

# **13-moment-equations from nonequilibrium thermodynamics and kinetic theory: Comparison for non-linear one-dimensional flows**

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# 13-moment-equations from nonequilibrium thermodynamics and kinetic theory: Comparison for non-linear one-dimensional flows

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## AFFILIATIONS

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## ABSTRACT

The GENERIC-13 moment equations (general equation for the non-equilibrium reversible-irreversible coupling) [Struchtrup & Öttinger, Phys. Fluids **34**, 017105 (2022)] were developed to have complete thermodynamic structure, in contrast to Grad's 13-moment equations which are not accompanied by a suitable formulation of the second law of thermodynamics and loose hyperbolicity for larger deviations from equilibrium. With GENERIC-13 constructed to agree with Grad-13 to second order in the Knudsen number, both sets are considered and compared for hyperbolicity and plane heat transfer, and Couette and Poiseuille flows. It is shown that the GENERIC-13 equations are unconditionally hyperbolic. Jump and slip boundary conditions for GENERIC-13 are developed from the second law with coefficients adapted from kinetic theory. Additional *asymptotically vanishing* boundary conditions are constructed such that solutions of the GENERIC-13 equations reduce to those of Grad-13 to second and of Navier–Stokes–Fourier equations to first order in the Knudsen number.

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## I. INTRODUCTION

This contribution concerns macroscopic equations for the description or rarefied gas flows, that is, flows beyond the traditional hydrodynamic regime. Specifically, we compare solutions of the recently presented GENERIC-13 equations<sup>1,2</sup> to those of the Grad-13 moment equations<sup>3–5</sup> and the Navier–Stokes–Fourier equations.

The most accurate description for rarefied gas flows is given through the Boltzmann equation, which describes the gas behavior on the microscopic level, such that the solution of the equation yields the velocity distribution function of the particles.<sup>6–8</sup> While the Boltzmann equation provides excellent description on all scales, it requires costly numerical solutions and does not allow insightful analytical solutions for problems in simple geometries.

Relevant macroscopic flow properties such as mass density  $\rho$ , velocity  $v_i$ , and temperature  $T$  are obtained as suitable moments of the distribution function. Thus, one can either first solve the Boltzmann equation and then determine the macroscopic properties from the solution or, as an alternative, one might derive transport equations for the macroscopic properties from the Boltzmann equations and then solve these.

The Navier–Stokes–Fourier (NSF) equations of classical hydrodynamics are obtained by Chapman–Enskog expansion of the Boltzmann

equation as the first-order approximation in the Knudsen number  $\text{Kn}$ , which is defined as the ratio between mean free path and required length of resolution.<sup>6–8</sup> Thus, the NSF equations provide an excellent description of gas flows as long as the Knudsen number is sufficiently small.<sup>6–10</sup> For the smaller relative scales encountered in rarefied gas flows, such as micro and nano flows as well as in vacuum flows, for which the Knudsen number is not small, the NSF equations lose validity, and analysis and simulation of such flows must rely on more elaborate models.

Higher order approximations based on the Chapman–Enskog expansion yield unstable equations<sup>8,11</sup> and thus must be discarded. An alternative approach is offered by Grad's moment method, which yields stable equations.<sup>3,4,7,8</sup> In the moment method, the set of hydrodynamic variables, i.e., mass density  $\rho$ , flow velocity  $v_i$ , and temperature  $T$ , is extended by adding higher moments of the distribution function and deriving their transport equations from the Boltzmann equation with a suitable closure. Grad's famous 13-moment equations are obtained by extending the set of variables with stress tensor  $\sigma_{ij}$  and heat flux vector  $q_i$ , while addition of higher moments produces Grad-type moment systems with, e.g., 14, 20, 21, 26, 35, and more variables.<sup>8,12</sup> By combining the ideas of the Grad and Chapman–Enskog methods it is seen<sup>5,9,13</sup> that the choice of variables in the Grad method

is linked to orders in the Knudsen number, such that the Grad-13 equations are accurate to second order  $\mathcal{O}(\text{Kn}^2)$  and the Grad-26 equations are  $\mathcal{O}(\text{Kn}^4)$ , while the NSF equations are  $\mathcal{O}(\text{Kn})$ , and the regularized 13-moment equations (R13) are  $\mathcal{O}(\text{Kn}^3)$ .

As approximations to the Boltzmann equation, Grad-type moment equations do not fully inherit the properties of the Boltzmann equation but reflect these only in approximation. Most importantly, the Boltzmann equation is in full agreement with the second law of thermodynamics: Boltzmann's famous H-theorem guarantees proper approach to stable equilibrium states.<sup>6–8</sup> In contrast, only the fully linearized Grad-type moment equations are accompanied by a formulation of the second law.<sup>10,14</sup> Non-linear Grad equations yield excellent results for a wide range of conditions,<sup>10,15</sup> where they behave as if accompanied by the second law, but under extreme non-linearity they might give unreasonable results. Moreover, Grad moment systems form sets of generally hyperbolic partial differential equations, but hyperbolicity breaks down under strong non-linearities.<sup>12</sup>

The loss of thermodynamic and mathematical structure in the Grad equations is related to Grad's closure by a perturbation of the equilibrium distribution function, which unavoidably loses positivity for fast particles, the more so as the non-equilibrium becomes stronger. An alternative closure is offered by entropy maximization (MaxEnt), which yields a strictly positive distribution for closure, and is equivalent to the principles of *Rational Extended Thermodynamics*.<sup>12,16</sup> The MaxEnt closure guarantees unrestricted validity of the second law and global hyperbolicity of its closed transport equations<sup>12</sup>; however, the closure can be performed analytically only for ten moments ( $\rho$ ,  $v_i$ ,  $T$ ,  $\sigma_{ij}$ ) but not for higher moment numbers. Thus, one must either restore to cost on-the-fly numerical closure or circumvent the difficulty by constructing best fit closures numerically.<sup>17,18</sup>

The most general formulation of nonequilibrium thermodynamics is offered by GENERIC (general equation for the non-equilibrium reversible-irreversible coupling),<sup>19–21</sup> which guarantees proper thermodynamic structure. While most thermodynamic models fall within GENERIC—including the NSF equations and the Boltzmann equation<sup>21</sup>—the alignment of extended moment systems with GENERIC proved to be difficult. Although a first set of extended transport equations for 13 moments within GENERIC<sup>22</sup> turned out to be incompatible with the moment equations in kinetic theory,<sup>23,24</sup> its derivation introduced most of the tools for later success, most importantly the expression for nonequilibrium entropy. Detailed consideration of the MaxEnt system for ten moments, which has proper thermodynamic structure, showed compatibility with GENERIC when irreversible but non-entropy-producing contributions (Casimir symmetry) were allowed in the formalism.<sup>25</sup>

Combination of elements of these previous approaches led to the GENERIC-13 equations.<sup>1</sup> Specifically, these are based on the 13-moment entropy of Ref. 22, following Ref. 25 include contributions with Casimir symmetry and are constructed such that they agree with the original Grad-13 equations to second order in the Knudsen number in the spirit of Ref. 13. The GENERIC-13 equations contain more and different terms than the Grad-13 equations, but the differences are of order  $\mathcal{O}(\text{Kn}^3)$  or higher.

While Ref. 1 presents the derivation of GENERIC-13 and the asymptotic matching to Grad-13, until now the equations were not further evaluated. Thus, to evaluate the usefulness of GENERIC-13, this contribution aims to study the mathematical properties and

solution behavior of this thermodynamically consistent set of equations. Specifically, we show that, for one-dimensional transport, in contrast to Grad-13 the GENERIC-13 equations are unconditionally hyperbolic. Furthermore, we consider classical one-dimensional steady-state boundary value problems for plane flows, i.e., heat transfer, Couette flow, and Poiseuille flow, with GENERIC-13 and compare their predictions to those of NSF and Grad-13 for small to larger Knudsen numbers.

For the solution of flow problems, thermodynamically consistent jump and slip boundary conditions (BC) for GENERIC-13 are derived following the methods of linear irreversible thermodynamics.<sup>26</sup> Here, the mathematical properties lead to an interesting problem: For the chosen geometries, the NSF and reduced Grad-13 equations require just five BC, which are temperature jump and velocity slip conditions at both sides of the flow plus a filling condition,<sup>27</sup> while GENERIC-13 requires additional BC. With GENERIC-13 reducing to Grad-13 and NSF to second and first order in Kn, the additional BC for GENERIC-13 must be constructed such that they effectively vanish in the limit of smaller Knudsen numbers. Hence, we present an approach for the construction of *asymptotically vanishing boundary conditions*. Due to their mathematical structure, in the plane flows studied, the GENERIC-13 equations require three additional boundary conditions for the two boundaries confining the flows. Thus, some asymmetry is induced through the boundary conditions, which for the parameter space studied is almost negligible.

As discussed, it is well known that the agreement of moment equations with the Boltzmann equation depends on the Knudsen number such that more moments are needed for larger Knudsen numbers, e.g., to describe Knudsen layers and other rarefaction effects. Thus, for larger Knudsen numbers one will not expect good agreement with the Boltzmann equation for system with 13 moments. Our results show very good agreement between the Grad-13 and GENERIC-13 for  $\text{Kn} = 0.1$ , which is close to the limit at which agreement with the Boltzmann equation is expected [recall that the Grad equations are of order  $\mathcal{O}(\text{Kn}^2)$ ]. Nevertheless, in order to study the differences between the two systems of equations, we include results for Knudsen numbers up to  $\text{Kn} = 1$ .

The remainder of this paper is structured as follows. In Sec. II, we briefly present the three sets of equations considered: NSF, Grad-13, and GENERIC-13. Next, in Sec. III, we evaluate the GENERIC-13 equations for hyperbolicity in one-dimensional problems, where it is shown that in contrast to Grad-13 the GENERIC-13 equations are unconditionally hyperbolic. In Sec. IV, the NSF, Grad-13, and GENERIC-13 equations are reduced for plane flow geometry, and written as first-order non-linear ordinary differential equations. Section V explores the question of boundary conditions in detail. The coefficient matrices of the transport equations are used to determine the required number of boundary conditions. Velocity slip and jump conditions are constructed from kinetic theory (for NSF and Grad-13) and the second law of thermodynamics (for GENERIC-13); construction of additional conditions for GENERIC-13 is carefully discussed. Finally, Sec. VI presents numerical solutions for heat transfer, and Couette and Poiseuille flows for Knudsen numbers up to unity. The paper ends with our conclusions.

## II. EQUATIONS

In the following, three sets of transport equations for ideal gases are considered and compared: Navier–Stokes–Fourier (NSF), Grad-13,

and GENERIC-13. We write the equations in tensor index notation with Einstein summation.

### A. Conservation laws

All three sets share the conservation laws for mass, momentum, and energy, which are written as<sup>1,2,10,26</sup>

$$\frac{D\rho}{Dt} + \rho \frac{\partial v_k}{\partial x_k} = 0, \quad (1)$$

$$\rho \frac{Dv_i}{Dt} + \rho \frac{\partial \theta}{\partial x_i} + \theta \frac{\partial \rho}{\partial x_i} + \frac{\partial \sigma_{ik}}{\partial x_k} = \rho F_i, \quad (2)$$

$$\frac{3}{2} \rho \frac{D\theta}{Dt} + \rho \theta \frac{\partial v_k}{\partial x_k} + \frac{\partial q_k}{\partial x_k} + \sigma_{kl} \frac{\partial v_l}{\partial x_l} = 0. \quad (3)$$

Here,  $x_i$  denotes the spatial variable,  $t$  is time,  $\rho$  is mass density,  $v_i$  is velocity,  $\theta = RT$  is thermodynamic temperature with the gas constant  $R$ ,  $\sigma_{ij}$  is the symmetric and trace-free stress tensor, and  $q_k$  is the heat flux vector; the gas pressure is given through the ideal gas law  $p = \rho\theta$ , and  $F_i$  denotes the body force. For compact notation we use the convective time derivative  $\frac{D}{Dt} = \frac{\partial}{\partial t} + v_k \frac{\partial}{\partial x_k}$ .

The differences between the three models considered lie in the equations for stress tensor and heat flux. Moreover, the GENERIC-13 equations use an alternative set of variables that will be introduced further as follows.

As was shown in Ref. 5, the original Grad-13 equations are valid only for Maxwell molecules. Since the GENERIC-13 equations were constructed to agree with the Grad-13 equations to second order in the Knudsen number, these are also valid for Maxwell molecules. Thus, in the following we restrict the discussion to Maxwell molecules for which shear viscosity  $\mu$  and heat conductivity  $\lambda$  depend only on temperature as<sup>8</sup>

$$\mu = \mu_0 \frac{\theta}{\theta_0}, \quad \lambda = \frac{15}{4} \mu, \quad (4)$$

where  $\mu_0$  is the viscosity at reference temperature  $\theta_0$ . The Knudsen number is defined relative to the reference equilibrium state as<sup>8</sup>

$$\text{Kn} = \frac{l_0}{L} = \frac{\mu_0}{\rho_0 \sqrt{\theta_0} L}, \quad (5)$$

with the mean free path  $l_0$  and the characteristic length  $L$ .

### B. Navier–Stokes–Fourier equations

The NSF equations are well known and widely used, they are highly effective in applications of low Knudsen number and provide an excellent base case for comparison.

In the Navier–Stokes–Fourier equations, the conservation laws are closed by means of the Newton stress tensor and the Fourier heat flux<sup>8,26</sup>

$$\sigma_{ij} = -2\mu \frac{\partial v_{(i}}{\partial x_{j)}}, \quad q_i = -\frac{15}{4} \mu \frac{\partial \theta}{\partial x_i}. \quad (6)$$

Here, indices in angular brackets denote the symmetric and trace-free part of a tensor, i.e.,  $\frac{\partial v_{(i}}{\partial x_{j)}} = \frac{1}{2} \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} - \frac{2}{3} \frac{\partial v_k}{\partial x_k} \delta_{ij} \right)$ .

### C. Grad-13 equations

In the Grad-13, equations stress and heat flux are thermodynamic variables with their own balance laws,<sup>8</sup> which we write as

$$\mu \left[ \frac{D\sigma_{ij}}{Dt} + \frac{4}{5} \frac{\partial q_{(i}}{\partial x_{j)}} + \sigma_{k(i} \frac{\partial v_{j)}}{\partial x_k} + \sigma_{ij} \frac{\partial v_k}{\partial x_k} \right] = -\rho\theta \left[ \sigma_{ij} + 2\mu \frac{\partial v_{(i}}{\partial x_{j)}} \right], \quad (7)$$

$$\begin{aligned} \mu \left[ \frac{Dq_i}{Dt} + \frac{5}{2} \sigma_{ik} \frac{\partial \theta}{\partial x_k} - \sigma_{ik} \theta \frac{\partial \ln \rho}{\partial x_k} + \theta \frac{\partial \sigma_{ik}}{\partial x_k} + \frac{7}{5} q_i \frac{\partial v_k}{\partial x_k} \right. \\ \left. + \frac{7}{5} q_k \frac{\partial v_i}{\partial x_k} + \frac{2}{5} q_k \frac{\partial v_k}{\partial x_i} \right] = -\frac{2}{3} \rho\theta \left[ q_i + \frac{15}{4} \mu \frac{\partial \theta}{\partial x_i} \right]. \end{aligned} \quad (8)$$

On the left of the heat flux balance, we have omitted a term  $-\frac{\sigma_{ij}}{\rho} \frac{\partial \sigma_{jk}}{\partial x_k}$ , which in Knudsen number expansion is the only term at order  $\mathcal{O}(\text{Kn}^3)$  and was ignored for the matching between Grad-13 and GENERIC-13, see the discussion in Ref. 1.

