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Nonlinear coupled constitutive relations model and its applications

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Abstract. In the hypersonic expansion flow, multiscale non-equilibrium effects always exist The well-known NS equation is no longer applicable based on the continuum assumption. In order to get the real physical solution of the challenging flow problems, Eu proposed a set of generalized hydrodynamic equations (GHE) from the viewpoint of generalized hydrodynamics formulated in the non-equilibrium ensemble method. However, when it comes to multidimensional problems, GHE seems difficult to be put into the hyperbolic conservation system of partial differential equations. For this reason, Myong takes a form of nonlinear algebraic system and can be solved more easily coupled with the hyperbolic conservation laws by an uncoupled iterative method. In this paper, the hypersonic flow over expanding corner is studied. The NCCR model is used to analyze the flow field with different expansion angles ($45°, 90°, 135°$) by comparing flow field properties (velocity, temperature, density and pressure). The NCCR results are basically identical with the NS results at low Knudsen numbers. As the Knudsen number increasing, the gap between these two methods increases gradually and the NCCR result is much closer to the DSMC results.

Keyword. Nonlinear coupled constitutive relations; non-equilibrium effects; coupled solutions; expansion tube

1 Introduction

In the flow of hypersonic expansion tube, there exists complex flow mechanism, such as the incident expansion wave and the reflection on the wall boundary. At the same time, due to the rapid expansion into the low density, the flow experiences continuum, transition and free molecular regions, which means traditional NS equation is no longer applicable due to the breakdown of continuum assumption.

In order to remedy this issue, Eu proposed a set of generalized hydrodynamic equations (GHE) from the viewpoint of generalized hydrodynamics formulated in the non-equilibrium ensemble method[1,2]. However, the scope of GHE's application is limited in the study of one-dimensional problems. Myong developed a set of nonlinear coupled algebraic equations based on GHE which is called nonlinear coupled constitutive relations (NCCR) model[3]. This model is validated subsequently by the cases of one-dimensional shock wave structure and multidimensional flat plate and blunt-cone flows[3]. It proves the potential of this model to simulate the high-speed rarefied gas dynamic flows. In addition, the NCCR model is consistent with the generalized Newton's law and the Fourier heat conduction law in continuum region, and the non-linear effect increases gradually in the rarefied region. Therefore, it could be widely used to describe the multi-scale effects in the hypersonic rarefied flow.

2 Numerical methods

2.1 Governing equation and nonlinear coupled constitutive relations

In order to simulate non-equilibrium flows, Eu proposed a set of generalized hydrodynamic equations (GHE) based on the generalized theory of fluid dynamics and the unbalanced integration method. Starting from the Boltzmann equation, GHE skillfully constructs a non-equilibrium distribution function and accumulates the integrals of its collisions. The unbalanced distribution function is as follows:

$$f = \exp\left[-\frac{1}{k_B T}\left(\frac{1}{2}mC^2 + H_{rot} + \sum_{k=1}^{\infty} X_k h^{(k)} - \mu\right)\right] \tag{1}$$

where μ is the normalization factor. X_k are functions of macroscopic variables and occupy the status similar to the coefficients of Maxwell-Grad moment method. T , k_B, m and H_{rot} represent temperature, Boltzmann constant, molecular mass and rotational Hamiltonian of molecule respectively. Finally, a set of evolution equations of non-conserved variables for diatomic gases (GHE) could be obtained as

$$\begin{aligned}
&\rho\frac{D(\mathbf{\Pi}/\rho)}{Dt} + \nabla\cdot\psi_4 = -2[\mathbf{\Pi}\cdot\nabla\mathbf{u}]^{(2)} - \frac{p}{\eta}\mathbf{\Pi}q(\kappa) - 2(p+\Delta)[\nabla\mathbf{u}]^{(2)} \\
&\rho\frac{D(\Delta/\rho)}{Dt} + \nabla\cdot\psi_5 = -2\gamma'(\Delta\mathbf{I}+\mathbf{\Pi}):\nabla\mathbf{u} - \frac{2}{3}\gamma' p\nabla\cdot\mathbf{u} - \frac{2}{3}\gamma'\frac{p}{\eta_b}\Delta q(\kappa) \\
&\rho\frac{D(\mathbf{Q}/\rho)}{Dt} + \nabla\cdot\psi_6 = -\mathbf{\Pi}\cdot c_p\nabla T - \mathbf{Q}\cdot\nabla\mathbf{u} - \frac{pc_p}{\lambda}\mathbf{Q}q(\kappa) - (p+\Delta)c_p T\nabla\ln T \\
&\qquad\nabla\cdot[(p+\Delta)\mathbf{I}+\mathbf{\Pi}]\cdot\frac{(\mathbf{\Pi}+\Delta\mathbf{I})}{\rho}
\end{aligned} \tag{2}$$

