] Qualitative visualization and identification of shock locations has also been performed by researchers.[7] However, reliable measurements of velocity and turbulence quantities for hot firing jets are not at present available. Hence computational fluid dynamics (CFD) method was wildly applied to modeling of underexpanded jets. The pioneering studies of Dash and Wolf[8] are a good example of numerical methods by using a parabolized Navier–Stokes method with two-equation turbulent model.

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To improve the accuracy and robustness of prediction for highly underexpanded jets numerically, a series of investigations was followed by some researchers.[9–13]

As a matter of fact, the modeling of real hot underexpanded jet flow has more difficulties. Generally, the rocket combustion is optimized at an oxidizer–fuel (O/F) ratio considerably less than stoichiometric, consequently some exhaust species burn when mixed with the air entering the mixing layer. Considering the supersonic flow state, the turbulent mixing and the nonlinear source terms, only a few methods are effective for these chemically reacting jet flows. The finite-rate chemistry method is one of these frequently used models in recent investigations.[14,15] Furthermore, it is clear that the afterburning in jet flows would influence the jet structure significantly and lead to some extra-effects to launcher vehicles. These effects such as contamination and radiation have been investigated by some researchers.[16,17] Nonetheless, the detailed differences between underexpanded jets with or without afterburning models were seldom reported.

The main goal of this work is to achieve a detailed understanding of underexpanded supersonic jet structures influenced by afterburning and examine the difference between the jet flow with or without chemical reactions. The reason for the detailed analysis of afterburning is that the ultraviolet and infrared radiations of exhausted jet flows are concerned in some fields and more accuracy of the flow prediction is needed for these researches. The CFD methodology is described in detail in the following section. Following this, computational conditions and CFD results are discussed based on the distributions of flow parameters. Conclusions are given in the last section.

2. Methodology

2.1. Governing equations

For the prediction of high-speed turbulent combustion jet flows, the expanded Navier–Stokes equations, containing transport equations of species are expressed in axisymmetric form by

$$\frac{\partial \boldsymbol{U}}{\partial t}+\frac{\partial \boldsymbol{E}}{\partial x}+\frac{\partial \boldsymbol{F}}{\partial y}+\boldsymbol{H}=\frac{\partial \boldsymbol{E}_{\mathrm{v}}}{\partial x}+\frac{\partial \boldsymbol{F}_{\mathrm{v}}}{\partial y}+\boldsymbol{H}_{\mathrm{v}}+\boldsymbol{S} \tag{1}$$

where $\boldsymbol{U}$ is conservative variable vector; $\boldsymbol{E}$, $\boldsymbol{F}$ and $\boldsymbol{H}$ are the convective flux vectors; $\boldsymbol{E}_{\mathrm{v}}$, $\boldsymbol{F}_{\mathrm{v}}$ and $\boldsymbol{H}_{\mathrm{v}}$ are the viscid flux vectors; $\boldsymbol{S}$ is sources term. They are given as

$$\boldsymbol{U}=[\rho,\rho Y_i,\rho u,\rho v,e_{\mathrm{t}}]^{\mathrm{T}};$$

$$\boldsymbol{E}=[\rho u,\rho Y_i u,\rho u^2+p,\rho uv,(e_{\mathrm{t}}+p)u]^{\mathrm{T}};$$

$$\boldsymbol{F}=[\rho v,\rho Y_i v,\rho uv,\rho v^2+p,(e_{\mathrm{t}}+p)v]^{\mathrm{T}};$$

$$\boldsymbol{H}=\frac{1}{y}[\rho v,\rho Y_i v,\rho uv,\rho v^2,(e_{\mathrm{t}}+p)v]^{\mathrm{T}};$$

$$\boldsymbol{E}_{\mathrm{v}}=\left[0,\rho\frac{1}{Pr}\cdot\frac{\mu}{\rho}\cdot\frac{\partial Y_i}{\partial x},\tau_{xx},\tau_{xy},u\tau_{xx}+v\tau_{xy}+q_x\right]^{\mathrm{T}};$$