In the limit of small Knudsen numbers the left hand sides of both equations vanish, and the Grad-13 equations reduce to the NSF expressions.

### D. GENERIC-13 equations

While the Grad-13 variables are  $\{\rho, v_i, \theta, \sigma_{ij}, q_i\}$ , due to the underlying philosophy the GENERIC-13 equations are written in the alternative set of variables<sup>1,2</sup>

$$\{\rho, M_i, \Theta_{ij}, w_i\}, \quad (9)$$

where  $M_i = \rho v_i$  denotes momentum density, and  $\Theta_{ij} = \theta \delta_{ij} + \frac{\sigma_{ij}}{\rho}$  is the temperature tensor with  $\Theta_{kk} = 3\theta$  and  $\Theta_{(ij)} = \frac{\sigma_{ij}}{\rho}$ . Moreover, the vector variable  $w_i$  replaces heat flux through the non-linear relation

$$q_k = \frac{1}{5} \rho \left( \frac{3}{2} \theta \delta_{kl} + \Theta_{kl} \right) w_l = \left( \frac{1}{2} \rho \theta \delta_{kl} + \frac{1}{5} \sigma_{kl} \right) w_l, \quad (10)$$

which to leading order in Kn reduces to  $w_i = \frac{2q_i}{\rho\theta}$ .

With the abbreviations

$$\kappa_{ik} = \frac{\partial v_i}{\partial x_k}, \quad \omega_{ij} = \frac{\partial v_j}{\partial x_i} - \frac{\partial v_i}{\partial x_j}, \quad (11)$$

the GENERIC-13 equations read

$$\frac{\partial \rho}{\partial t} + \frac{\partial M_k}{\partial x_k} = 0, \quad (12)$$

$$\frac{\partial M_i}{\partial t} + \frac{\partial M_i v_k}{\partial x_k} + \frac{\partial \rho \Theta_{ki}}{\partial x_k} = \rho F_i, \quad (13)$$

$$\begin{aligned} \frac{\partial \Theta_{ij}}{\partial t} + \frac{\partial \Theta_{ij}}{\partial x_k} v_k + 2\kappa_{k(i} \Theta_{j)k} - \Theta_{ij} \omega_{ir} - \Theta_{ir} \omega_{jr} \\ + \frac{1}{\rho} \frac{\partial}{\partial x_s} \left[ \frac{\rho}{5} (w_i \Theta_{js} + w_j \Theta_{is} + \Theta_{ij} w_s) \right] \\ = -\frac{\rho\theta}{\mu} \left[ \frac{1}{3} \theta \Theta_{rr}^{-1} + \frac{1}{30} \theta \Theta_{kr}^{-1} w_r \Theta_{ks}^{-1} w_s \right] \Theta_{(ij)}, \end{aligned} \quad (14)$$

$$\begin{aligned} & \frac{\partial w_i}{\partial t} + v_k \frac{\partial w_i}{\partial x_k} + w_i \frac{\partial v_i}{\partial x_k} + \left( 2 \frac{\partial \Theta_{ik}}{\partial x_k} + \Theta_{is} \Theta_{kl}^{-1} \frac{\partial \Theta_{kl}}{\partial x_s} \right) \\ & - \frac{1}{5} (w_i \Theta_{sl} + \Theta_{il} w_s + \Theta_{is} w_l) \frac{\partial w_n \Theta_{nl}^{-1}}{\partial x_s} \\ & = -\frac{p}{\mu} \left[ \frac{1}{6} \theta \Theta_{kk}^{-1} \delta_{ir} - \frac{1}{15} \theta \Theta_{ir}^{-1} + \frac{7}{30} \theta^2 \Theta_{ik}^{-1} \Theta_{rk}^{-1} \right. \\ & \left. + \frac{1}{60} \theta \Theta_{kr}^{-1} \Theta_{ks}^{-1} w_s w_i \right] w_r. \end{aligned} \quad (15)$$

The first two equations above are the mass and momentum balances; the energy balance appears as the trace of the equation for  $\Theta_{ij}$ ; by Knudsen number expansion to second order the trace-free part of the  $\Theta_{ij}$ -balance and the  $w_i$ -balance reduces to the Grad equations [(7), (8)], respectively.

The GENERIC-13 equations are accompanied by the entropy balance

$$\frac{\partial \eta}{\partial t} + \frac{\partial \eta v_k}{\partial x_k} + \frac{\partial \phi_k}{\partial x_k} = \Sigma, \quad (16)$$

with entropy density  $\eta$ , entropy flux  $\phi_i$ , and entropy generation rate  $\Sigma$  related to the variables (9) through the relations

$$\eta = \rho R \left( \frac{1}{2} \ln [\det \Theta] - \ln \rho - \frac{1}{20} \Theta_{rs}^{-1} w_r w_s + \eta_0 \right), \quad (17)$$

$$\phi_k = \frac{1}{2} \rho R \left( 1 + \frac{3}{50} \Theta_{rs}^{-1} w_r w_s \right) w_k, \quad (18)$$

$$\begin{aligned} \Sigma = & \frac{p^2}{\mu} R \left[ \frac{1}{2} \left( \frac{1}{3} \theta \Theta_{rr}^{-1} - 1 \right) \Theta_{rr}^{-1} + \frac{17}{300} \left( \frac{10}{17} \theta \Theta_{rr}^{-1} - 1 \right) \Theta_{ij}^{-1} \Theta_{ik}^{-1} w_j w_k \right. \\ & \left. + \frac{7}{300} \theta \Theta_{ij}^{-1} \Theta_{jk}^{-1} \Theta_{kl}^{-1} w_l w_i + \frac{1}{600} \theta \left( \Theta_{ij}^{-1} \Theta_{ik}^{-1} w_j w_k \right)^2 \right] \geq 0. \end{aligned} \quad (19)$$

According to the second law of thermodynamics, the entropy generation rate  $\Sigma$  vanishes in equilibrium and is positive in non-equilibrium states.

### III. HYPERBOLICITY IN 1-D

#### A. General

Famously, the Grad-13 equations are hyperbolic for processes not too far from equilibrium states but lose hyperbolicity for processes involving large stresses and heat fluxes.<sup>12</sup> In this section, we revisit this behavior to show that the extension of Grad-13 to GENERIC-13 yields a generally hyperbolic system.

Specifically, we study time dependent one-dimensional transport in  $x$ -direction, where all variables depend on  $(x, t)$  only and vector variables point into the direction of transport, that is,

$$v_i = [v(x, t), 0, 0], \quad q_i = [q(x, t), 0, 0], \quad w_i = [w(x, t), 0, 0]. \quad (20)$$

As well, the temperature tensor is diagonal

$$\Theta_{ij} = \begin{bmatrix} \theta \left( 1 + \frac{\sigma}{\rho \theta} \right) & 0 & 0 \\ 0 & \theta \left( 1 - \frac{1}{2} \frac{\sigma}{\rho \theta} \right) & 0 \\ 0 & 0 & \theta \left( 1 - \frac{1}{2} \frac{\sigma}{\rho \theta} \right) \end{bmatrix}. \quad (21)$$

Due to its definition,<sup>1</sup> the diagonal elements must be non-negative, hence the normal stress  $\sigma$  is restricted to the interval  $-1 \leq \frac{\sigma}{\rho \theta} \leq 2$ .

For both sets of equations, Grad-13 and GENERIC-13, the 1-D balance laws can be written in the compact form

$$\frac{\partial u_A}{\partial t} + \mathcal{A}_{AB} \frac{\partial u_B}{\partial x} = -\mathcal{C}_{AB} \frac{\rho \theta}{\mu} u_B, \quad (22)$$

where  $u_A$  is the vector of 1-D variables,  $\mathcal{A}_{AB}$  is the flux matrix, and the damping factors  $\mathcal{C}_{AB}$  are dimensionless weights on the collision frequency  $\frac{\rho \theta}{\mu}$ . A system of this form is hyperbolic, if the eigenvalues  $\Lambda^z$ —which are the characteristic speeds of disturbances—of the matrix  $\mathcal{A}_{AB}$  are real, it loses hyperbolicity when the eigenvalues are complex.

Moreover, if the matrix  $\mathcal{A}_{AB}$  is symmetric, the set of equations is called symmetric hyperbolic, which is ensured when the equations are accompanied by an entropy balance with concave entropy  $\eta(u_A)$  and non-negative production. Symmetric hyperbolic systems have desirable mathematical properties, such as well-posedness of initial value problems, see Ref. 12 for further discussion and references. For the Grad-13 and GENERIC-13 equations as written below, the matrices are not symmetric but are diagonalizable with linearly independent eigenvectors, which is equivalent to symmetry.

For evaluation of the eigenvalues, we consider an observer resting with the flow, hence  $v = 0$ , and use dimensionless variables chosen such that  $\rho = \theta = 1$ , and dimensionless stress, heat flux, and  $w$ -vector are  $\frac{\sigma}{\rho \theta}, \frac{q}{\rho \theta^{3/2}}, \frac{w}{\sqrt{\theta}}$ .

#### B. Grad-13 equations

The variables for the 1-D Grad-13 equations are

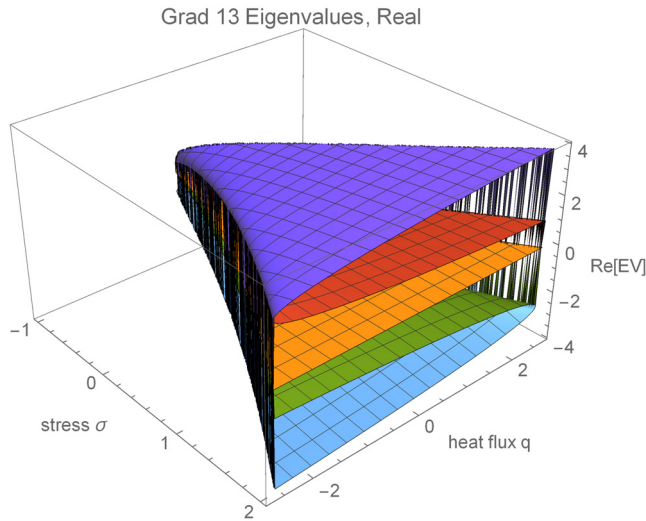
$$u_A = \{ \rho(x, t), v(x, t), \theta(x, t), \sigma(x, t), q(x, t) \}, \quad (23)$$

with the matrix

$$\mathcal{A}_{AB}^{\text{Grad}} = \begin{bmatrix} v & \rho & 0 & 0 & 0 \\ \frac{\theta}{\rho} & v & 1 & \frac{1}{\rho} & 0 \\ 0 & \frac{2}{3} \left( \theta + \frac{\sigma}{\rho} \right) & v & 0 & \frac{21}{3\rho} \\ 0 & \left( \frac{4}{3} \rho \theta + \frac{7}{3} \sigma \right) & 0 & v & \frac{8}{15} \\ -\frac{\theta \sigma}{\rho} & \frac{16}{5} q & \left( \frac{5}{2} \rho \theta + \frac{5}{2} \sigma \right) & \theta & v \end{bmatrix}. \quad (24)$$

Figure 1 shows the five eigenvalues of  $\mathcal{A}_{AB}^{\text{Grad}}$  as functions of dimensionless stress and heat flux in the admissible region for stress,  $-1 \leq \frac{\sigma}{\rho \theta} \leq 2$ . Eigenvalues are shown only where they are real, the vertical black lines (an artifact of the numerical plotting) indicate the boundary between the hyperbolic region with real eigenvalues, and the non-hyperbolic region with complex eigenvalues, which are not shown. Due to the omission of the third order term in (8) the hyperbolic region has a somewhat different shape than the one shown in Ref. 12, but the conclusion remains the same: for larger heat fluxes (in dependence on the value of  $\sigma$ ), the Grad-13 equations lose hyperbolicity and become physically meaningless.

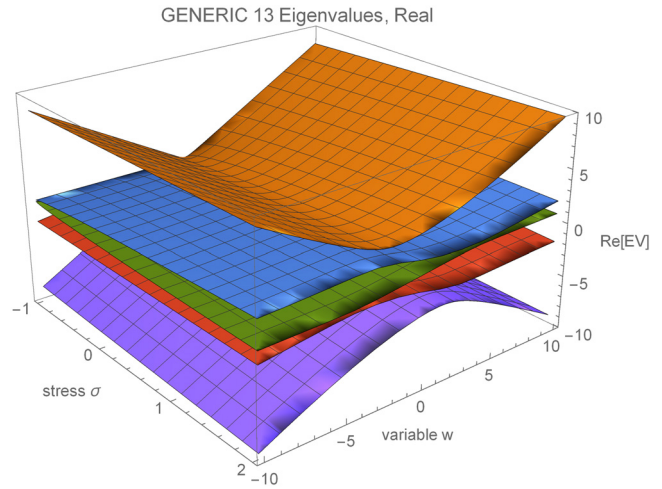
The only non-zero entries for the production matrix  $\mathcal{C}_{AB}$  are constant



**FIG. 1.** Eigenvalues  $\Lambda^\alpha$  for the Grad-13 matrix  $\mathcal{A}_{AB}^{\text{Grad}}$  for dimensionless variables. The eigenvalues are only shown where all are real, outside the plotted regions at least some of the  $\Lambda^\alpha$  are complex, and the Grad-13 equations lose hyperbolicity.

$$C_{44}^{\text{Grad}} = 1, \quad C_{55}^{\text{Grad}} = \frac{2}{3}, \quad (25)$$

that is, the damping of stress  $\sigma$  and heat flux  $q$  is linear.



**FIG. 2.** Eigenvalues  $\Lambda^\alpha$  for the GENERIC-13 matrix  $\mathcal{A}_{AB}^{\text{GEN13}}$  for dimensionless variables. All eigenvalues are real for all data.