where ρ, p, T, $\mathbf{\Pi}$, Δ and $\mathbf{Q}$ denote density, hydrostatic pressure, temperature, the shear stress, the excess normal stress and the heat flux respectively. γ' is equal to $(5-3\gamma)/2$ and the nonlinear dissipation factor $q(\kappa)=\sinh(\kappa)/\kappa$. ψ_4, ψ_5 and ψ_6 are the flux of high-order moments. In order to make above evolution equations closed, Eu provided a closure different from Grad's by assuming

$$\psi_4 = \psi_5 = \psi_6 = 0. \tag{3}$$

After applying the adiabatic approximation and omitting the term $\nabla\cdot[(p+\Delta)\mathbf{I}+\mathbf{\Pi}]\cdot\frac{(\mathbf{\Pi}+\Delta\mathbf{I})}{\rho}$ and $\mathbf{Q}\cdot\nabla\mathbf{u}$, the above equation reduces to the form as

$$-2[\mathbf{\Pi}\cdot\nabla\mathbf{u}]^{(2)} - \frac{p}{\eta}\mathbf{\Pi}q(\kappa) - 2(p+\Delta)[\nabla\mathbf{u}]^{(2)} = 0 \tag{4}$$

$$-2\gamma'(\Delta\mathbf{I}+\mathbf{\Pi}):\nabla\mathbf{u} - \frac{2}{3}\gamma' p\nabla\cdot\mathbf{u} - \frac{2}{3}\gamma'\frac{p}{\eta_b}\Delta q(\kappa) = 0 \tag{5}$$

$$-\mathbf{\Pi}\cdot c_p\nabla T - \frac{pc_p}{\lambda}\mathbf{Q}q(\kappa) - (p+\Delta)c_p T\nabla\ln T = 0 \tag{6}$$

In present work, the non-dimensional parameters[4] can be introduced as

$$x^* = \frac{x}{L_0}, y^* = \frac{y}{L_0}, z^* = \frac{z}{L_0}, u^* = \frac{u}{a_\infty}, v^* = \frac{v}{a_\infty}, w^* = \frac{w}{a_\infty}, t^* = \frac{t}{L_0 / a_\infty}, p^* = \frac{p}{\rho_\infty a_\infty^2},$$
$$\rho^* = \frac{\rho}{\rho_\infty}, T^* = \frac{T}{T_\infty}, E^* = \frac{E}{a_\infty^2}, h^* = \frac{h}{a_\infty^2}, \eta^* = \frac{\eta}{\eta_\infty}, \eta_b^* = \frac{\eta_b}{\eta_\infty}, \lambda^* = \frac{\lambda}{\lambda_\infty}, R^* = \frac{R}{a_\infty^2 / T_\infty} = \frac{1}{\gamma}, \tag{7}$$
$$c_p^* = \frac{c_p}{a_\infty^2 / T_\infty} = \frac{1}{\gamma - 1}, c_v^* = \frac{c_v}{a_\infty^2 / T}, \mathbf{\Pi}^* = \frac{\mathbf{\Pi}}{\eta_\infty a_\infty / L_0}, \Delta^* = \frac{\Delta}{\eta_\infty a_\infty / L_0}, \mathbf{Q}^* = \frac{\mathbf{Q}}{\lambda_\infty T_\infty / L_0},$$

where the subscript ∞ represents the reference value of the free stream state. Here L_0 is the characteristic length; a denotes the speed of sound; x, y, z, u, v, w denote the coordinate and the velocity components in three directions respectively; t, p, ρ, T, E and h stand for time, pressure, density, temperature, inner energy and enthalpy respectively; η, η_b, λ mean the coefficients of viscosity, bulk viscosity and heat conduction and R, γ, c_p, c_v represent the gas constant, specific heat ratio, specify heat capacity per mass at constant pressure and at constant volume respectively. For notational brevity, the asterisks are omitted in following non-dimensional equations and the final forms are

