On the Stability of Higher-Order Continuum (HOC) Equations for Hybrid HOC/DSMC Solvers

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Abstract. Our interest in the stability analysis of the high-order continuum (HOC) equations is motivated by the relevance to the development of a hybrid method combining such equations with the Direct Simulation Monte-Carlo (DSMC) technique for the computation of hypersonic flows in all regimes – continuum, transition, and rarefied. The hybrid approach allows the effects of thermophysics (thermal and chemical non-equilibrium) and turbulence to be included much more easily than in other approaches, and can easily be developed into a robust and efficient engineering tool for practical 3D hypersonic computations. Stability characteristics of model HOC equations when subjected to small disturbances are investigated. We explore the feasibility of simplified, yet accurate and numerically stable, versions of the HOC equations and extend our previous work[2] to include multidimensional Burnett equations, with the specific example of the Augmented Burnett models. The latter is shown to have a much wider stability regime than Lumpkin's model.

INTRODUCTION

Hypersonic flows about space vehicles produce flow fields with local Knudsen numbers, K_n, which may lie in all the three regimes – continuum, transition, and rarefied. The Navier-Stokes (NS) equations and the direct simulation Monte-Carlo (DSMC) methods can accurately and efficiently model flows in the continuum and rarefied regimes, respectively. The kinetic approach considers an ensemble of small particles or molecules whose distribution function can be determined as a solution of the Boltzmann equation, while the continuum approach is based on the representation of the gas as a fluid continuum governed by the mass, momentum, and energy conservation laws. Though, theoretically, the kinetic approach is appropriate for simulating gas flows in any regime, in practice, it can require large computer resources if the gas flow is dense. DSMC remains the most efficient numerical technique for solving the Boltzmann equation [1]. It enables the computation of flows with high Knudsen number. Nevertheless, DSMC computations are still too expensive in many cases, especially for 3D engineering applications. Although a rather efficient tool for supersonic and particularly hypersonic flows, the DSMC procedure becomes more resource-consuming for low Mach number subsonic flows, due to difficulties with boundary condition implementation on subsonic inflow/outflow boundaries. Furthermore, obtaining gas interactions with DSMC is a difficult task. The continuum approach is much cheaper and more versatile in these regards. There is, therefore, a strong motivation for its utilization at the low K_n values. The traditional continuum model is based on the Navier-Stokes equations, which are the first order approximations to the Boltzmann equation with respect to the (small) parameter K_n. Coupled with no velocity slip/no temperature jump solid wall boundary conditions, they are valid if the Knudsen number is small, say, less than 0.001. More rarefied flows should be described using the Navier-Stokes equations with velocity slip/temperature jump boundary conditions.

The flows in the transitional regime require higher-order continuum (HOC) models; the most well-known being the Burnett equations, obtained as second order approximations. Though there are some difficulties with the stability of their solutions and the development of relevant solid wall boundary conditions, recent advancements [2] allow the consideration of the (properly modified) Burnett equations as a potential continuum model for transitional flows. In recent years, Burnett equations have been successfully employed to compute 3D hypersonic flows in continuum-transition regime [3], although it has been difficult to compute flows for K_n>1.

The other high-order continuum (HOC) equations, such as Eu's [4] and Grad's 13-moment equations [5], are significantly more expensive to compute than the Burnett equations, and have been tested only for 1D and for 2D geometrically simple problems. Another approach is due to Aristov and Tcheremissin [6],

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wherein the left-hand side of the Boltzmann equation is solved with a finite-difference scheme and a special quadrature formula is employed for the collision integral on the right-hand side. This method has recently been applied to solve 2D problems involving a mono-atomic gas. Application of the approach to gases with internal degrees of freedom is problematic at the moment because of the difficulty with the inclusion of chemical reactions. We therefore investigate the Burnett equations for use as the HOC component of our hybrid procedure.

In this paper, we examine the stability of a few versions of the Burnett equations, to guide the selection of the model for a robust hybrid procedure for hypersonic flows. In specifics, we will examine Lumpkin's simplified model [7], the generalized Burnett equations, and the Augmented Burnett equations for their relative stability characteristics. Although the stability analysis of the Burnett equations have been reported in the literature,[8] the studies did not include Lumpkin's model or considered the presence of rotational temperature in the analysis.