### C. GENERIC-13 equations

For the GENERIC-13 equations, we chose the variables

$$u_A = \{\rho(x, t), v(x, t), \theta(x, t), \sigma(x, t), w(x, t)\}, \quad (26)$$

which yields the matrix

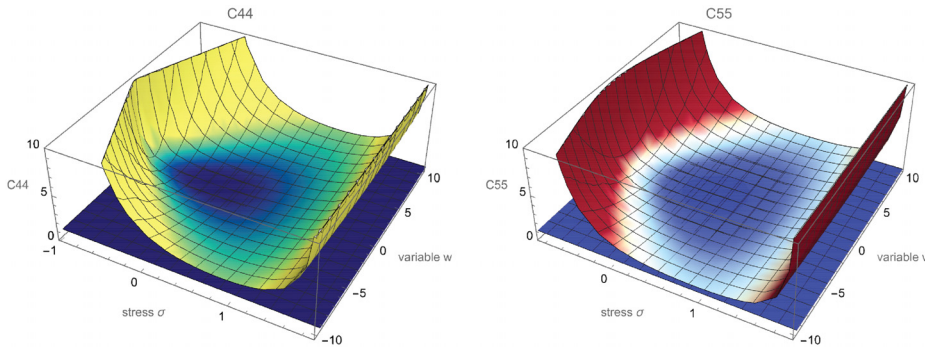
$$\mathcal{A}_{AB}^{\text{GEN13}} = \begin{bmatrix} v & \rho & 0 & 0 & 0 \\ \frac{\theta}{\rho} & v & 1 & \frac{1}{\rho} & 0 \\ \frac{1}{3} \frac{\theta w}{\rho} & \frac{2}{3} \left( \theta + \frac{\sigma}{\rho} \right) & v + \frac{1}{3} w & \frac{2}{15} \frac{w}{\rho} & \frac{1}{3} \theta + \frac{2}{15} \frac{\sigma}{\rho} \\ \frac{4}{15} \theta w & \left( \frac{4}{3} \rho \theta + \frac{7}{3} \sigma \right) & \frac{4}{15} \rho w & v + \frac{7}{15} w & \frac{4}{15} \rho \theta + \frac{7}{15} \sigma \\ - \left[ \frac{2 - \frac{5}{2} \frac{\sigma}{\rho \theta}}{1 - \frac{1}{2} \frac{\sigma}{\rho \theta}} + \frac{3}{5} \frac{1}{\left( 1 + \frac{\sigma}{\rho \theta} \right)} \frac{w^2}{\theta} \right] \frac{\sigma}{\rho^2} & w & \frac{5 + \frac{1}{2} \frac{\sigma}{\rho \theta}}{1 - \frac{1}{2} \frac{\sigma}{\rho \theta}} + \frac{3}{5} \frac{w^2}{\theta \left( 1 + \frac{\sigma}{\rho \theta} \right)} & \left[ \frac{2 - \frac{5}{2} \frac{\sigma}{\rho \theta}}{1 - \frac{1}{2} \frac{\sigma}{\rho \theta}} + \frac{3}{5} \frac{w^2}{\theta \left( 1 + \frac{\sigma}{\rho \theta} \right)} \right] \frac{1}{\rho} & v - \frac{3}{5} w \end{bmatrix}. \quad (27)$$

Figure 2 shows the five eigenvalues of  $\mathcal{A}_{AB}^{\text{GEN13}}$  as functions of dimensionless stress and  $w$ -vector in the admissible region for stress,  $-1 \leq \frac{\sigma}{\rho \theta} \leq 2$ , for  $w$ -vectors in the range  $-10 \leq \frac{w}{\sqrt{\theta}} \leq 10$ , which refer to extremely large heat fluxes that will not be reached in physical processes. Further numerical tests show that all eigenvalues are real for all values of  $w$  [or heat flux  $q = \left( \frac{\rho \theta}{2} + \frac{\sigma}{5} \right) w$ ], hence the GENERIC-13 equations remain hyperbolic for all possible processes.

The damping terms for GENERIC-13 are strongly non-linear, with the only non-zero elements

$$C_{44}^{\text{GEN13}} = \frac{\left( 1 + \frac{1}{2} \frac{\sigma}{\rho \theta} \right)}{\left( 1 + \frac{\sigma}{\rho \theta} \right) \left( 1 - \frac{1}{2} \frac{\sigma}{\rho \theta} \right)} + \frac{1}{30} \frac{\theta w^2}{\left( \theta + \frac{\sigma}{\rho} \right)^2}, \quad (28)$$

$$C_{55}^{\text{GEN13}} = \frac{\frac{2}{3} + \frac{3}{5} \frac{\sigma}{\rho \theta} + \frac{17}{60} \left( \frac{\sigma}{\rho \theta} \right)^2}{\left( 1 + \frac{\sigma}{\rho \theta} \right)^2 \left( 1 - \frac{1}{2} \frac{\sigma}{\rho \theta} \right)} + \frac{1}{60} \frac{w^2}{\theta \left( 1 + \frac{\sigma}{\rho \theta} \right)^2}. \quad (29)$$



**FIG. 3.** Damping factors  $C_{44}$  and  $C_{55}$  for GENERIC-13 and Grad-13 equations. While Grad-13 factors are constant, GENERIC-13 factors are non-linear with strong damping for processes far from equilibrium.

Interestingly, as shown in Fig. 3, both factors become large when stress approaches the boundaries of the admissible region,  $-1 \leq \frac{\sigma}{\rho\theta} \leq 2$ , and for large  $w$ . Thus, the GENERIC-13 equations ensure strong damping for processes far from the equilibrium state  $\sigma = q = w = 0$ . Meaningless values for stress, that is, those outside the interval  $(-1, 2)$ , are unattainable.

#### IV. STEADY-STATE PLANE FLOWS

##### A. Flow geometries

The remainder of this contribution concerns solutions of the NSF, Grad-13, and GENERIC-13 equations for steady-state plane flows between two parallel plates as sketched in Fig. 4. The plate distance is  $L$  and the plate temperatures and velocities are prescribed as  $\theta_0, \theta_L$  and  $V_0, V_L$ , respectively. Moreover, there might be a body force or pressure gradient  $F$  driving the flow.

We will consider the following standard flow configurations.<sup>26</sup>

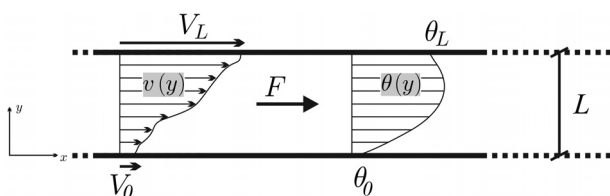
- *Heat transfer:* Plates at rest,  $V_0 = V_L = 0$ ; plate temperatures  $\theta_0 = 1 - \Delta\theta, \theta_L = 1 + \Delta\theta$ ; no driving force,  $F = 0$ .
- *Couette flow:* Lower plate moves at  $V_0 = -\Delta v$ , upper plate at  $V_L = \Delta v$ ; equal temperatures,  $\theta_L = \theta_0$ ; no driving force,  $F = 0$ .
- *Poiseuille flow:* Plates at rest,  $V_0 = V_L = 0$ ; equal temperatures,  $\theta_L = \theta_0$ ; flow driven by body force  $F$ .

Due to geometry, all variables depend only on the normal direction,  $y$ , the velocity vector reduces to

$$v_i = [v(y), 0, 0], \tag{30}$$

but the heat flux vector will have contributions in  $x$ - and  $y$ -direction

$$q_i = [q_1(y), q_2(y), 0], \quad w_i = [w_1(y), w_2(y), 0]. \tag{31}$$



**FIG. 4.** Geometry for steady-state plane flows between two parallel planes in distance  $L$  with prescribed boundary temperatures  $\theta_0, \theta_L$ , velocities  $V_0, V_L$ , and driving force  $F$ .

The three sets of equations can be reduced to systems of first-order differential equations of the form

$$\mathcal{A}_{AB} \frac{du_B}{dy} = \mathcal{P}_A, \tag{32}$$

with variables  $u_A$ , matrices  $\mathcal{A}_{AB}$ , and production vectors  $\mathcal{P}_A$  specified as follows. This notation is particularly useful for the discussion of boundary conditions in Sec. V.

It is convenient to use dimensionless variables relative to an equilibrium rest state  $\rho_0, \theta_0$ , and use the length  $L$  to further non-dimensionalize, that is, we introduce dimensionless space coordinate, Knudsen number, and body force as

$$\frac{x}{L} = \hat{x}, \quad \frac{\mu}{\rho_0 \sqrt{\theta_0} L} = \text{Kn} \hat{\theta}, \quad \frac{LF}{\theta_0} \rightarrow \hat{F}, \tag{33}$$

and the dimensionless thermodynamic variables

$$\frac{\rho}{\rho_0} = \hat{\rho}, \quad \frac{v}{\sqrt{\theta_0}} = \hat{v}, \quad \frac{\theta}{\theta_0} = \hat{\theta}, \quad \frac{\sigma_{ij}}{\rho_0 \theta_0} = \hat{\sigma}_{ij}, \quad \frac{q_i}{\rho_0 \sqrt{\theta_0}^3} = \hat{q}_i; \tag{34}$$

or for GENERIC-13

$$\frac{\Theta_{ij}}{\theta_0} = \hat{\Theta}_{ij}, \quad \frac{w_i}{\sqrt{\theta_0}} = \hat{w}_i. \tag{35}$$

For the sake of better readability the hats that indicate dimensionless variables will be omitted in the sequel.

##### B. NSF

In the NSF case, the only non-vanishing variables are

$$u_A^{\text{NSF}} = \{\rho(y), v(y), \theta(y), \sigma_{12}(y), q_2(y)\}. \tag{36}$$

The mass balance is identically fulfilled, and the conservation laws for momentum in  $x$ - and  $y$ -direction and energy reduce to

$$\frac{d\sigma_{12}}{dy} = \rho F, \quad \theta \frac{d\rho}{dy} + \rho \frac{d\theta}{dy} = 0, \quad \frac{dq_2}{dy} + \sigma_{12} \frac{dv}{dy} = 0, \tag{37}$$

with stress and heat flux given by

$$\text{Kn} \theta \frac{dv}{dy} = -\sigma_{12}, \quad \frac{15}{4} \text{Kn} \theta \frac{d\theta}{dy} = -q_2. \tag{38}$$

The above equations are of the form (32), with

$$\mathcal{A}_{AB}^{\text{NSF}} = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 \\ \theta & 0 & \rho & 0 & 0 \\ 0 & \sigma_{12} & 0 & 0 & 1 \\ 0 & \rho\theta & 0 & 0 & 0 \\ 0 & 0 & \frac{5}{2}\rho\theta & 0 & 0 \end{bmatrix}, \quad \mathcal{P}_A^{\text{NSF}} = \begin{bmatrix} \rho F \\ 0 \\ 0 \\ -\frac{\rho}{\text{Kn}}\sigma_{12} \\ -\frac{2}{3}\frac{\rho}{\text{Kn}}q_2 \end{bmatrix}. \tag{39}$$

**C. Grad-13 equations**

Due to higher order terms accounting for gas rarefaction, the Grad-13 equations contain additional variables, such as normal stresses and heat flux parallel to the flow, which vanish in NSF; the variables are

$$u_A^{\text{Grad}} = \{\rho(y), v(y), \theta(y), \sigma_{11}(y), \sigma_{12}(y), \sigma_{22}(y), q_1(y), q_2(y)\}. \tag{40}$$

The complete Grad-13 equations in plane flow geometry are highly non-linear, with

$$\mathcal{A}_{AB}^{\text{Grad}} = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ \theta & 0 & \rho & 0 & 0 & 1 & 0 & 0 \\ 0 & \sigma_{12} & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & \frac{4}{3}\sigma_{12} & 0 & 0 & 0 & 0 & 0 & -\frac{4}{15} \\ 0 & \rho\theta + \sigma_{22} & 0 & 0 & 0 & 0 & \frac{2}{5} & 0 \\ 0 & -\frac{2}{3}\sigma_{12} & 0 & 0 & 0 & 0 & 0 & \frac{8}{15} \\ -\frac{\theta\sigma_{12}}{\rho} & \frac{7}{5}q_2 & \frac{5}{2}\sigma_{12} & 0 & \theta - \frac{\sigma_{11}}{\rho} & -\frac{\sigma_{12}}{\rho} & 0 & 0 \\ -\frac{\theta_{22}}{\rho} & \frac{2}{5}q_1 & \frac{5}{2}(\rho\theta + \sigma_{22}) & 0 & -\frac{\sigma_{12}}{\rho} & \theta - \frac{\sigma_{11}}{\rho} & 0 & 0 \end{bmatrix}, \quad \mathcal{P}_A^{\text{Grad}} = \begin{bmatrix} \rho F \\ 0 \\ 0 \\ -\frac{\rho}{\text{Kn}}\sigma_{11} \\ -\frac{\rho}{\text{Kn}}\sigma_{12} \\ -\frac{\rho}{\text{Kn}}\sigma_{22} \\ -\frac{2}{3}\frac{\rho}{\text{Kn}}q_1 \\ -\frac{2}{3}\frac{\rho}{\text{Kn}}q_2 \end{bmatrix}. \tag{41}$$

As will be discussed below, these equations are not accompanied by a complete theory of boundary conditions. Thus, while we will discuss the properties of the matrix  $\mathcal{A}_{AB}^{\text{Grad}}$ , we will not consider their solutions.

**D. Grad-13 bulk equations**

A simplified form of the Grad-13 equations in plane flow geometry is obtained from applying the Chapman–Enskog expansion to second order, which shows that in plane flow geometry some contributions are of higher than second order. Removal of these higher order terms results in the Grad-13 Bulk equations,<sup>8,27</sup> we will consider their solutions for comparison. The variables are the same as for the full Grad-13 equations but with a simpler matrix

$$\mathcal{A}_{AB}^{\text{GradB}} = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ \theta & 0 & \rho & 0 & 0 & 1 & 0 & 0 \\ 0 & \sigma_{12} & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & \frac{4}{3}\sigma_{12} & 0 & 0 & 0 & 0 & 0 & -\frac{4}{15} \\ 0 & \rho\theta & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{2}{3}\sigma_{12} & 0 & 0 & 0 & 0 & 0 & \frac{8}{15} \\ 0 & \frac{7}{5}q_2 & \frac{7}{2}\sigma_{12} & 0 & \theta & 0 & 0 & 0 \\ 0 & 0 & \frac{5}{2}\rho\theta & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \quad \mathcal{P}_A^{\text{Grad}} = \begin{bmatrix} \rho F \\ 0 \\ 0 \\ -\frac{\rho}{\text{Kn}}\sigma_{11} \\ -\frac{\rho}{\text{Kn}}\sigma_{12} \\ -\frac{\rho}{\text{Kn}}\sigma_{22} \\ -\frac{2}{3}\frac{\rho}{\text{Kn}}q_1 \\ -\frac{2}{3}\frac{\rho}{\text{Kn}}q_2 \end{bmatrix}. \tag{42}$$

A closer look at the bulk equations shows that these can be combined to yield algebraic relations between the non-hydrodynamic variables  $\sigma_{11}$ ,  $\sigma_{22}$ ,  $q_1$  and the hydrodynamic variables  $\sigma_{12}$  and  $q_2$ , as<sup>8,27</sup>

$$\sigma_{11} = \frac{8 \sigma_{12}^2}{5 \rho \theta}, \quad \sigma_{22} = -\frac{6 \sigma_{12}^2}{5 \rho \theta}, \quad q_1 = \frac{7 \sigma_{12} q_2}{2 \rho \theta} - \frac{3}{2} \text{Kn} \theta F, \quad (43)$$

while the remaining equations read

$$\frac{d\sigma_{12}}{dy} = \rho F, \quad \theta \frac{d\rho}{dy} + \rho \frac{d\theta}{dy} + \frac{d\sigma_{22}}{dy} = 0, \quad \frac{dq_2}{dy} + \sigma_{12} \frac{dv}{dy} = 0, \quad (44)$$

$$\text{Kn} \theta \frac{dv}{dy} = -\sigma_{12}, \quad \frac{15}{4} \text{Kn} \theta \frac{d\theta}{dy} = -q_2; \quad (45)$$

apart from the contribution  $\frac{d\sigma_{22}}{dy}$  in the momentum balance these are identical with the NSF equations.