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}_c + N_\delta \nabla \cdot \mathbf{F}_v = 0, \tag{8}$$

$$\mathbf{U} = \begin{pmatrix} \rho \\ \rho \mathbf{u} \\ \rho E \end{pmatrix} \quad \mathbf{F}_c = \begin{pmatrix} \rho \mathbf{u} \\ \rho \mathbf{u}\mathbf{u} + p\mathbf{I} \\ (\rho E + p)\mathbf{u} \end{pmatrix} \quad \mathbf{F}_v = \begin{pmatrix} 0 \\ \mathbf{\Pi} + \Delta \mathbf{I} \\ (\mathbf{\Pi} + \Delta \mathbf{I}) \cdot \mathbf{u} + \varepsilon \mathbf{Q} \end{pmatrix},$$

and

$$\hat{\mathbf{\Pi}} q\left(c\hat{R}\right) = (1 + \hat{\Delta})\hat{\mathbf{\Pi}}_0 + \left[\hat{\mathbf{\Pi}} \cdot \nabla \hat{\mathbf{u}}\right]^{(2)}, \tag{9}$$

$$\hat{\Delta} q\left(c\hat{R}\right) = \hat{\Delta}_0 + \frac{3}{2} f_b (\hat{\Delta}\mathbf{I} + \hat{\mathbf{\Pi}}) : \nabla \hat{\mathbf{u}}, \tag{10}$$

$$\hat{\mathbf{Q}} q\left(c\hat{R}\right) = (1 + \hat{\Delta})\hat{\mathbf{Q}}_0 + \hat{\mathbf{\Pi}} \cdot \hat{\mathbf{Q}}_0, \tag{11}$$

where $\hat{\mathbf{\Pi}}_0$, $\hat{\Delta}_0$ and $\hat{\mathbf{Q}}_0$ denote shear stress of the linear Newtonian law, linear excess normal stress and heat conduction of the Fourier law, respectively,

$$\mathbf{\Pi}_0 = -2\eta [\nabla \mathbf{u}]^{(2)}, \quad \Delta_0 = -\eta_b \nabla \cdot \mathbf{u}, \quad \mathbf{Q}_0 = -\lambda \nabla T \tag{12}$$

where

$$\frac{\eta_\infty}{\rho_\infty a_\infty L_0} = N_\delta = \frac{\mathrm{Ma}}{\mathrm{Re}}, \quad \hat{\mathbf{\Pi}} = \frac{N_\delta}{p}\mathbf{\Pi}, \quad \hat{\Delta} = \frac{N_\delta}{p}\Delta, \quad \hat{\mathbf{Q}} = \frac{N_\delta}{p} \frac{\mathbf{Q}}{\sqrt{T/(2\varepsilon)}}$$
$$\hat{R} = \left[\hat{\mathbf{\Pi}} : \hat{\mathbf{\Pi}} + \frac{2\gamma'}{f_b}\hat{\Delta}^2 + \hat{\mathbf{Q}} \cdot \hat{\mathbf{Q}}\right]^{1/2}, \nabla \hat{\mathbf{u}} = -2\eta \frac{N_\delta}{p} \nabla \mathbf{u}, \varepsilon = \frac{1}{\Pr(\gamma - 1)}.$$

2.2 Modified coupled solutions of nonlinear coupled constitutive relations

Based on Myong's uncoupled computational method, three-dimensional problems are simplified approximately into three one-dimensional non-interfering problems in *x*, *y*, *z* directions and the computation of stress and heat flux components on a surface is achieved by the two uncoupled solvers[5, 6]. Nevertheless, this method overlooks the interactional effect of three directions in real flows and weakens the coupled effect of non-conserved variables $\left(\Pi_{xx}, \Pi_{xy}, \Pi_{xz}, \Delta, Q_x\right)$ in constitutive relations. The most unsatisfied feature is the computational instability caused by the existence of a phenomenon that density might come to be negative particularly in some expansion flow regions of wake stream. Therefore, our work would rather focus on the direct solutions of the nonlinear coupled constitutive equations by a coupled solver. Owning to the computation complexity of the coupled constitutive equations, above three equations have to be merged into one formulation firstly by using the Rayleigh-Onsager dissipation function[7]. From tensor expressions above, we can get