ANALYSIS OF LUMPKIN'S SIMPLIFIED BURNETT EQUATIONS

The one-dimensional equations are considered for the analysis of Lumpkin's simplified model, with $\varpi = 8$ and $\theta = \left(\theta_1 + \frac{8}{3}\theta_2 + \frac{2}{3}\theta_3 + \frac{2}{3}\theta_5\right)$ in the standard Burnett equations.[2,3,8] The resulting equations can be written as follows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} = 0\,, \tag{1}$$

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial}{\partial x}\left(p + \rho u^2\right) = -\frac{\partial \tau_{xx}}{\partial x}\,, \tag{2}$$

$$\frac{\partial(\rho E)}{\partial t} + \frac{\partial}{\partial x}\left(pu + \rho E u\right) = -\frac{\partial}{\partial x}\left(u\,\tau_{xx}\right) - \frac{\partial q}{\partial x}\,, \tag{3}$$

$$\frac{\partial(\rho T_R)}{\partial t} + \frac{\partial}{\partial x}\left(\rho u T_R\right) = \mu\frac{\partial^2 T_R}{\partial x^2} + \frac{4\rho p(6T_t - T_R)}{5\pi\mu Z_R}\,, \tag{4}$$

where

$$\tau_{xx} = \left(-\frac{4}{3}\mu + \frac{\pi\mu(\gamma-1)^2 Z_R}{4}\right)\frac{\partial u}{\partial x} + \frac{8\mu^2}{p}\left(\frac{\partial u}{\partial x}\right)^2, \tag{5}$$

$$q = -\frac{15}{4}\mu R\frac{\partial T_t}{\partial x} + \frac{40}{9}\frac{\mu^2}{\rho T_t}\left(\frac{\partial u}{\partial x}\right)\left(\frac{\partial T_t}{\partial x}\right) - \mu R\frac{\partial T_R}{\partial x}\,, \tag{6}$$

and $E = \frac{1}{2}\left(3RT_t + 2RT_R + u^2\right)$, $p = \rho R T_t$, T_R, T_t, μ, and Z_R are the total energy/unit mass, hydrodynamic pressure, rotational temperature, translational temperature, molecular viscosity, and the rotational collision number. Note that τ_R is the relaxation time for rotational energy, so that $Z_R\tau_c = Z_R\left(\frac{\pi\mu}{4p}\right)$, where τ_c is the mean collision time.

Linearization of the Equations

Consider a diatomic gas in equilibrium with density ρ_0, pressure p_0, translational temperature T_{t0} and rotational temperature T_{R0}. The gas is subjected to small perturbations defined as the non-dimensional variables:

$$\rho' = \frac{\rho - \rho_0}{\rho_0}\,,\; T_t' = \frac{T_t - T_{t0}}{T_{t0}}\,,\; T_R' = \frac{T_R - T_{R0}}{T_{R0}}\,,\; u' = \frac{u}{\sqrt{RT_{t0}}}\,,\; t' = \frac{t}{\mu_0/\rho_0}\,,\; x' = \frac{x}{L_0}\,,$$

$L_0 = \dfrac{\mu_0}{\rho_0\sqrt{RT_{t0}}}$. Note that $T_{R0} = T_{t0}$ is assumed.

The linearized equations can be written as:

$$\frac{\partial V'}{\partial t'} + L_1\frac{\partial V'}{\partial x'} + L_2\frac{\partial^2 V'}{\partial x'^2} + L_0 V' = A, \tag{7}$$

where $V' = [\rho' \quad u' \quad T_t' \quad T_R']^T$ and

$$L_1 = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 2/3 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad L_2 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & \left\{-\frac{4}{3} + \frac{\pi}{4}(\gamma-1)^2 Z_R\right\} & 0 & 0 \\ 0 & 0 & -5/2 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}, \quad L_0 = C\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{20}{3} & 0 & \frac{22}{3} & -\frac{2}{3} \\ -10 & 0 & -11 & 1 \end{bmatrix}, \tag{8}$$

and $A = [0, 0, -\frac{10}{3}C, 5C]^T$, where "T" denotes the transpose operator.