### E. GENERIC-13

Due to the strong non-linearity of the GENERIC-13 equations, their reduced form for plane flows is quite lengthy, see the [Appendix](#)

for details. The eight non-vanishing variables correspond to those in Grad-13, they are

$$u_A^{\text{GEN}} = \{\rho(y), v(y), \theta(y), \Theta_{11}(y), \Theta_{12}(y), \Theta_{22}(y), w_1(y), w_2(y)\}, \quad (46)$$

with the temperature tensor

$$\Theta_{ij} = \begin{bmatrix} \theta + \frac{\sigma_{11}}{\rho} & \frac{\sigma_{12}}{\rho} & 0 \\ \frac{\sigma_{12}}{\rho} & \theta + \frac{\sigma_{22}}{\rho} & 0 \\ 0 & 0 & \theta - \frac{\sigma_{11}}{\rho} - \frac{\sigma_{22}}{\rho} \end{bmatrix}. \quad (47)$$

The expressions for  $\mathcal{A}_{AB}^{\text{GEN}13}$  and  $\mathcal{P}_A^{\text{GEN}13}$  given below include abbreviations  $\alpha_i, \beta_i, \gamma_i, \delta_i, \epsilon_i$  used for compactness as the full expressions are too long to write explicitly in matrix form. Along with the full equations, the abbreviations are provided in [Subsection 3](#) of the [Appendix](#). Matrix and production vectors read

$$\mathcal{A}_{AB}^{\text{GEN}13} = \begin{bmatrix} \Theta_{12} & 0 & 0 & 0 & \rho & 0 & 0 & 0 \\ \Theta_{12} & 0 & 0 & 0 & 0 & \rho & 0 & 0 \\ \frac{1}{5\rho} \left[ \Theta_{12} w_1 + \left( \frac{3}{2} \theta + \Theta_{22} \right) w_2 \right] & \Theta_{12} & \frac{3}{10} w_2 & 0 & \frac{1}{5} w_1 & \frac{1}{5} w_2 & \frac{1}{5} \Theta_{12} & \left( \frac{1}{5} \Theta_{22} + \frac{3}{10} \theta \right) \\ \frac{1}{5\rho} (2\Theta_{12} w_1 + \Theta_{11} w_2) & 2\Theta_{12} & 0 & \frac{1}{5} w_2 & \frac{2}{5} w_1 & 0 & \frac{2}{5} \Theta_{12} & \frac{1}{5} \Theta_{11} \\ \frac{1}{5\rho} (\Theta_{22} w_1 + 2\Theta_{12} w_2) & \Theta_{22} & 0 & 0 & \frac{2}{5} w_2 & \frac{1}{5} w_1 & \frac{1}{5} \Theta_{22} & \frac{2}{5} \Theta_{12} \\ \frac{3}{5\rho} \Theta_{22} w_2 & 0 & 0 & 0 & 0 & \frac{3}{5} w_2 & 0 & \frac{3}{5} \Theta_{22} \\ 0 & w_2 & 3\Theta_{12} \Theta_{33}^{-1} & \alpha_1 & \beta_1 & \gamma_1 & \delta_1 & \epsilon_1 \\ 0 & 0 & 3\Theta_{22} \Theta_{33}^{-1} & \alpha_2 & \beta_2 & \gamma_2 & \delta_2 & \epsilon_2 \end{bmatrix}, \quad (48)$$

$$\mathcal{P}_A^{\text{GEN}13} = \begin{bmatrix} \rho F \\ 0 \\ 0 \\ -\frac{1}{3\text{Kn}} \left[ \theta \Theta_{rr}^{-1} + \frac{1}{10} \theta \Theta_{kr}^{-1} w_r \Theta_{ks}^{-1} w_s \right] \Theta_{(11)} \\ -\frac{1}{3\text{Kn}} \left[ \theta \Theta_{rr}^{-1} + \frac{1}{10} \theta \Theta_{kr}^{-1} w_r \Theta_{ks}^{-1} w_s \right] \Theta_{(12)} \\ -\frac{1}{3\text{Kn}} \left[ \theta \Theta_{rr}^{-1} + \frac{1}{10} \theta \Theta_{kr}^{-1} w_r \Theta_{ks}^{-1} w_s \right] \Theta_{(22)} \\ -\frac{\rho \theta}{6\text{Kn}} \left[ \Theta_{kk}^{-1} w_1 - \frac{2}{5} \Theta_{1r}^{-1} w_r + \frac{7}{5} \theta \Theta_{1k}^{-1} \Theta_{rk}^{-1} w_r + \frac{1}{10} \Theta_{kr}^{-1} \Theta_{ks}^{-1} w_s w_r w_1 \right] \\ -\frac{\rho \theta}{6\text{Kn}} \left[ \Theta_{kk}^{-1} w_2 - \frac{2}{5} \Theta_{2r}^{-1} w_r + \frac{7}{5} \theta \Theta_{2k}^{-1} \Theta_{rk}^{-1} w_r + \frac{1}{10} \Theta_{kr}^{-1} \Theta_{ks}^{-1} w_s w_r w_2 \right] \end{bmatrix}. \quad (49)$$

V. BOUNDARY CONDITIONS

Solutions of the plane flow configurations result from integration of Eq. (32) and consideration of proper boundary conditions (BCs) that relate the parameters controlled at the boundary to the variables in the domain. As will be discussed further in Sec. VF, the number of boundary conditions required equals the number of constants of integration which equals the number of non-zero eigenvalues of the coefficient matrices  $\mathcal{A}_{AB}$ .

A. Controlled boundary parameters

As indicated in Fig. 4, in plane flow geometry one will naturally control the plate velocities  $V_0, V_L$  and the plate temperatures  $\theta_0, \theta_L$ . The corresponding boundary conditions are velocity-slip and temperature-jump conditions at both walls of the channel, which appear quite naturally from arguments in kinetic theory as well as from the second law of thermodynamics. In the numerical solutions below, the slip condition is implemented in the boundary cells of the tangential momentum balance, and the jump condition in the boundary cells of the energy balance.

Furthermore, the filling condition prescribes the average mass density of the flow through the integral

$$\rho_0 = \frac{1}{L} \int_0^L \rho(y) dy; \tag{50}$$

where in dimensionless formulation  $\rho_0 \rightarrow 1$ . Prescription of the value of  $\rho_0$  effectively serves as an additional boundary condition, instead of vanishing normal velocities  $v_2 = 0$  at the boundaries, which is guaranteed throughout.

The body force  $F$  is applied throughout the domain and does not affect boundary conditions.

Thus, all boundary conditions for the various systems of transport equations must be related to these five parameters.

B. The number of required boundary conditions

The first step in developing suitable BC for the transport equations is to ask how many BC are required for a particular set. We explore this for the steady plane flows of interest, for which the transport equations reduce to (32)

$$\mathcal{A}_{AB} \frac{du_B}{dy} = \mathcal{P}_A, \tag{51}$$

hence the fields  $u_A$  are determined from integration. Each integration introduces a constant of integration which must be determined from BC; hence, the number of BC required equals the number of independent integrations. This number follows from the properties of the matrix  $\mathcal{A}_{AB}$ .

We introduce the eigenvalues (EVs)  $\Lambda^\alpha$  and the corresponding left eigenvectors  $L_A^\alpha$  of  $\mathcal{A}_{AB}$ , such that

$$L_A^\alpha \mathcal{A}_{AB} = \Lambda^\alpha L_B^\alpha, \tag{52}$$

where summation over Latin letters is implied but not over Greek letters. We assume that the left eigenvectors are all independent. In hyperbolic systems, the EV of the matrix of coefficients is the characteristic speeds of the system.

With this, multiplication of the transport equations with the left eigenvectors  $L_A^\alpha$  yields

$$\Lambda^\alpha L_B^\alpha \frac{du_B}{dy} = L_A^\alpha \mathcal{P}_A \quad (\alpha = 1, \dots, n). \tag{53}$$

The eigenvalues  $\Lambda^\alpha$  might either be equal to zero, positive, or negative, which we indicate by writing

$$\Lambda^{\alpha_0} = 0, \quad \Lambda^{\alpha_+} > 0, \quad \Lambda^{\alpha_-} < 0; \tag{54}$$

the numbers of such EV we denote by  $n_0, n_+$ , and  $n_-$ , respectively, with  $n_0 + n_+ + n_- = n$ .

For vanishing EV, the transport equations reduce to algebraic relations between the variables

$$0 = L_A^{\alpha_0} \mathcal{P}_A \quad (\alpha_0 = 1, \dots, n_0); \tag{55}$$

for these no integration is required. Indeed, Eqs. (43) from the Grad-13 bulk equations can be obtained in this manner. Note that these algebraic relations hold in all points of the domain, including the boundaries.

It follows that the number of independent integrations equals the number of non-zero eigenvalues, hence the number of boundary conditions required is

$$\# \text{ of BC} = n - n_0. \tag{56}$$

We discuss the eigenvalues for the individual systems in the subsections below. To develop insight about the eigenvalues of the various matrices, we considered the analytical solution of the Grad-13B equations for Couette flow and evaluated the matrices at different conditions for Knudsen number and velocity difference.

1. NSF equations

The matrix  $\mathcal{A}_{AB}$  for NSF (39) has five independent eigenvalues, which appear as one pair of real EV, one pair of conjugate complex EV, and one individual EV. The pair structure is particularly clear in the linear limit (small differences between the plate velocities and temperatures, small force) where the real pair have the same value but opposite sign.

Relating the EV to the controlled parameters, the two pairs are linked to velocity slip and temperature jump conditions at the two sides of the domain, and the single EV is linked to the filling condition.

It is worthwhile to note that the complex conjugate EV is never used in computations, only for counting of BC.

2. Grad-13 bulk equations

Similar to NSF, the matrix (42) of the Grad-13 bulk equations yields two pairs and one individual EV, where, however, it might happen that both pairs of EV are conjugate complex while the individual EV remains real. Again, we attribute the pairs of EVs to slip and jump conditions, and the individual to the filling condition (50).

3. Grad-13 original equations

The matrix (41) of the full Grad-13 equations yields one additional pair of eigenvalues. Extending our observation from NSF and Grad-13B, the extra pair should be linked to another boundary condition that must be applied on both sides of the domain.

There is no theory of BC for the Grad-13 equations available in the literature, and we will not explore the possibilities for the development of the required additional BC of higher order. In our cursory

evaluation of the EV, this extra pair was always conjugate complex, with corresponding eigenvectors complex. With that, it is not possible to extend the method discussed below for GENERIC-13, which relies on real EV and eigenvectors, to the case of Grad-13. A complete set of proper BC for the full Grad-13 equations remains elusive.

#### 4. GENERIC-13 equations

The matrix (48) exhibits a surprising behavior, in which it has eight (8) non-zero eigenvalues.

Numerical evaluation shows that these eigenvalues depend on the Knudsen number as follows: five eigenvalues—one real pair, one conjugate complex pair, and one individual—are always distinct from zero—these correspond to the non-vanishing EV of NSF and Grad-13B, and thus are linked to slip, jump, and filling conditions.

The three additional EVs appearing, however, are generally smaller and vanish with the Knudsen number. The signs of the extra EV depend on location. At the left boundary ( $x = 0$ ), we find two negative and one positive EV, on the right ( $x = 1$ ), one EV is negative and two are positive.

In other words, as the Knudsen number decreases, the GENERIC-13 equations approach the Grad-13B or even the NSF equations, and their extra eigenvalues become smaller and smaller until they effectively vanish. As the number of BC required equals the number of non-zero EVs, the number of BC required changes from eight to five with Knudsen number decreasing.

From this observation, we derive the *BC consistency requirement*:

Solving GENERIC-13 demands additional BC that give meaningful results for all Knudsen numbers, specifically the BC must reduce to, or be compatible with,  $0 = L_A^w \mathcal{P}_A$  for small Kn.

We specifically note that the second law of thermodynamics—which we use below to motivate jump and slip conditions—does not provide any additional BC. These, therefore, must be constructed in a rational manner without the help of the second law.

While the slip and jump BC for each boundary together with the filling condition (50) suffice for the NSF and Grad-13 equations, three additional BC are mathematically required for GENERIC-13. From physical considerations, one would expect that additional BC is required on both sides of the domain, linked to pairs of EV. With three additional EVs, the need for three additional BC cannot be satisfied by symmetrically prescribing BC to both sides of the domain.

The formulation of the additional BC must be compatible with the Knudsen number ordering: as GENERIC-13 reduces to Grad-13 for smaller Knudsen numbers, the number of required BC decreases, and the slip and jump BC suffice. That is, the additional BC should be compatible such that its influence vanishes with Knudsen number. We will return to this question after the discussion of jump and slip boundary conditions.

#### C. Slip and jump BC for GENERIC-13 from the second law

We proceed with the construction of jump and slip BC for GENERIC-13 from the second law of thermodynamics, following the procedures of Linear Irreversible Thermodynamics, as, e.g., outlined in Ref. 26. Denoting stress tensor and heat flux vector in the wall by  $t_{ik}^W$ ,  $q_k^W$  conservation of tangential momentum and normal energy flux at the wall-gas boundary read

$$\rho \Theta_{\tau n} = -t_{\tau n}^W, \tag{57}$$

$$q_n + \rho \Theta_{\tau n} v_\tau = q_n^W - t_{\tau n}^W v_\tau^W. \tag{58}$$

In these equations,  $\tau$  and  $n$  indicate tangential and normal vector and tensor components, respectively, e.g.,  $q_n = q_i n_i$ ,  $q_\tau = q_i - q_n n_i$ . The velocities of the wall and the gas at the wall are only tangential, that is,  $v_n^W = v_n = 0$ . Note that with the wall normal pointing into the gas, we have, e.g.,  $q_n = q_2$  at  $x = 0$  and  $q_n = -q_2$  at  $x = L$ .

The corresponding entropy generation rate  $\Sigma_S$  is the difference between normal entropy fluxes leaving and entering, where the wall entropy flux is given by the classical ratio of heat flux and wall temperature<sup>26</sup>

$$\phi_n - \frac{q_n^W}{T_W} = \Sigma_S \geq 0. \tag{59}$$

The second law of thermodynamics requires that also the wall entropy generation rate is non-negative.

The three equations above are combined by eliminating wall stress and heat flux, and the expression for the GENERIC-13 entropy flux  $\phi_k$  (18) is inserted to obtain the dimensionless entropy generation rate  $\hat{\Sigma}_S = \Sigma_S/R$  as

$$\left[ \frac{1}{\theta} \left( 1 + \frac{3}{50} \Theta_{rs}^{-1} w_r w_s \right) - \frac{1}{\theta_W} \left( 1 + \frac{2}{5} \frac{\sigma_{nn}}{\rho \theta} \right) \right] \frac{1}{2} \rho \theta w_n + \left[ -V_\tau - \frac{1}{5} w_\tau \right] \frac{\sigma_{n\tau}}{\theta_W} = \hat{\Sigma}_S \geq 0, \tag{60}$$

where

$$V_\tau = v_\tau - v_\tau^W \tag{61}$$

is the purely tangential slip velocity.