$$\hat{R}^2 q\left(c\hat{R}\right) = F \tag{13}$$

where

$$F = (1+\hat{\Delta})\hat{\mathbf{\Pi}}:\hat{\mathbf{\Pi}}_0 + \hat{\mathbf{\Pi}}:\left[\hat{\mathbf{\Pi}}\cdot\nabla\hat{\mathbf{u}}\right]^{(2)} + \frac{2\gamma'}{f_b}\hat{\Delta}\hat{\Delta}_0 + 3\gamma'\hat{\Delta}(\hat{\Delta}\mathbf{I}+\hat{\mathbf{\Pi}}):\nabla\hat{\mathbf{u}} + (1+\hat{\Delta})\hat{\mathbf{Q}}\cdot\hat{\mathbf{Q}}_0 + \hat{\mathbf{\Pi}}:\hat{\mathbf{Q}}_0\hat{\mathbf{Q}}\,.$$

Here a simple iterative method will be adopted to solve equation (14) as

$$\begin{aligned}
\hat{R}_n &= \left[\hat{\mathbf{\Pi}}_n:\hat{\mathbf{\Pi}}_n + \frac{2\gamma'}{f_b}\hat{\Delta}_n^2 + \hat{\mathbf{Q}}_n\cdot\hat{\mathbf{Q}}_n\right]^{1/2} \\
\hat{R}_{n+1} &= \frac{1}{c}\sinh^{-1}\left(\frac{cF_n}{\hat{R}_n}\right) \\
\hat{\mathbf{\Pi}}_{n+1} &= \left((1+\hat{\Delta}_n)\hat{\mathbf{\Pi}}_0 + \left[\hat{\mathbf{\Pi}}_n\cdot\nabla\hat{\mathbf{u}}\right]^{(2)}\right)\frac{\hat{R}_n\hat{R}_{n+1}}{F_n} \\
\hat{\Delta}_{n+1} &= \left(\hat{\Delta}_0 + \frac{3}{2}f_b(\hat{\Delta}_n\mathbf{I}+\hat{\mathbf{\Pi}}_n):\nabla\hat{\mathbf{u}}\right)\frac{\hat{R}_n\hat{R}_{n+1}}{F_n} \\
\hat{\mathbf{Q}}_{n+1} &= \left((1+\hat{\Delta}_n)\hat{\mathbf{Q}}_0 + \hat{\mathbf{\Pi}}_n\cdot\hat{\mathbf{Q}}_0\right)\frac{\hat{R}_n\hat{R}_{n+1}}{F_n}
\end{aligned} \tag{14}$$

And the initial values of shear stress, excess normal stress and heat flux in above equation are calculated below by the linear values $\mathbf{\Pi}_0$, Δ_0 and $\mathbf{Q}_0$ from NSF model as

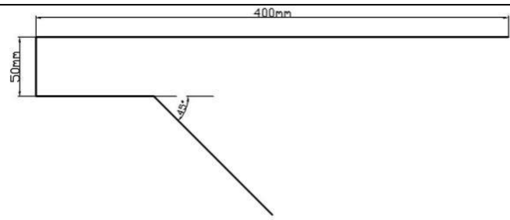
$$\begin{aligned}
\hat{R}_0 &= \left[\hat{\mathbf{\Pi}}_0:\hat{\mathbf{\Pi}}_0 + \frac{2\gamma'}{f_b}\hat{\Delta}_0^2 + \hat{\mathbf{Q}}_0\cdot\hat{\mathbf{Q}}_0\right]^{1/2} \\
\hat{\mathbf{\Pi}}_1 &= \frac{\sinh^{-1}\left(c\hat{R}_0\right)}{c\hat{R}_0}\hat{\mathbf{\Pi}}_0 \\
\hat{\Delta}_1 &= \frac{\sinh^{-1}\left(c\hat{R}_0\right)}{c\hat{R}_0}\hat{\Delta}_0 \\
\hat{\mathbf{Q}}_1 &= \frac{\sinh^{-1}\left(c\hat{R}_0\right)}{c\hat{R}_0}\hat{\mathbf{Q}}_0
\end{aligned} \tag{15}$$

The complete solutions of NCCR model[8,9] are also considered to be converged when $\left|\hat{R}_{n+1}-\hat{R}_n\right| \le 10^{-5}$.