Solution of the Linearized Equations

Consider the homogeneous portion of the linearized equations and assume $V' = \bar{V}e^{i\omega x'}e^{\phi t'}$, where $\phi = \alpha + i\beta$ and $\omega = \frac{2\pi}{L/L_0}$. Since $L_0 = \frac{\mu_0}{\rho_0\sqrt{RT_0}} = 0.783\lambda$, we have $\omega = 4.92\frac{\lambda}{L} = 4.92K_n$, where K_n is the Knudsen number. The dispersion relation is

$$\det\left|\phi I + i\omega L_1 - \omega^2 L_2 + L_0\right| = 0, \tag{9}$$

which can be simplified to

$$\phi^4 + \left[\left(\frac{29}{6} - \frac{\gamma-1}{5C}\right)\omega^3 + \frac{25}{3}C\right]\phi^3 + \omega^2\left[\omega^2\left\{\frac{43}{6} - \frac{7}{10}\frac{\gamma-1}{C}\right\}\omega^2 + \frac{377}{18}C - \frac{5\gamma}{3} + \frac{10}{3}\right]\phi^2$$
$$+\omega^2\left[\left(\frac{10}{3} - \frac{\gamma-1}{2C}\right)\omega^4 + \left\{59\left(\frac{2C}{9} - \frac{\gamma-1}{30}\right) + \frac{25}{6}\right\}\omega^2 + \frac{7}{3}C\right]\phi$$
$$+\frac{5}{2}\omega^6 + \frac{19}{6}\omega^4 C = 0; \quad C \equiv \frac{4}{5\pi Z_R}. \tag{10, 11}$$

This equation was solved using MATLAB to determine the stability boundaries for Z_R = 4, 10, 18, and 23. Note that Lumpkin recommended $18 \le Z_R \le 23$ for his model and that Jean's equation has been used in the source term.

The stability boundaries are shown in figures 1 and 2 for various values of Z_R. Regions with $\alpha < 0$ (on the *x*-axis) are stable, whereas regions with $\alpha > 0$ are unstable. γ is taken as 1.4 for a diatomic gas.

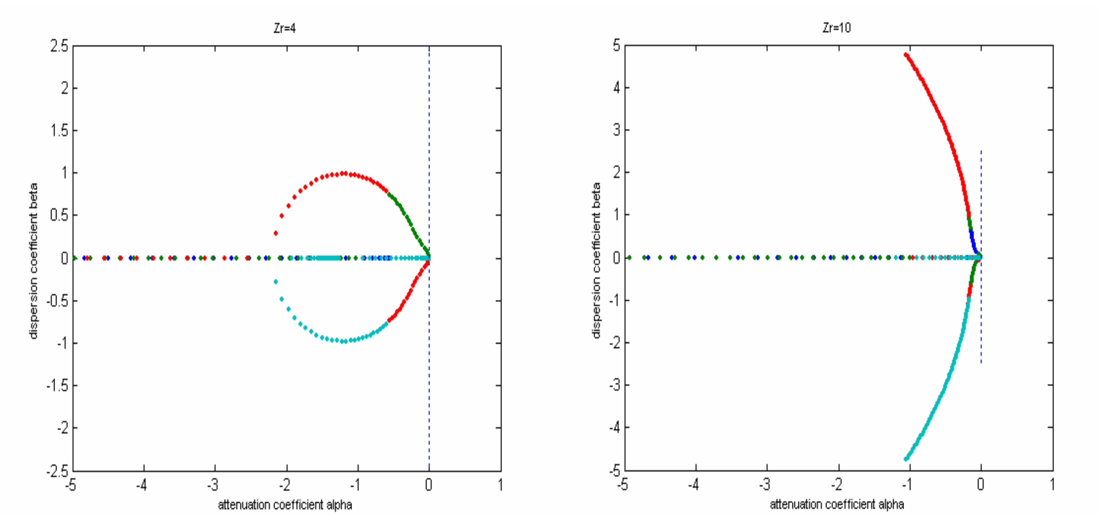

FIGURE 1. Stability boundaries of Lumpkin's simplified Burnett model for Z_R =4 and 10