In Linear Irreversible Thermodynamics, the entropy generation is interpreted as the sum of products of thermodynamic fluxes  $\mathcal{J}_A$  and thermodynamic forces  $\mathcal{F}_A$ , that is, we write

$$\hat{\Sigma}_S = \sum_A \mathcal{J}_A \mathcal{F}_A \geq 0. \tag{62}$$

We follow Ref. 28 where it was argued that the force-flux splitting is such that properties that are even in normal tensor components are the forces, and properties that are odd in normal component are the fluxes, hence we identify the forces as

$$\mathcal{F}_V = -V_\tau - \frac{1}{5} w_\tau, \tag{63}$$

$$\mathcal{F}_\theta = \frac{1}{\theta} \left( 1 + \frac{3}{50} \Theta_{rs}^{-1} w_r w_s \right) - \frac{1}{\theta_W} \left( 1 + \frac{2}{5} \frac{\sigma_{nn}}{\rho \theta} \right), \tag{64}$$

with the corresponding fluxes

$$\mathcal{J}_V = \sigma_{n\tau}, \quad \mathcal{J}_\theta = \frac{1}{2} \rho \theta w_n. \tag{65}$$

Positive entropy generation rate at the wall-gas interface in non-equilibrium is guaranteed by linear force-flux relations between expressions of identical tensor structure, that is, with suitable positive phenomenological coefficients  $\psi_V, \psi_\theta$  we write<sup>26</sup>

$$\sigma_{n\tau} = -\psi_V \left[ V_\tau + \frac{1}{5} w_\tau \right], \tag{66}$$

$$w_n = \psi_\theta \left[ \frac{1}{\theta} \left( 1 + \frac{3}{50} \Theta_{rs}^{-1} w_r w_s \right) - \frac{1}{\theta_W} \left( 1 + \frac{2}{5} \frac{\sigma_{nn}}{\rho\theta} \right) \right]. \quad (67)$$

The coefficients  $\psi_V$  and  $\psi_\theta$  will be determined from matching to the kinetic theory BC presented next.

#### D. Slip and jump BC from kinetic theory

For NSF and Grad-13, we consider kinetic theory boundary conditions based on the well-known Maxwell model, which considers a sharp wall-gas interface, where gas particles colliding with the wall are either diffusely or specularly reflected; the accommodation coefficient  $\chi$  gives the likelihood of diffusive reflection, the wall normal points toward the gas. Jump and slip boundary conditions for the Grad-13B equations were derived from this model, ignoring Knudsen layers corrections, in Ref. 8, which reduced to order  $\mathcal{O}(\text{Kn}^2)$  for plane flow geometry read

$$\sigma_{n\tau} = -\frac{\chi}{2-\chi} \sqrt{\frac{2}{\pi\theta}} \rho\theta \left[ V_\tau + \frac{1}{5} \frac{q_\tau}{\rho} \right], \quad (68)$$

$$q_n = -\frac{2\chi}{2-\chi} \sqrt{\frac{2}{\pi\theta}} \rho\theta \left[ \theta - \theta_W + \frac{1}{4} \frac{\sigma_{nn}}{\rho} - \frac{1}{4} V_\tau^2 \right]. \quad (69)$$

Considering only first-order terms in Kn yields the appropriate slip and jump conditions for the NSF equations as

$$\sigma_{n\tau} = -\frac{\chi}{2-\chi} \sqrt{\frac{2}{\pi\theta}} \rho\theta V_\tau, \quad q_n = -\frac{2\chi}{2-\chi} \sqrt{\frac{2}{\pi\theta}} \rho\theta (\theta - \theta_W). \quad (70)$$

#### E. Matching of Grad-13 and GENERIC-13 slip and jump BC

For a sound comparison of results, we match the phenomenological coefficients  $\psi_V, \psi_\theta$  to the kinetic theory boundary conditions for Grad-13 [(68), (69)]. From (69) and (43), we find to second order in Kn that

$$-\frac{1}{4} V_\tau^2 = -\frac{1}{4} \left( \frac{2-\chi}{\chi} \right)^2 \frac{\pi\theta \sigma_{n\tau} \sigma_{n\tau}}{2(\rho\theta)^2} = \left( \frac{2-\chi}{\chi} \right)^2 \frac{5\pi \sigma_{nn}}{48 \rho}. \quad (71)$$

With this, and the approximation of (10) as  $q_n = \frac{1}{2} \rho\theta w_n$ , the Grad-13 BC can be written as

$$\sigma_{n\tau} = -\frac{\chi}{2-\chi} \sqrt{\frac{2}{\pi}} \rho\sqrt{\theta} \left[ V_\tau + \frac{1}{10} w_\tau \right], \quad (72)$$

$$w_n = -\frac{4\chi}{2-\chi} \sqrt{\frac{2}{\pi}} \sqrt{\theta}\theta_W \left[ \frac{1}{\theta_W} \left( 1 + \xi \frac{\sigma_{nn}}{\rho\theta} \right) - \frac{1}{\theta} \right], \quad (73)$$

with the abbreviation

$$\xi = \frac{1}{4} \left( 1 + \frac{5\pi}{12} \left( \frac{2-\chi}{\chi} \right)^2 \right). \quad (74)$$

This is sufficiently similar to the GENERIC-13 BC [(66), (67)] to identify coefficients  $\psi_V, \psi_\theta$  so that the slip and jump BC for GENERIC-13 finally read

$$\sigma_{n\tau} = -\frac{\chi}{2-\chi} \sqrt{\frac{2}{\pi}} \sqrt{\theta}\rho \left[ V_\tau + \frac{1}{5} w_\tau \right], \quad (75)$$

$$w_n = -\frac{4\chi}{2-\chi} \sqrt{\frac{2}{\pi}} \sqrt{\theta}\theta_W \left[ \frac{1}{\theta_W} \left( 1 + \frac{2}{5} \frac{\sigma_{nn}}{\rho\theta} \right) - \frac{1}{\theta} \left( 1 + \frac{3}{50} \Theta_{rs}^{-1} w_r w_s \right) \right]. \quad (76)$$

Note that for  $\chi \in (0, 1)$  we have  $\xi \in (\infty, 0.577)$ , that is compared to the simplified kinetic theory model GENERIC-13 generally gives a smaller value (2/5) for this factor.

#### F. Additional BC for GENERIC-13

##### 1. Asymptotically vanishing BC

The BC consistency requirement can be guaranteed by the following procedure. Let  $\Lambda^\epsilon$  be an asymptotically vanishing eigenvalue, that is,

$$\lim_{\text{Kn} \rightarrow 0} \Lambda^\epsilon = 0, \quad (77)$$

with the associated characteristic transport equation

$$\Lambda^\epsilon L_B^\epsilon \frac{du_B}{dy} = L_A^\epsilon \mathcal{P}_A. \quad (78)$$

We interpret

$$\frac{dW^\epsilon}{dy} = L_B^\epsilon \frac{du_B}{dy} \quad (79)$$

as the characteristic gradient for the EV  $\Lambda^\epsilon$ .

A consistent BC is obtained by setting the characteristic gradient at the boundary to zero

$$\frac{dW^\epsilon}{dy} = 0, \quad (80)$$

so that at the boundary ( $\mathfrak{B}$ , that is, at  $x = 0$  and  $x = L$ )

$$\left[ \Lambda^\epsilon L_B^\epsilon \frac{du_B}{dy} \right]_{\mathfrak{B}} = \left[ \Lambda^\epsilon \frac{dW^\epsilon}{dy} \right]_{\mathfrak{B}} = [L_A^\epsilon \mathcal{P}_A]_{\mathfrak{B}} = 0. \quad (81)$$

With this, we arrive at the boundary condition

$$[L_A^\epsilon \mathcal{P}_A]_{\mathfrak{B}} = 0, \quad (82)$$

which ensures that independently of the actual value of  $\Lambda^\epsilon$  this algebraic equation is fulfilled at the boundary. At larger Kn, the algebraic relation does not hold in the interior but is enforced only at the boundary. As the Knudsen number decreases, GENERIC-13 is reduced toward Grad-13B so that the EV approaches zero and the solution in the interior approaches the algebraic relation, which then is valid in all locations.

With three asymptotically vanishing EV we must choose EV for the construction of the boundary condition (82). Closer (numerical) evaluation showed that at the left side ( $x = 0$ ) one EV is positive and two EV are negative, while on the right ( $x = L$ ) one EV is negative and two are positive. As the eigenvalues are interpreted as the characteristic speeds of the equations, negative EV on the left (or positive EV on the right) refers to characteristics leaving the system, while positive (negative on the right) EV refers to characteristics entering.

Prescribing a BC for an incoming characteristic implies an external manipulation of the system, that is, the characteristic is set to a value at the boundary that propagates into the system. In contrast,

values of characteristics traveling outward are created within the system, as expressed through the transport equations. Setting  $\frac{dW^c}{dy} = 0$  for such a characteristic implies free flow of the characteristic out of the system and was chosen as the least impactful BC.

With three BC required and two boundaries, we are facing some asymmetry introduced in the solution by prescribing one characteristic BC on one side of the domain, and two on the other, or one pair of BCs and one singular one. Thus, for the two EVs describing existing characteristics on either side, we decided to choose that with the larger absolute value on both sides of the domain and the one with the smaller absolute value on just one side (left). Indeed, the BC (82) is closer to the actual equation (78) for the smaller EV, and we expect this choice to create less asymmetry.

It worked well to implement the corresponding pair of BCs (82) in the boundary cells of the discretization of the  $\Theta_{22}$  balance and the single BC in the  $\Theta_{11}$  balance.

Obviously, while they appear intuitively plausible, we have no strong reasons for the choices laid out above that lead to the described implementation of additional BC for GENERIC-13. The need for additional BC beyond slip and jump was encountered before for the R13-moment equations, where it could be circumvented by a reformulation of the transport equations that kept the Knudsen order intact but reduced the number of BC.<sup>29,30</sup> A similar reformulation of GENERIC-13 is not possible, since this would impact the thermodynamic structure that is at the core of the equations. We are not aware of a similar problem elsewhere, hence had to develop our own approach.

In our numerical solutions, we experimented with other choices, e.g., BC for different characteristics, implemented into other equations, but differences between results were generally small and did not warrant a deeper evaluation. The results presented below show that the chosen approach produces sensible results.

A deeper consideration of the construction of a full set of BC for GENERIC-13 might be warranted but is beyond the scope of this contribution.

## 2. Kinetic theory

Just as the jump and slip conditions [(68), (69)] for NSF and Grad-13 are obtained from the Maxwell boundary condition, one can derive boundary conditions for higher moments of the distribution function of kinetic theory.<sup>10,28,29</sup> By extension of the derivation of slip and jump conditions, such BC for higher moments might be meaningful as the additional BC required.

Kinetic theory BC is not linked to the EV discussed above; hence, there is no guideline as to which particular higher order BC one might choose. Thus, we explored several options before settling on a BC developed for the fourth moment,  $R_{ij}$ , of the distribution function as part of the regularized 13-moment (R13) equations, adjusted to stand in agreement with the second law of thermodynamics.<sup>28</sup> In our notation, and for Maxwell molecules, the BC reads [Eq. (12b) of Ref. 28]

$$-\frac{12}{5}\text{Kn}\frac{dq_\tau}{dn} = \frac{\chi}{2-\chi}\sqrt{\frac{2}{\pi\theta}}\left(V_\tau - \frac{11}{5}\frac{q_\tau}{\rho\theta} - \frac{16}{15}\text{Kn}\frac{d\sigma_{\tau n}}{dn}\right), \quad (83)$$

where  $\frac{d}{dn} = n_i \frac{d}{dx_i}$  denotes the derivative in direction of the wall normal. This BC is implemented in the boundary cells of the  $w_2$ -balance.

With its background in kinetic theory, this BC is not linked to the eigen-structure of the matrix  $\mathcal{A}_{AB}$ , hence the consistency requirement

is not guaranteed. We note that the fourth moment has no physical meaning but is found in the regularized 13-moment equations as the gradient of the heat flux vector.<sup>5,9,13</sup>

## VI. NUMERICAL SIMULATIONS

We now present and discuss numerical solutions of steady-state plane flow configurations for NSF, Grad-13B, and GENERIC-13. Numerical solutions are generated through an iterative process using fourth-order finite difference approximations on a uniform grid with  $n = 200$  grid points. To simplify the approach, MATLAB's `fsolve` (`eqs, z0`) function is used in which initial guesses  $z0$  must be provided along with a tolerance; more specifically, the function uses the Levenberg–Marquardt algorithm. For our applications, initial guesses are selected from the previous model and a conservative convergence tolerance of  $10^{-15}$  is implemented. Consistency between our solutions and previously published work gives confidence of excellent convergence. The number of significant figures is dependent on the variable of interest and is unique to each curve; therefore, they can vary on the presented results.

A good initial guess is crucial for finding reliable results and for this the hierarchy of models in terms of Knudsen number offers a natural multi-step approach to determine useful guesses. For NSF we chose the well-known analytical results for constant coefficients<sup>26</sup> as initial guesses. The numerical solution for NSF then serves as an initial guess for Grad-13, and the result of that calculation serves as the initial guess for GENERIC-13. All calculations are performed in dimensionless variables, with set Knudsen numbers.

Accuracy is high, and differences between the results of the various sets of equations are due to differences in the equations themselves and their boundary conditions.

This method of solution is quite forgivable about the prescription of boundary conditions. We show solutions of GENERIC-13 with the full set of eight properly compatible BC as discussed above, and with the extra BC (83) on two sides added to jump, slip, and mass conditions, that is one BC less than mathematically required. These results are included to show that the incompatibility of the extra kinetic BC leads to unwelcome jumps at the boundaries in the limit of small Knudsen numbers.

### A. Heat transfer

In the case of pure heat transfer, flow velocity  $v$ , shear stress  $\sigma_{12}$ , and parallel heat flux  $q_1$  vanish, and only the temperature jump boundary conditions are required, where we set the wall temperatures to  $\theta_B = 1 \pm \Delta\theta$ .

For this simple geometry NSF and Grad-13B equations agree, hence no separate curves for Grad-13B are shown in Figs. 5 and 6, which compare NSF and GENERIC-13 curves for mass density  $\rho$ , temperature  $\theta$ , normal stress  $\sigma_{22}$ , normal heat flux  $q_2$ , and pressure  $p$ . No extra BC is required for GENERIC-13.

Figure 5 shows results at  $\text{Kn} = 0.05$  with a small temperature deviation  $\Delta\theta = 0.05$ . At this small Knudsen number, we are in the NSF regime, and as expected, NSF and GENERIC-13 agree very well; the difference of below 0.01% between pressures and heat fluxes is only visible due to the chosen scale. There are small temperature jumps at the walls, and normal stresses vanish.