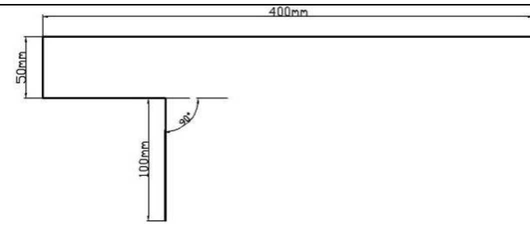
3 Computational results

In this section, the computation results of expending tubes with different expansion angles using nonlinear coupled constitutive relations（NCCR）are presented and compared with DSMC and NS validation data. The configurations of different tubes are depicted in Fig. 1. Maxwell-Smoluchowski slip and jump boundary conditions are applied at the solid surface. The working diatomic gas is assumed pure nitrogen with $Pr = 0.72$, $\gamma = 1.4$, $c = 1.02029$ and $s = 0.74$. The specific inputs for the inflow conditions are listed as

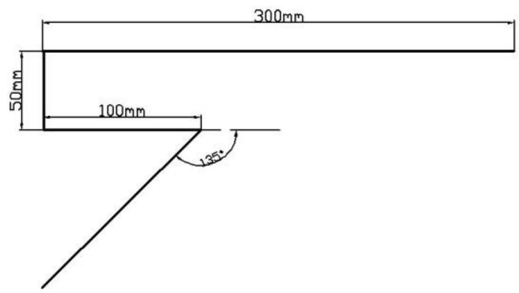
$$
\begin{array}{ll}
U_\infty = 6596.5\,\mathrm{m/s} & P_\infty = 79.7791\,\mathrm{Pa} \\
T_\infty = 270.65\,\mathrm{K} & \rho_\infty = 1.027\times10^{-3}\,\mathrm{kg/m^3} \\
T_w = 300\,\mathrm{K} & R = 296.72\,\mathrm{m^2}/\left(\mathrm{sec^2}\cdot\mathrm{K}\right). \\
Kn_\infty = 1.58\times10^{-3} & Ma_\infty = 20 \\
\eta_{ref} = 1.656\times10^{-5}\,\mathrm{N\cdot s/m^2} & T_{ref} = 273\,\mathrm{K}
\end{array}
$$



(a) *expansion degree* $\alpha = 45°$



(b) *expansion degree* $\alpha = 90°$



(c) *expansion degree* $\alpha = 135°$

FIGURE 1. *Schematic of expansion tube configurations*

The Mach number fields predicted by both NCCR and NS equation can be seen in Figures 2, 3, and 4. As it is compared, in the region of stream entrance, the Mach number simulated by the NCCR solver is coincident with NS solver. However, it exists great difference in the expansion region, especially the cases with larger expending corner. Before we start to research the reason that results in this kind of phenomenon, the contour of continuum breakdown parameter is shown in Fig. 3. The gradient-length-local Knudsen number6 is above 0.05 extremely at the expending region. In this condition, NSF equation will lose its accuracy and be no longer validated. We assume that in the low Knudsen number part, the NCCR result is in good agreement with NS solver and they will be vary with the increasing of non-equilibrium.