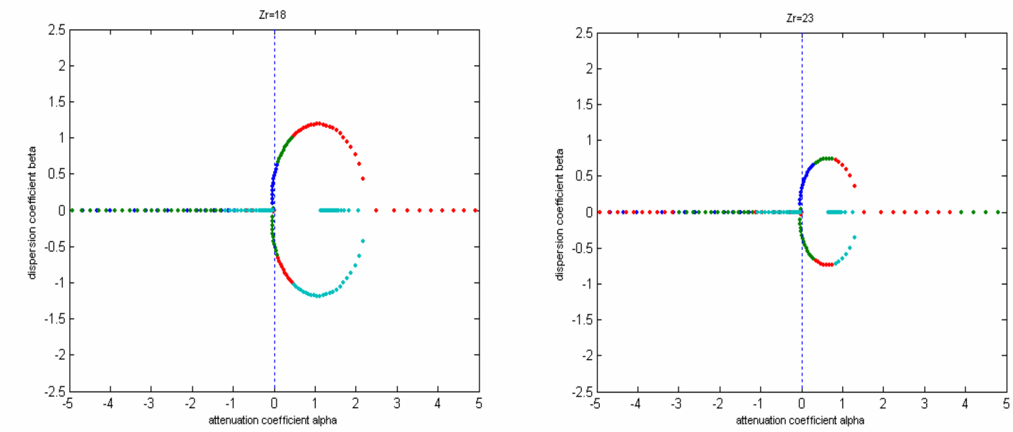

FIGURE 2. Stability boundaries of Lumpkin's simplified Burnett model for Z_R =18 and 23

ANALYSIS OF THE GENERALIZED 3D BURNETT EQUATIONS

The governing equations considered for the stability analysis of the 3D Burnett equations with translational and rotational thermal non-equilibrium are as follows:

$$\frac{\partial \rho}{\partial t}+\frac{\partial(\rho u)}{\partial x}+\frac{\partial(\rho v)}{\partial y}+\frac{\partial(\rho w)}{\partial z}=0, \tag{12}$$

$$\frac{\partial(\rho u)}{\partial t}+\frac{\partial}{\partial x}\left(P+\rho u^2\right)+\frac{\partial}{\partial y}(\rho uv)+\frac{\partial}{\partial z}(\rho uw)=-\frac{\partial \tau_{xx}}{\partial x}-\frac{\partial \tau_{xy}}{\partial y}-\frac{\partial \tau_{xz}}{\partial z}, \tag{13}$$

$$\frac{\partial(\rho v)}{\partial t}+\frac{\partial}{\partial x}(\rho vu)+\frac{\partial}{\partial y}\left(\rho v^2+P\right)+\frac{\partial}{\partial z}(\rho vw)=-\frac{\partial \tau_{xy}}{\partial x}-\frac{\partial \tau_{yy}}{\partial y}-\frac{\partial \tau_{yz}}{\partial z}, \tag{14}$$

$$\frac{\partial(\rho w)}{\partial t}+\frac{\partial}{\partial x}(\rho wu)+\frac{\partial}{\partial y}(\rho wv)+\frac{\partial}{\partial z}\left(\rho w^2+P\right)=-\frac{\partial \tau_{xz}}{\partial x}-\frac{\partial \tau_{yz}}{\partial y}-\frac{\partial \tau_{zz}}{\partial z}, \tag{15}$$

$$\frac{\partial(\rho E)}{\partial t}+\frac{\partial}{\partial x}(pu+\rho Eu)+\frac{\partial}{\partial y}(pv+\rho Ev)+\frac{\partial}{\partial z}(pw+\rho Ew)=$$

$$-\left\{\frac{\partial}{\partial x}\left(u\tau_{xx}+v\tau_{xy}+w\tau_{xz}\right)+\frac{\partial}{\partial y}\left(u\tau_{xy}+v\tau_{yy}+w\tau_{yz}\right)+\frac{\partial}{\partial z}\left(u\tau_{xz}+v\tau_{yz}+w\tau_{zz}\right)\right\}-\left(\frac{\partial q_x}{\partial x}+\frac{\partial q_y}{\partial y}+\frac{\partial q_z}{\partial z}\right),$$

$$\frac{\partial(\rho e_r)}{\partial t}+\frac{\partial}{\partial x}(\rho Eu)+\frac{\partial}{\partial y}(\rho e_r v)+\frac{\partial}{\partial z}(\rho e_r w)=-\left(\frac{\partial q_r}{\partial x}+\frac{\partial q_r}{\partial y}+\frac{\partial q_r}{\partial z}\right)+\frac{\rho \Delta e_r}{Z_r \tau_c}. \tag{16}$$