Figure 6 shows results at  $\text{Kn} = 1$  and a significant temperature deviation  $\Delta\theta = 0.5$ . At this large Knudsen number, NSF is not valid, and this is seen in the significant differences in the curves.

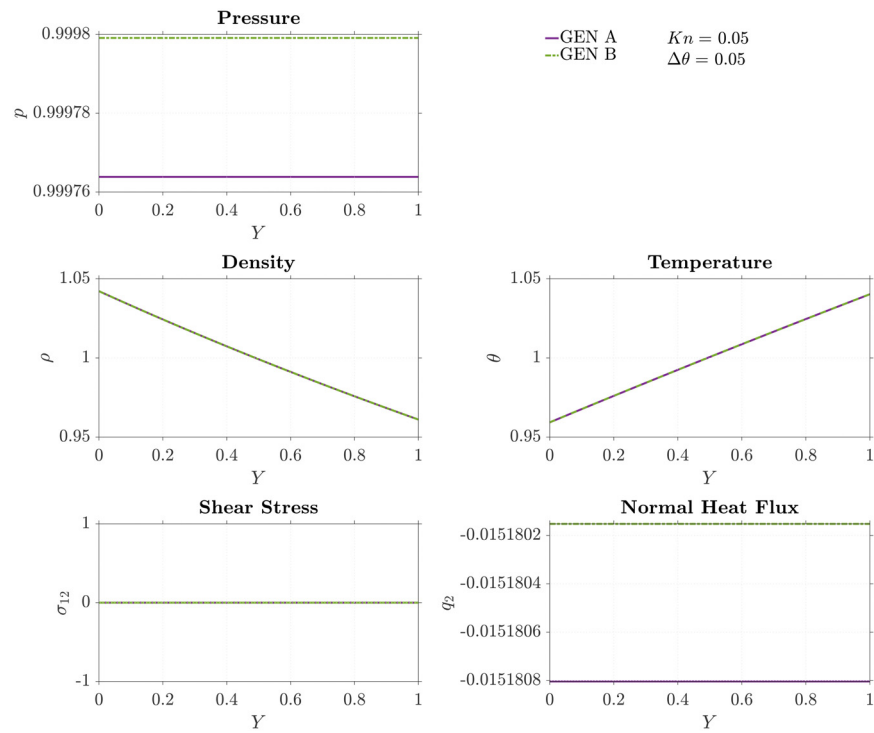


FIG. 5. Heat transfer for NSF and GENERIC-13 at  $Kn = 0.05$ ,  $\Delta\theta = 0.05$ .

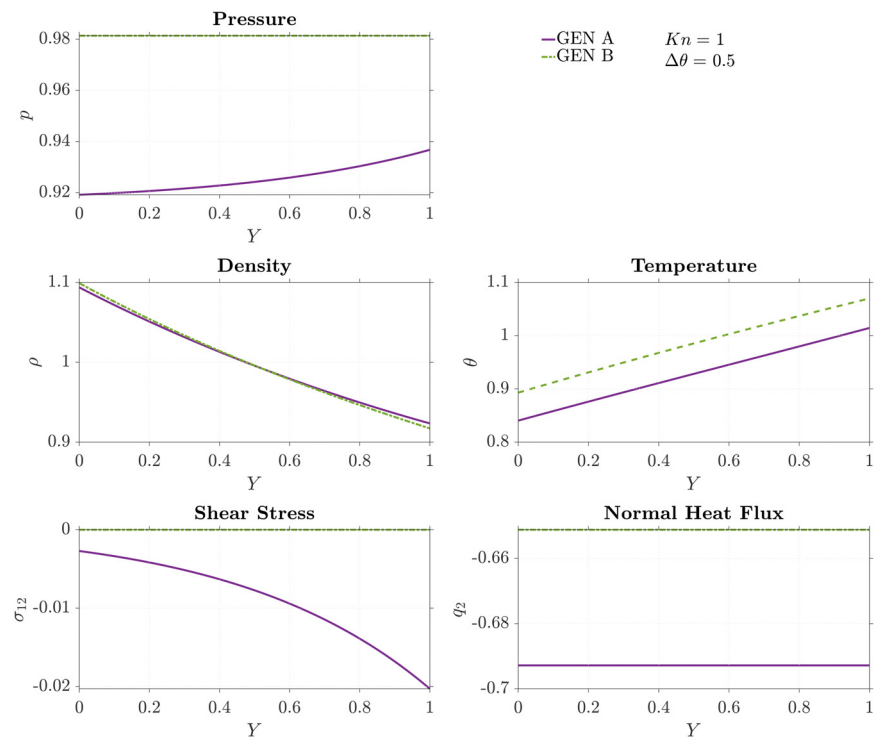


FIG. 6. Heat transfer for NSF and GENERIC-13 at  $Kn = 1$ ,  $\Delta\theta = 0.5$ .

Temperature jumps are large (the boundary temperatures are  $\theta_B = 0.5, 1.5$ ), and due to the large temperature difference non-linear effects in GENERIC-13 induce normal stress and pressure deviation (of course,  $p + \sigma_{22} = \text{const.}$ ).

**B. Couette flow**

Next, we consider Couette flow, for which NSF and Grad-13B equations differ, and solutions for GENERIC-13 are based on (a) the asymptotically vanishing BC (82) and (b) the kinetic theory boundary condition

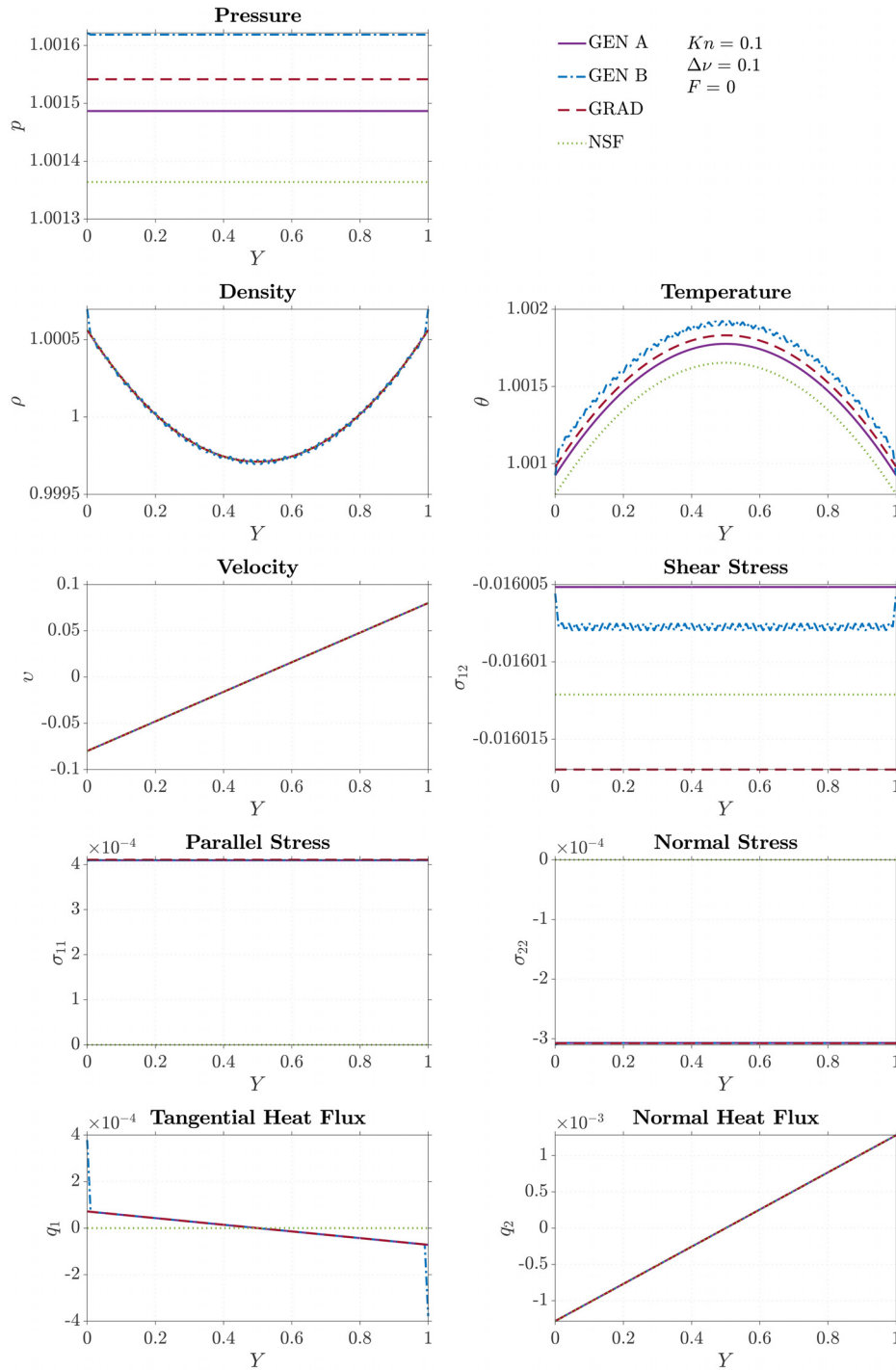


FIG. 7. Couette flow for NSF, Grad-13, and GENERIC-13 at  $Kn = 0.1$ ,  $\Delta v = 0.1$ .

(83), which in the plots are indicated as GEN-A and GEN-B, respectively. The plots show the eight relevant variables (40) as well as pressure.

We begin with flows at low Knudsen number  $Kn = 0.1$  which is large enough as that some discrepancy between NSF and the higher

order models is expected, but no difference between Grad-13 and GENERIC-13. Temperatures and velocities of the plates are set to  $\theta = 1$  and  $V_B = \pm \Delta v$ . Figures 7 and 8 show results for  $\Delta v = 0.1$  and  $\Delta v = 0.5$ , respectively.

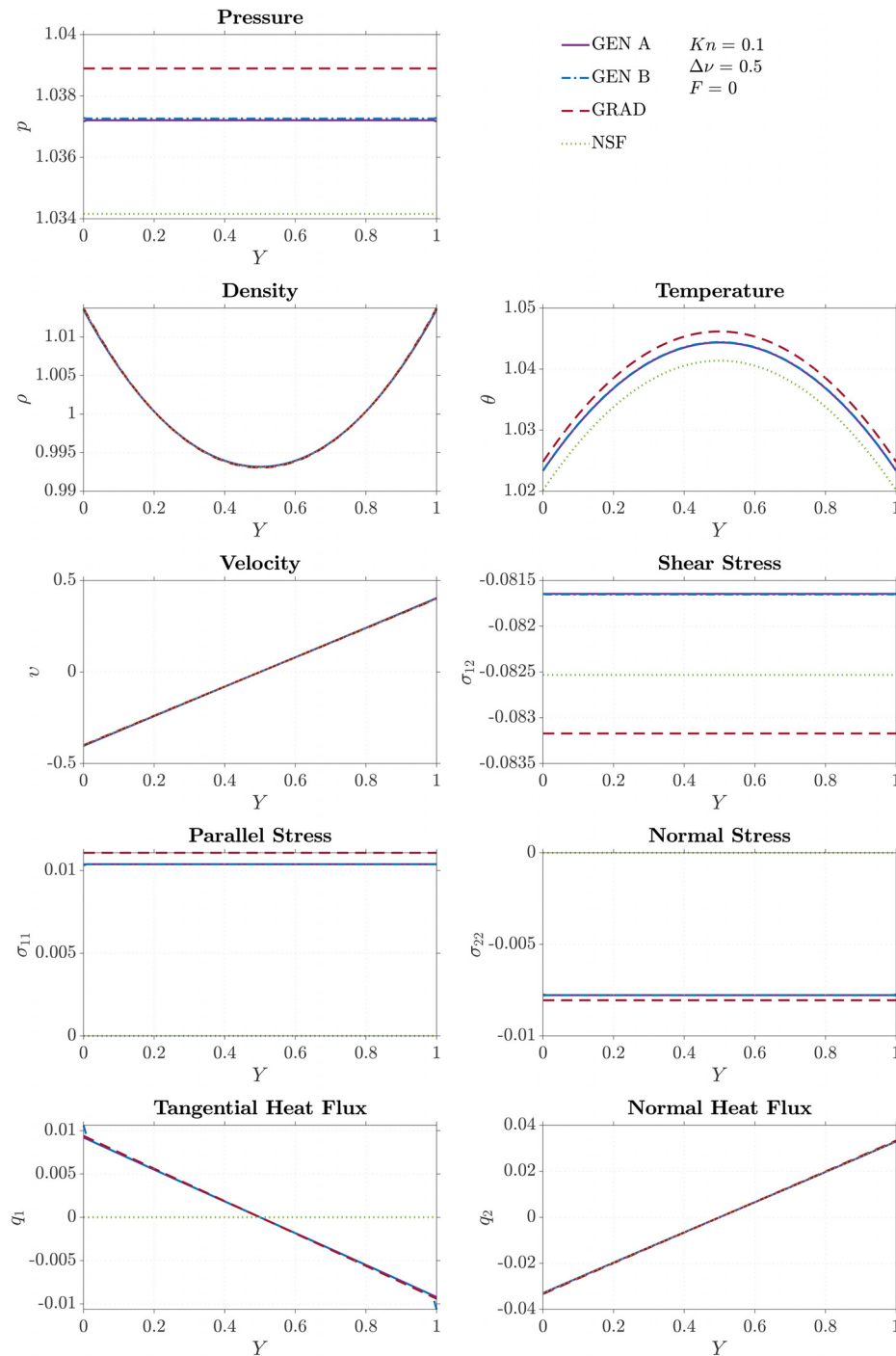


FIG. 8. Couette flow for NSF, Grad-13, and GENERIC-13 at  $Kn = 0.1$ ,  $\Delta v = 0.5$ .