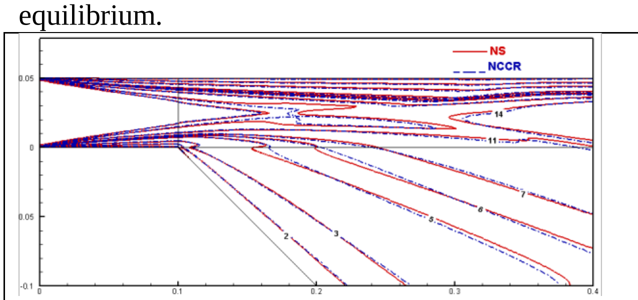


FIG 2. *Mach number contour* $(\alpha = 45°)$

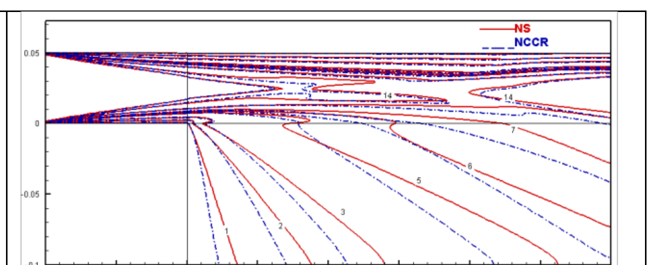


FIG 3. *Mach number contour* $(\alpha = 90°)$

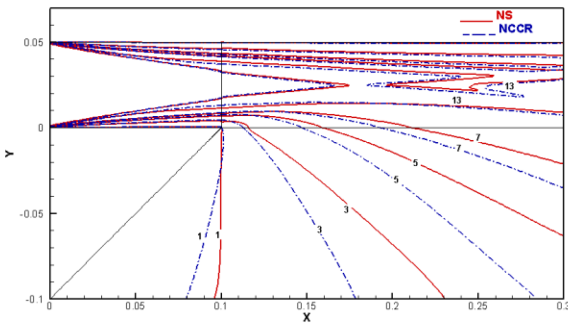


FIG 4. *Mach number contour* $(\alpha = 135°)$

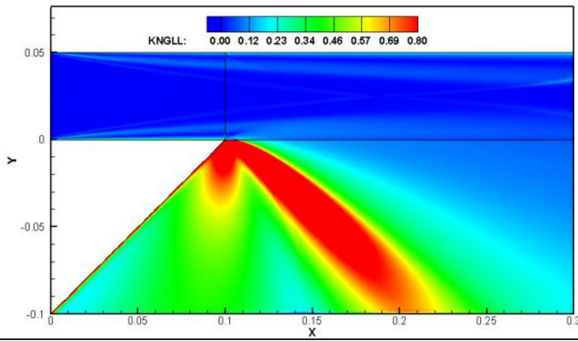
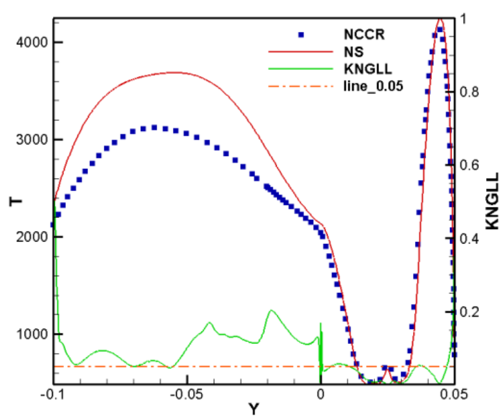
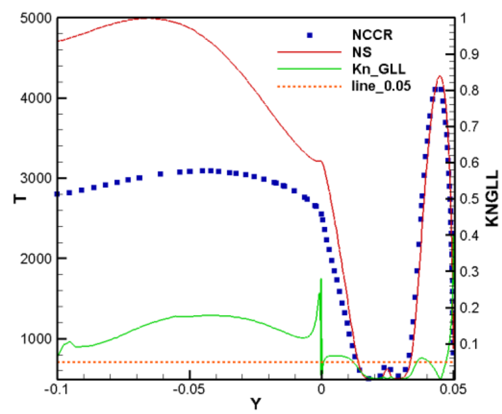


FIG 5. Kn_{GLL} *contour*

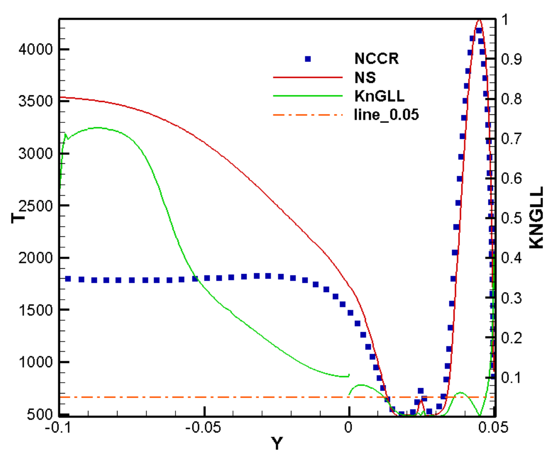
These assumptions are confirmed by the results that are shown in Figure 6, which are extracted at the line of $X = 0.2mm$. As it is displayed, the temperature is sensitive to non-equilibrium of the flow field. In the section from 0.01 to 0.05 mm, the Kn_{GLL} less than 0.05, value provides well agreement. In the rest expending region, as the flow becomes more rarefied, temperature of two methods becomes totally different. The result simulated by NS solver exceeds the NCCR equation, especially in the part with high Kn_{GLL}.