Note that the last equation is for the rotational energy and that

$$\tau_{ij}=\left(\tau_{ij}\right)_{N.S}+\left(\tau_{ij}\right)_{Burnett}+\left(\tau_{ij}\right)_{augmented}, \tag{17}$$

$$q_i=\left(q_i\right)_{N.S}+\left(q_i\right)_{Burnett}+\left(q_i\right)_{augmented}, \quad E=\frac{3}{2}RT_t+RT_R+\frac{1}{2}\left(u^2+v^2+w^2\right), \tag{18}$$

$\Delta e_r=\frac{4}{5}\left[E-\frac{1}{2}\left(u^2+v^2+w^2\right)\right]-e_r=\frac{R}{5}\left(6T_t-T_R\right)$, $\tau_c=\frac{\pi\mu}{4p}$ is mean collision time, as before, so that

$$\frac{\rho \Delta e_r}{Z_R \tau_c}=\frac{4p\rho R\left(6T_t-T_R\right)}{5\pi\mu Z_R}. \tag{19}$$

The Linearized Equations

Using a similar non-dimensionalization scheme as above, the equations can be written as

$$\frac{\partial V'}{\partial t'} + L_1 \frac{\partial V'}{\partial x'} + M_1 \frac{\partial V'}{\partial y'} + N_1 \frac{\partial V'}{\partial z'} + L_2 \frac{\partial^2 V'}{\partial x'^2} + M_2 \frac{\partial^2 V'}{\partial y'^2} + N_2 \frac{\partial^2 V'}{\partial z'^2} + L_3 \frac{\partial^3 V'}{\partial x'^3}$$
$$+ M_3 \frac{\partial^3 V'}{\partial y'^3} + N_3 \frac{\partial^3 V'}{\partial z'^3} + M_4 \left(\frac{\partial^4 V'}{\partial x'^4} + \frac{\partial^4 V'}{\partial y'^4} + \frac{\partial^4 V'}{\partial z'^4} \right) + L_o V' = S \quad (20)$$

Define $A = \frac{4}{3} + \frac{\pi}{4}(\gamma - 1)^2 Z_R$, $V' = [\rho, u', v', w', T_t', T_R']^T$, where

$$L_1 = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2/3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \quad M_1 = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2/3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \quad N_1 = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 2/3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \quad L_2 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -A & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -5/2 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix},$$

$$M_2 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -A & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -5/2 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix}, \quad N_2 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -A & 0 & 0 \\ 0 & 0 & 0 & 0 & -5/2 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix}, \quad L_3 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ -4/3 & 0 & 0 & 0 & 2/3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -7/6 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \quad M_3 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -4/3 & 0 & 0 & 0 & 2/3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -7/6 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix},$$

$$N_3 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -4/3 & 0 & 0 & 0 & 2/3 & 0 \\ 0 & 0 & 0 & -7/6 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \quad M_4 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \omega_7 & 0 & 0 & 0 & 0 \\ 0 & 0 & \omega_7 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \omega_7 & 0 \\ 2/3\,\theta_6 & 0 & 0 & 0 & 2/3\,\theta_7 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix},$$

$$L_o = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{20}{3}C & 0 & 0 & 0 & \frac{22}{3}C & \frac{-2}{3}C \\ -10C & 0 & 0 & 0 & -11C & C \end{bmatrix}, \quad S = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \frac{-10}{3}C \\ 5C \end{bmatrix}. \quad (21)$$

We assume a solution of the form $V' = \overline{V} e^{i\varpi x'} e^{i\varpi y'} e^{i\varpi z'} e^{\phi t'}, \phi = \alpha + i\beta, \varpi = \frac{2\pi}{L/L_o}$ and obtain the characteristic equation for ϕ:

$$\left| \phi I + i\varpi(L_1 + M_1 + N_1) - \varpi^2(L_2 + M_2 + N_2) - i\varpi^3(L_3 + M_3 + N_3) + 3\varpi^4 M_4 \right| = 0 \cdot \quad (22)$$