At the smaller velocities (Fig. 7) we observe good agreement between Grad, GEN-A and GEN-B, with the important difference that these show normal and parallel stresses and tangential heat flux, which are not described by NSF. While GEN-A and GEN-B

agree in the bulk, they disagree at the boundary. Indeed, the kinetic theory BC used for GEN-B produces a jump in the tangential heat flux at the boundary, which must be attributed to violation of the BC consistency requirement of Sec. VB. At this Knudsen number

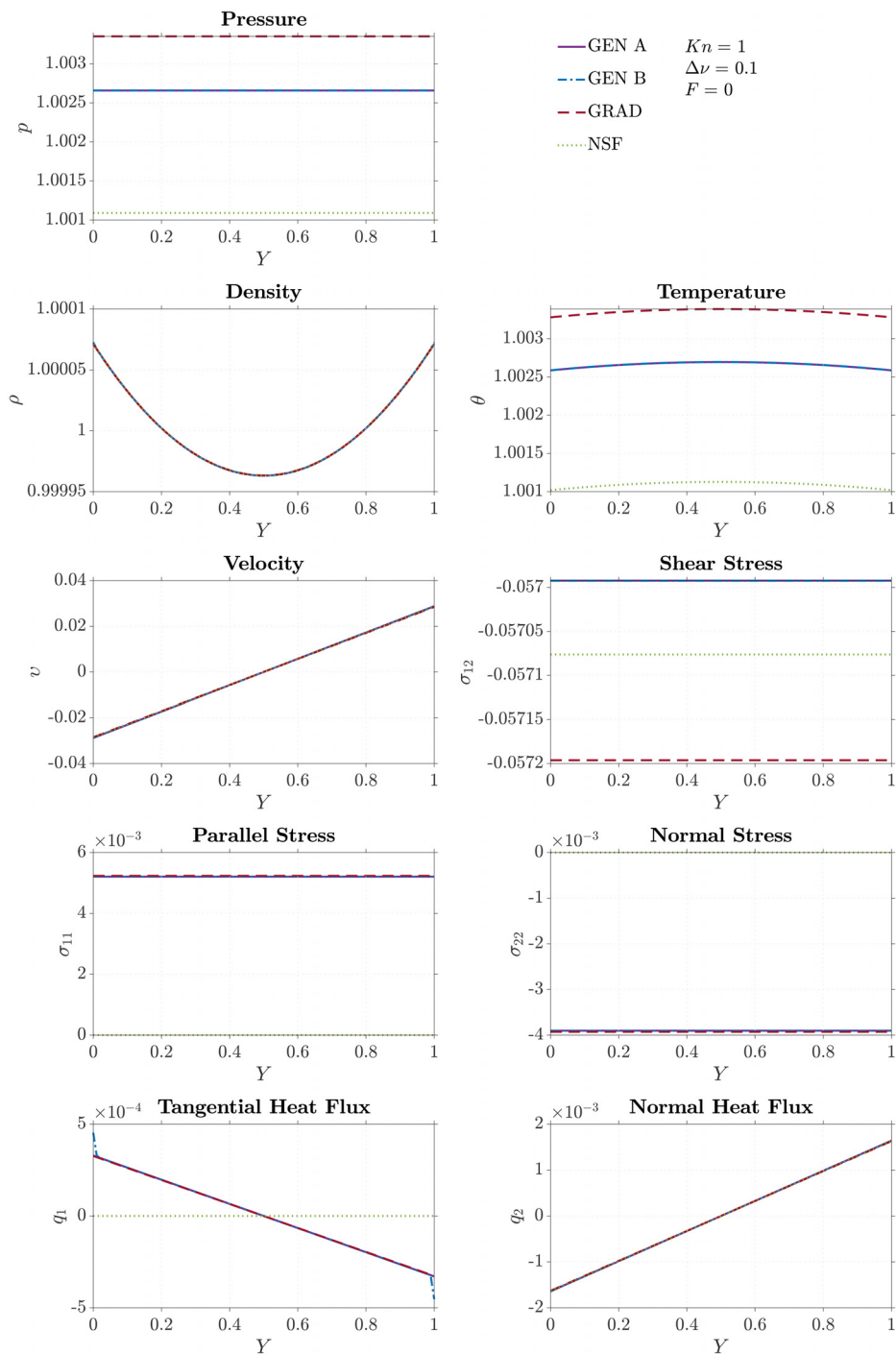


FIG. 9. Couette flow for NSF, Grad-13, and GENERIC-13 at  $Kn = 1$ ,  $\Delta\nu = 0.1$ .

the parallel and normal stresses  $\sigma_{11}$ ,  $\sigma_{22}$ , and the tangential heat flux  $q_1$  are given by the bulk equations (43), which hold for Grad-13 as well as for GENERIC-13 (for small Kn). Thus, the extra BC's are not needed, and with the kinetic BC not consistent we observe

the jump in  $q_1$  for GEN-B, while no such jump appears for GEN-A which uses the consistent BC (82). No asymmetry is observed in GEN-A, since the extra BC does not have any influence on the flow.

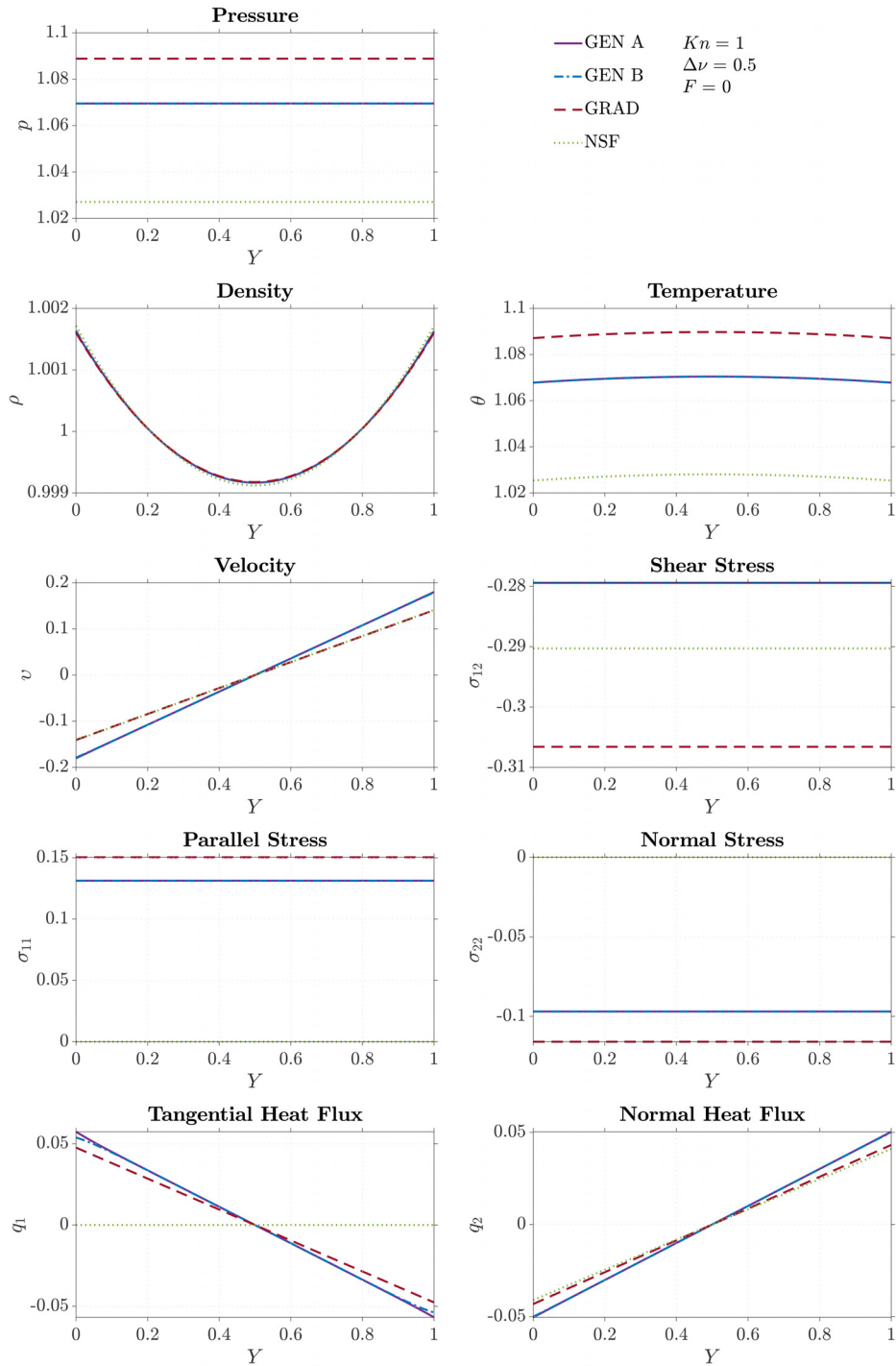


FIG. 10. Couette flow for NSF, Grad-13, and GENERIC-13 at  $Kn = 1$ ,  $\Delta\nu = 0.5$ .

For the larger velocity difference of Fig. 8 the relative mismatch for GEN-B at the boundary is less pronounced, and GEN-A and GEN-B agree. Probably due to non-linear effects, we observe some differences between GENERIC-13 and Grad-13 in the curves for temperature and shear stress but excellent agreement else.

Next, we consider two cases with Knudsen number  $Kn = 1$  where more pronounced differences between Grad-13 and GENERIC-13 are expected. For  $\Delta v = 0.1$  as shown in Fig. 9, the general behavior is quite similar to those at smaller  $Kn$ , again with boundary jumps for GEN-B. For larger boundary velocity  $\Delta v = 0.5$ , as shown in (Fig. 10),

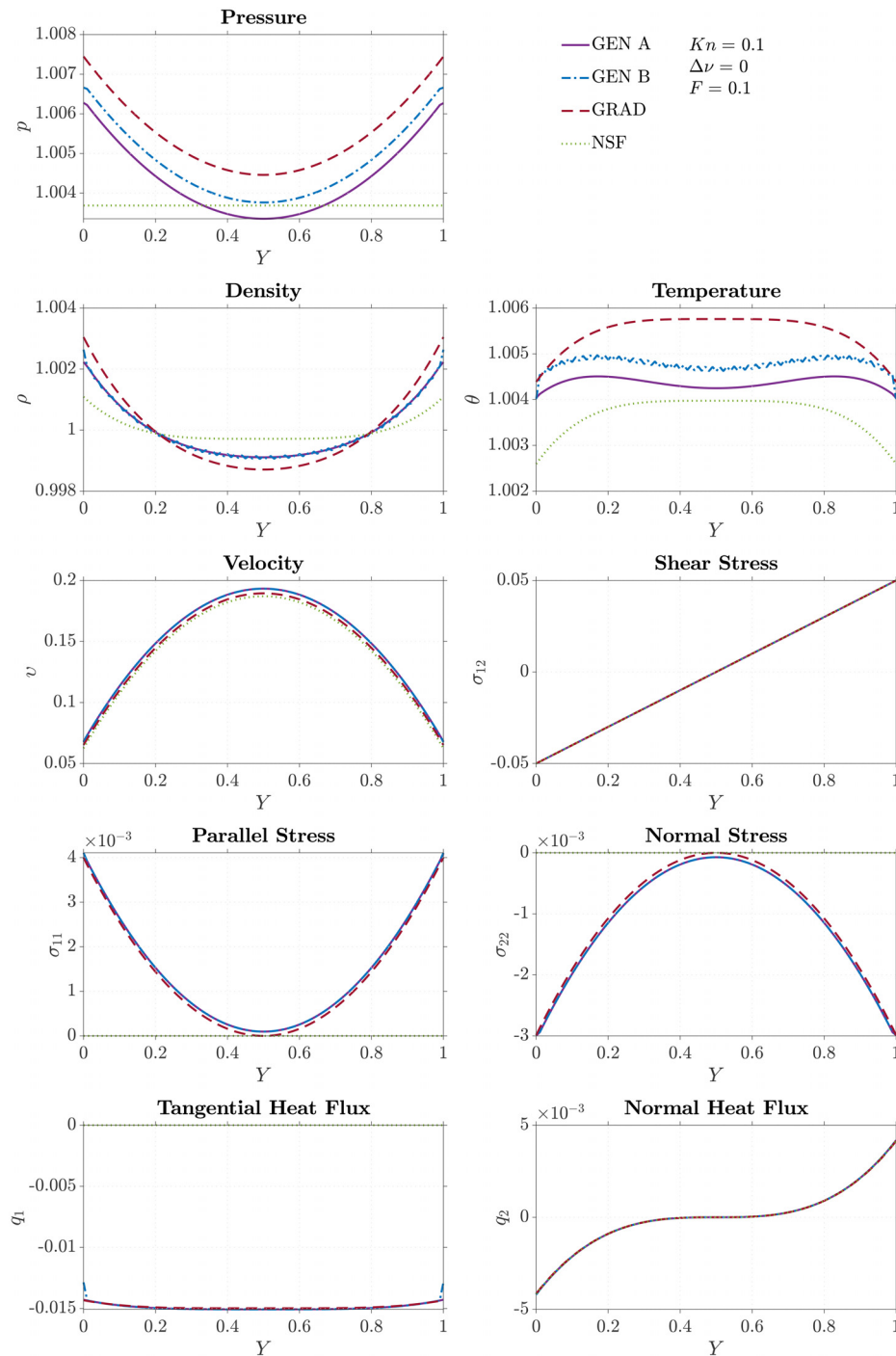


FIG. 11. Poiseuille flow for NSF, Grad-13, and GENERIC-13 at  $Kn = 0.1, F = 0.1$ .

most of the behavior is as for the cases discussed before, but the different extra BC leads to visible differences in the tangential heat flux  $q_1$  in the vicinity of the wall. While the kinetic BC of GEN-B now does not induce a jump, the compatible BC of GEN-A induces some extra curvature toward the boundary. While the tangential heat flux curve is

similar to curves with Knudsen layers known for the R-13 equations of kinetic theory,<sup>10,30</sup> the latter result from linear effects and are present also for small velocities, while the curvature for GEN-A is due to non-linearities and vanishes for smaller velocities. Although one BC is prescribed only on the left side, there is no visible asymmetry in the curves.

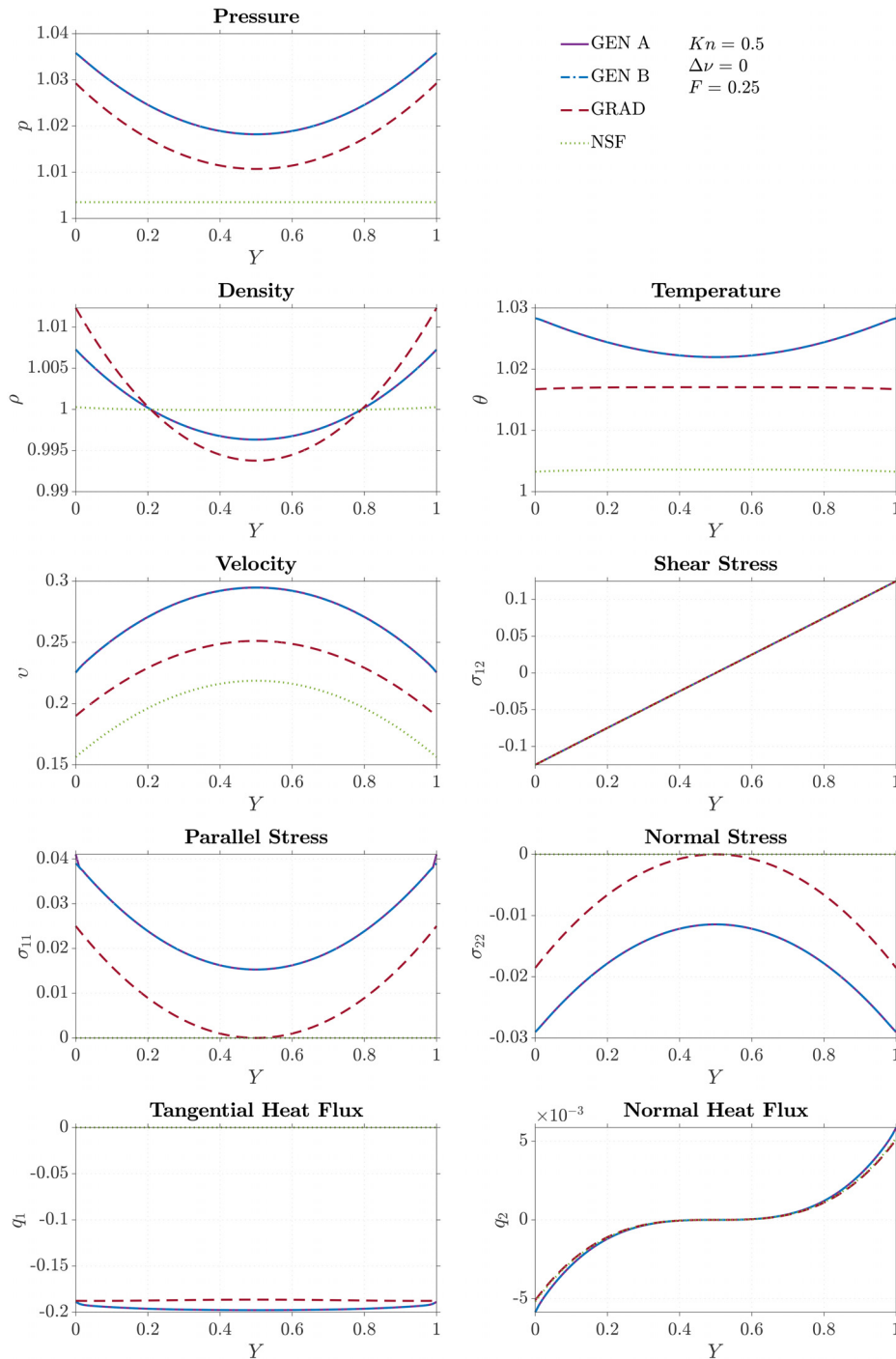


FIG. 12. Poiseuille flow for NSF, Grad-13, and GENERIC-13 at  $Kn = 0.5$ ,  $F = 0.25$ .