(a) *expansion degree* $\alpha = 45°$



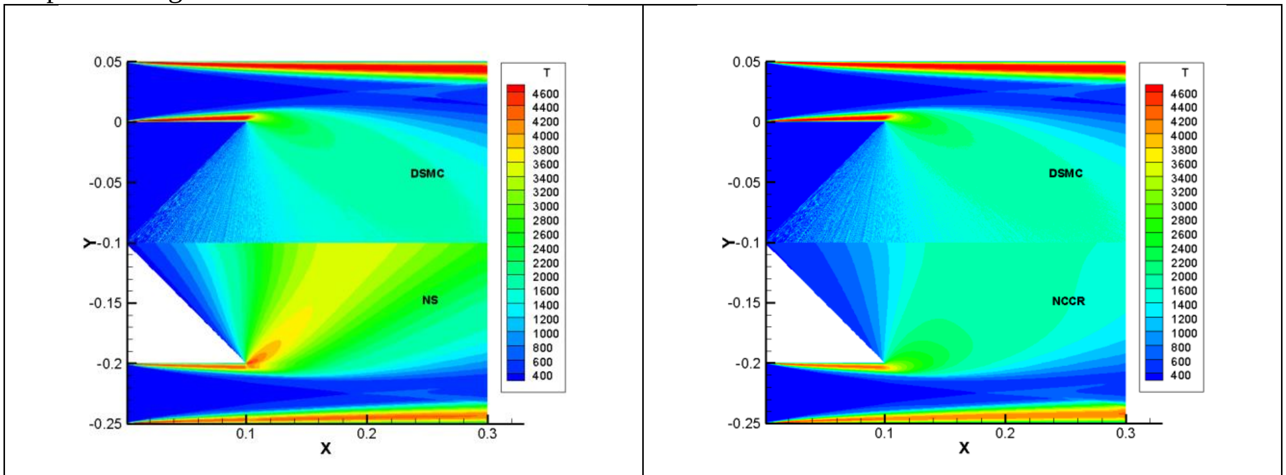
(b) *expansion degree* $\alpha = 90°$



(c) *expansion degree* $\alpha = 135°$

FIG 6. *Distribution profiles of temperature and* Kn_{GLL}

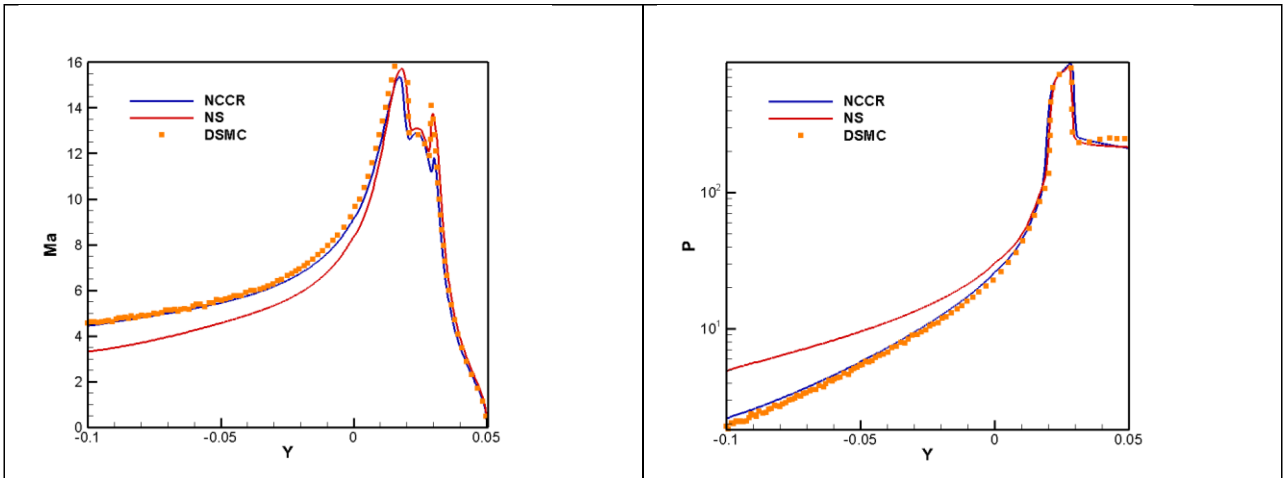
To verify the accuracy of NCCR model in non-equilibrium flow region, we use the open-source software SPARTA to model the same cases. SPARTA is a Direct Simulation Montel Carlo (DSMC) simulator, developed at Sandia National Laboratories, a US Department of Energy facility in 2014. Figure 7 compare the whole flow field temperature of DSMC with NCCR and NS method. It is obviously that temperature simulated by DSMC method is lower than NS solver and in accord with NCCR model in the expansion region.