This results in a sixth-order polynomial in ϕ, whose trajectories determine the stability boundary. The following three limits can be observed:

A. L_3, M_3, N_3, $M_4 = 0$ → Navier-Stokes equations with translational and rotational non-equilibrium. This limit has been analyzed for various values of Z_R, and they are known to be stable for $Z_R = 0$.
B. $M_4 = 0$ → conventional Burnett equations with translational and rotational non-equilibrium. The equations are known to be unstable for all Z_R including $Z_R = 0$.
C. $M_4 \neq 0$ → Augmented Burnett equations. We studied their stability for various values of Z_R. For $Z_R = 0$, they are known to be stable if

$$\omega_7 = \frac{2}{9} \quad \theta_6 = \frac{-5}{8} \quad \theta_7 = \frac{11}{16} \cdot \quad (23)$$

We will consider $0 < Z_R < 23$ in Case C. By changing the values of ω_7, θ_6, and θ_7, we will try to extend the stability for the largest Z_R value.

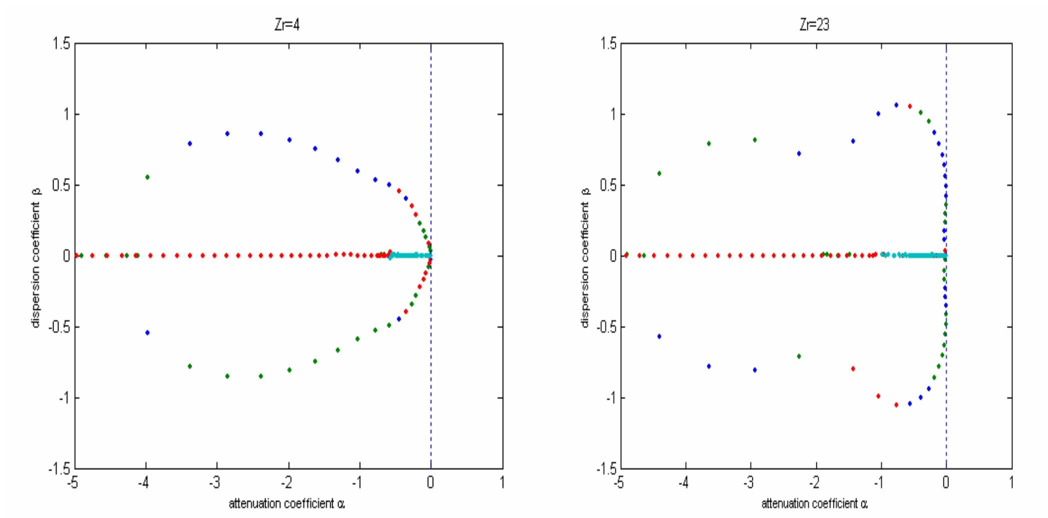

FIGURE 3. Stability boundaries of the Augmented Burnett equations for Z_R =4 and 23

RESULTS SUMMARY

It is apparent that the Lumpkin's equations are unstable to small perturbations in a quiescent fluid when $Z_R > 0$ and stable otherwise. Although the simplified model seems to work well in some cases,[2] it will be necessary to use either the Augmented or BGK-Burnett model to include the rotational non-equilibrium. However, detailed stability characteristics of these equations are of interest and will be carried out in further studies. Note that $\omega = 4.92K_n$, and that the stability boundaries have been determined by varying K_n from 0 to 1 using 100 points. We have also examined the stability of the 1D Augmented Burnett equations for Z_R =4, 18, and 23. The results for Z_R =4 and 3 are shown in figure 3. The results for the Case Z_R =18 are similar to those for Z_R = 23 and are therefore not shown in this paper. As the figures show, we have found that, with the appropriate coefficients, the Augmented equations are stable for Z_R values up to 23. This suggests the superiority of the Augmented Burnett equations over Lumpkin's simplified model. Hence, the former might be more appropriate for subsequent work on hybrid HOC/DMSC procedures. We have incorporated a few physically realizable and computationally stable versions of the Burnett equations into LAURA [9] and combined this with a DSMC procedure. Details are available in [10].

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