$$\boldsymbol{F}_{\mathrm{v}}=\left[0,\rho\frac{1}{Pr}\cdot\frac{\mu}{\rho}\cdot\frac{\partial Y_i}{\partial y},\tau_{yx},\tau_{yy},u\tau_{xy}+v\tau_{yy}+q_y\right]^{\mathrm{T}};$$

$$\boldsymbol{H}_{\mathrm{v}}=\left[0,\rho\frac{1}{Pr}\cdot\frac{\mu}{\rho}\cdot\frac{\partial Y_i}{\partial y},\tau_{yx},\tau_{yy}-\tau_{\theta\theta},u\tau_{xy}+v\tau_{yy}+q_y\right]^{\mathrm{T}};$$

$$\boldsymbol{S}=[0,\omega_i,0,0,0]^{\mathrm{T}}$$

The variables in these questions are the density ρ, the velocity components u and v, the pressure term p, the species mass fractions Y_i, the kinetic viscosity coefficient μ, the prandtl number Pr, the mass production rate of the ith species ω_i and the total internal energy e_{t}. τ_{xx}, τ_{yy}, τ_{xy}, τ_{yx} and $\tau_{\theta\theta}$ are shear and normal stresses. q_x and q_y represent the energy fluxes due to heat conduction and species diffusion. Sutherland law is used to calculate the viscosity. n_{s} is the number of species. Dalton's law was utilized to determined the mixture pressure of gases, which is given as

$$p=\sum_{i=1}^{n_{\mathrm{s}}}\rho_i\frac{R}{M_i}T \tag{2}$$

where T is the flow temperature; n_s is the number of species; R is the gas constant and M_i is the molar weight of the ith species. Similar to the form of pressure, connections of variables between mixture and individual species are given as

$$\begin{cases}\rho=\sum_{i=1}^{n_{\mathrm{s}}}\rho_i\\ c_p=\sum_{i=1}^{n_{\mathrm{s}}}\\ c_{pi}Y_i\sum_{i=1}^{n_{\mathrm{s}}}\omega_i=0\\ \sum_{i=1}^{n_{\mathrm{s}}}Y_i=1\end{cases} \tag{3}$$

The specific heat c_{pi} of the ith species is expressed as piecewise 4th degree polynomial functions. The total enthalpy of the ith species is given as

$$h_i=\int_{T_0}^{T}c_{pi}\mathrm{d}T+h_i^0 \tag{4}$$

where h_i^0 is the standard heat enthalpy of formation of the ith species at temperature of 298.15 K.

For the modeling of underexpanded jet flow without combustion, the axisymmetric Navier–Stocks equations without species transport equations are utilized in this research, and all flow variables are used in mixture forms.

In order to predict the spatial evolution of these gas jets, the k–ε model based on an eddy viscosity assumption is chosen as the turbulent model in this research. The axisymmetric transport equations for the turbulence kinetic energy k and the dissipation rate ε are given as

$$\begin{aligned}&\frac{\partial(\rho k)}{\partial t}+\frac{\partial(\rho uk)}{\partial x}+\frac{\partial(\rho vk)}{\partial y}+\frac{\rho vk}{y}\\&\quad=\frac{\partial}{\partial x}\left[\left(\mu+\frac{\mu_{\mathrm{t}}}{\sigma_k}\right)\frac{\partial k}{\partial x}\right]+\frac{\partial}{\partial y}\left[\left(\mu+\frac{\mu_{\mathrm{t}}}{\sigma_k}\right)\frac{\partial k}{\partial y}\right]\\&\qquad+\frac{1}{y}\left[\left(\mu+\frac{\mu_{\mathrm{t}}}{\sigma_k}\right)\frac{\partial k}{\partial y}\right]+G_k-\rho\varepsilon\end{aligned} \tag{5}$$