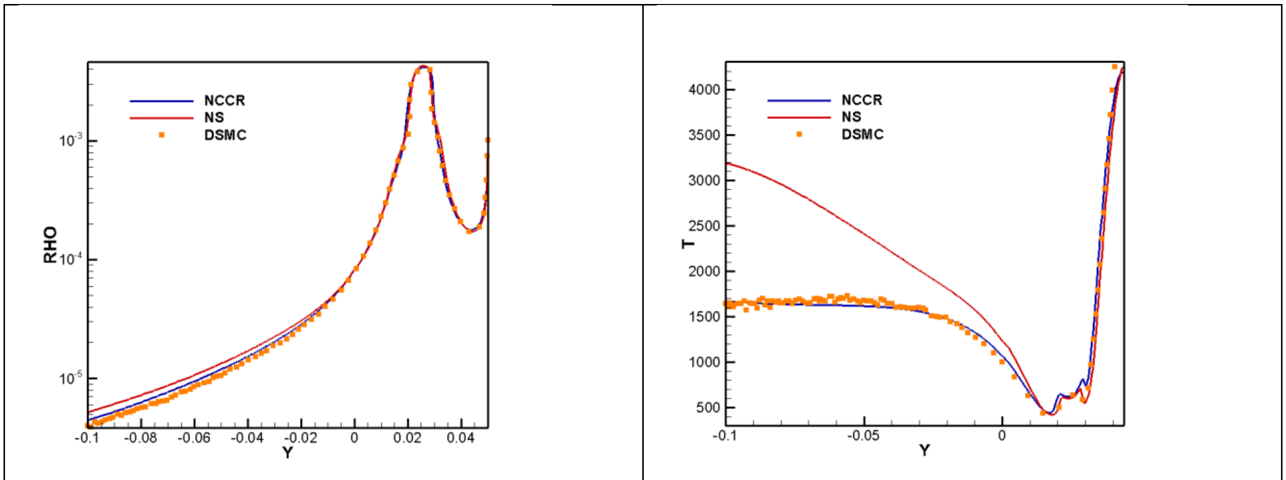
(a) *DSMC and NS* | (b) *DSMC and NCCR*

FIG 7. *Temperature contours by different methods*

In Figure 8, we extract the line of *x*=0.25mm to compare flow properties, such as Mach number, pressure, density and temperature. In Figure (b) and (c), log scale in y axis is used to make comparison much more fairly. All results show that NCCR results computed by the coupled iterative solver are in outstanding agreement with the DSMC results and the NSF results cannot match with DSMC results, especially in the expansion domain which is considered to be removed from local thermodynamic equilibrium based on continuum breakdown parameter Kn_{GLL} .



(a) *Mach number* | (b) *Pressure*



(c) *Density* | (d) *Temperature*

FIG 8. *Comparison of flow property profiles at x=0.25mm*

4 Conclusions

The main point of this paper is focused on the further extension of NCCR model into multi-scale problem and the validation of a reliable coupled solution for this model with three-dimensional FVM schemes. Based on the new modified solution, three kinds of expansion tubes for a diatomic gas are on detailed researches. The NCCR model is shown to yield some quantitative agreement with DSMC data in the prediction of hypersonic and rarefied flows compared with linear constitutive relation NSF. The successful applications in these far-from-equilibrium cases have implied the potential of NCCR model as an alternative to more computationally intensive DSMC and less accurate NSF linear constitutive relations in prediction of hypersonic and rarefied flow.

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