C. Poiseuille flow

Poiseuille flow proved to be more difficult for our numerical approach, where it was not possible to obtain reliable results for larger Knudsen number or driving force. Thus, we show only a few results, a more thorough examination will require an improved numerical approach.

Figure 11 shows results of  $Kn = 0.1, F = 0.1$ . This Knudsen number is sufficiently small so that GENERIC-13 and Grad-13B agree well in heat flux and stress components. Due to the simplification of Grad-13B through the second CE expansion, these cannot describe the characteristic convex dip in the temperature profile—a well-known rarefaction effect<sup>15</sup>—which is well reproduced by GENERIC-13. While GEN-A employs asymmetric BC, there is no visible asymmetry in the results. As for Couette flow, the kinetic boundary condition (GEN-B) has a mismatch at the boundary that induces boundary jumps in the heat flux  $q_1$ . NSF cannot describe parallel heat flux and normal stresses, underestimates temperature jumps, and yields the usual<sup>26</sup> concave temperature profile.

For other values of  $Kn$  and  $F$ , we were not able to produce proper results from GEN-A with eight BC as mathematically required. However, just as for the kinetic BC, the code yields reasonable results with seven BC prescribed (three pairs for jump, slip, extra BC, plus filling). For the case of Fig. 11, the corresponding results are indistinguishable from those shown. Figure 12 shows results for a case with larger Knudsen number and driving force, with  $Kn = 0.5, F = 0.25$ , where the temperature curve is dominated by the convex dip, but other variables are similar to the previous case.

VII. DISCUSSION AND OUTLOOK

We have studied the full non-linear GENERIC-13 equations, which were developed as a system with complete thermodynamic structure to describe mildly rarefied gases. Within second order in the Knudsen number the equations agree with Grad’s 13-moment equations.

Evaluation for one-dimensional propagation revealed that the GENERIC-13 equations are unconditionally hyperbolic for all values of the variables. Moreover, their non-linear production terms emphasize push-back toward equilibrium for larger deviation from equilibrium.

In order to solve GENERIC-13 for classic plane flow problems, we had to develop appropriate boundary conditions (BC). Jump and slip BC were found from the entropy generation at a solid-gas interface which suggests flux-force relations as in Linear Irreversible Thermodynamics. Phenomenological coefficients were matched to jump and slip boundary conditions from kinetic theory. However, due to their complex mathematical structure, the GENERIC-13 equations require additional BC, which must be formulated such that their influence fades as the Knudsen number decreases, and the equations reduce toward the Grad-13 or NSF equations. Based on this requirement and the structure of the equations, we proposed a set of *asymptotically vanishing BC*, which lead to meaningful solutions for heat transfer, and Couette and Poiseuille flows. We emphasize that, while reasonable, the additional BC is postulated, and additional justification, or working alternatives, would be welcome.

The results presented here indicate that the GENERIC-13 provides a set of meaningful equations for the description of mildly rarefied flows. Further numerical evaluation for more complex flow problems should be considered in the future.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

**Luke Bell:** Investigation (equal); Methodology (equal); Software (equal); Validation (equal); Writing – original draft (equal). **Henning Struchtrup:** Conceptualization (equal); Funding acquisition (equal); Investigation (equal); Methodology (equal); Writing – review & editing (equal).

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

APPENDIX: GENERIC-13 EQUATIONS FOR PLANE FLOWS

The following shows the fully reduced GENERIC-13 equations for both heat transfer and shear flow cases followed by the abbreviations used in the matrix  $\mathcal{A}_{AB}^{GEN13}$ .

1. Equations for heat transfer ( $V_0 = V_L = w_1 = F = 0$ )

Momentum balance

$$\frac{d\rho\Theta_{22}}{dy} = 0. \tag{A1}$$

$\Theta_{11}$ -balance

$$\begin{aligned} & \frac{w_2\Theta_{11}}{5\rho} \frac{d\rho}{dy} + \frac{w_2}{5} \frac{d\Theta_{11}}{dy} + \frac{\Theta_{11}}{5} \frac{dw_2}{dy} \\ & = -\frac{1}{Kn} \frac{\theta}{30} \left[ \left( \frac{w_2}{\Theta_{22}} \right)^2 + 10 \left( \frac{1}{\Theta_{11}} + \frac{1}{\Theta_{22}} + \frac{1}{3\theta - \Theta_{11} - \Theta_{22}} \right) \right] \\ & \quad \times (\rho\Theta_{11} - \rho\theta). \end{aligned} \tag{A2}$$

$\Theta_{22}$ -balance

$$\begin{aligned} & \frac{3w_2\Theta_{22}}{5\rho} \frac{d\rho}{dy} + \frac{3w_2}{5} \frac{d\Theta_{22}}{dy} + \frac{3\Theta_{22}}{5} \frac{dw_2}{dy} \\ & = -\frac{1}{Kn} \frac{\theta}{30} \left[ \left( \frac{w_2}{\Theta_{22}} \right)^2 + 10 \left( \frac{1}{\Theta_{11}} + \frac{1}{\Theta_{22}} + \frac{1}{3\theta - \Theta_{11} - \Theta_{22}} \right) \right] \\ & \quad \times (\rho\Theta_{22} - \rho\theta). \end{aligned} \tag{A3}$$

Energy balance

$$\begin{aligned} & \frac{1}{\rho} (2w_2\Theta_{22} + 3w_2\theta) \frac{d\rho}{dy} + (3w_2) \frac{d\theta}{dy} + (2w_2) \frac{d\Theta_{22}}{dy} \\ & \quad + (2\Theta_{22} + 3\theta) \frac{dw_2}{dy} = 0. \end{aligned} \tag{A4}$$

$w_2$ -balance

$$\begin{aligned} & \left( \frac{\Theta_{22}}{\Theta_{11}} - \frac{\Theta_{22}}{3\theta - \Theta_{11} - \Theta_{22}} \right) \frac{d\Theta_{11}}{dy} + \left( 3 + \frac{3w_2^2}{5\Theta_{22}} - \frac{\Theta_{22}}{3\theta - \Theta_{11} - \Theta_{22}} \right) \\ & \times \frac{d\Theta_{22}}{dy} + \frac{\Theta_{22}}{3\theta - \Theta_{11} - \Theta_{22}} \frac{d\theta}{dy} - \frac{12}{5} w_2 \frac{dw_2}{dy} \\ & = -\frac{\rho}{Kn} \frac{\theta}{30} \left[ \frac{5}{\Theta_{11}} - \frac{1}{\Theta_{22}} + \frac{5}{\Theta_{33}} + \frac{7\theta + 5w_2^2}{\Theta_{22}^2} \right] w_2. \end{aligned} \tag{A5}$$

2. Equations for shear flows

Momentum balance

$$\frac{d\rho\Theta_{12}}{dy} = \rho F, \quad \frac{d\rho\Theta_{22}}{dy} = 0.$$

To reduce the length of the expanded equations, use the abbreviation

$$\begin{aligned} \zeta &= -\frac{1}{Kn} \left[ \frac{1}{3} \theta \Theta_{rr}^{-1} + \frac{1}{30} \theta \Theta_{kr}^{-1} w_r \Theta_{ks}^{-1} w_s \right] \\ &= -\frac{1}{Kn} \left[ \frac{1}{3} \theta \Theta_{rr}^{-1} + \frac{1}{30} \theta (w_1^2 (\Theta_{11}^{-1} \Theta_{11}^{-1} + \Theta_{12}^{-1} \Theta_{12}^{-1}) \right. \\ & \quad \left. + w_2^2 (\Theta_{12}^{-1} \Theta_{12}^{-1} + \Theta_{22}^{-1} \Theta_{22}^{-1}) + 2w_1 w_2 (\Theta_{11}^{-1} \Theta_{12}^{-1} + \Theta_{12}^{-1} \Theta_{22}^{-1}) \right]. \end{aligned} \tag{A6}$$

$\Theta_{11}$ -balance

$$\frac{w_2 \Theta_{11}}{5\rho} \frac{d\rho}{dy} + 2\Theta_{12} \frac{dv}{dy} + \frac{w_2}{5} \frac{d\Theta_{11}}{dy} + \frac{2\Theta_{12}}{5} \frac{dw_1}{dy} + \frac{\Theta_{11}}{5} \frac{dw_2}{dy} = \zeta \sigma_{11}. \tag{A7}$$

$\Theta_{12}$ -balance

$$\Theta \frac{dv}{dy} + \frac{\Theta_{22}}{5} \frac{dw_1}{dy} + \frac{2\Theta_{12}}{5} \frac{dw_2}{dy} = \zeta \sigma_{12}. \tag{A8}$$

$\Theta_{22}$ -balance

$$3\Theta_{22} \frac{dw_2}{dy} = \zeta \sigma_{22}. \tag{A9}$$

$\Theta_{33}$ -balance

$$\begin{aligned} & \left( \frac{3w_2\theta}{5\rho} - \frac{w_2\Theta_{11}}{5\rho} \right) \frac{d\rho}{dy} - \frac{w_2}{5} \frac{d\Theta_{11}}{dy} + \frac{3w_2}{5} \frac{d\theta}{dy} \\ & + \left( \frac{3\theta}{5} - \frac{\Theta_{11}}{5} - \frac{\Theta_{22}}{5} \right) \frac{dw_2}{dy} = \zeta \sigma_{33}. \end{aligned} \tag{A10}$$

Energy balance ( $\theta$ )

$$\frac{3w_2\theta}{5\rho} \frac{d\rho}{dy} + 2\Theta_{12} \frac{dv}{dy} + \frac{3w_2}{5} \frac{d\theta}{dy} + \frac{2\Theta_{12}}{5} \frac{dw_1}{dy} + \left( \frac{3\theta}{5} + \frac{2\Theta_{22}}{5} \right) \frac{dw_2}{dy} = 0. \tag{A11}$$

$w_1$ -balance

$$\begin{aligned} & w_2 \frac{dv}{dy} + 2 \frac{d\Theta_{12}}{dy} + \Theta_{12} \left[ (\Theta_{11}^{-1} - \Theta_{33}^{-1}) \frac{d\Theta_{11}}{dy} + 2\Theta_{12}^{-1} \frac{d\Theta_{12}}{dy} + (\Theta_{22}^{-1} - \Theta_{33}^{-1}) \frac{d\Theta_{22}}{dy} + 3\Theta_{33}^{-1} \frac{d\theta}{dy} \right] \\ & - \frac{1}{5} \left[ (2w_1\Theta_{12} + w_2\Theta_{11}) \frac{dw_1\Theta_{11}^{-1}}{dy} + (2w_1\Theta_{12} + w_2\Theta_{11}) \frac{dw_2\Theta_{12}^{-1}}{dy} (w_1\Theta_{22} + 2w_2\Theta_{12}) \frac{dw_1\Theta_{12}^{-1}}{dy} + (w_1\Theta_{22} + 2w_2\Theta_{12}) \frac{dw_2\Theta_{22}^{-1}}{dy} \right] \\ & = \frac{-\rho\theta^{1-w}}{Kn} \left\{ \frac{1}{6} \theta \Theta_{kk}^{-1} w_1 - \frac{1}{15} \theta (\Theta_{11}^{-1} w_1 + \Theta_{12}^{-1} w_2) + \frac{7}{30} \theta^2 [(\Theta_{11}^{-1} \Theta_{11}^{-1} + \Theta_{12}^{-1} \Theta_{12}^{-1}) w_1 + (\Theta_{11}^{-1} \Theta_{12}^{-1} + \Theta_{12}^{-1} \Theta_{22}^{-1}) w_2] \right. \\ & \quad \left. + \frac{1}{60} \theta w_1 [(\Theta_{11}^{-1} \Theta_{11}^{-1} + \Theta_{12}^{-1} \Theta_{12}^{-1}) w_1^2 + (\Theta_{12}^{-1} \Theta_{12}^{-1} + \Theta_{22}^{-1} \Theta_{22}^{-1}) w_2^2 + (2\Theta_{11}^{-1} \Theta_{12}^{-1} + 2\Theta_{12}^{-1} \Theta_{22}^{-1}) w_1 w_2] \right\}. \end{aligned} \tag{A12}$$

$w_2$ -balance

$$\begin{aligned} & 2 \frac{d\Theta_{22}}{dy} + \Theta_{22} \left[ (\Theta_{11}^{-1} - \Theta_{33}^{-1}) \frac{d\Theta_{11}}{dy} + 2\Theta_{12}^{-1} \frac{d\Theta_{12}}{dy} + (\Theta_{22}^{-1} - \Theta_{33}^{-1}) \frac{d\Theta_{22}}{dy} + 3\Theta_{33}^{-1} \frac{d\theta}{dy} \right] \\ & - \frac{1}{5} \left[ (2w_2\Theta_{12} + w_1\Theta_{22}) \frac{dw_1\Theta_{11}^{-1}}{dy} + (2w_2\Theta_{12} + w_1\Theta_{22}) \frac{dw_2\Theta_{12}^{-1}}{dy} (3w_2\Theta_{22}) \frac{dw_1\Theta_{12}^{-1}}{dy} + (3w_2\Theta_{22}) \frac{dw_2\Theta_{22}^{-1}}{dy} \right] \\ & = \frac{-\rho\theta^{1-w}}{Kn} \left\{ \frac{1}{6} \theta \Theta_{kk}^{-1} w_2 - \frac{1}{15} \theta (\Theta_{12}^{-1} w_1 + \Theta_{22}^{-1} w_2) + \frac{7}{30} \theta^2 [(\Theta_{12}^{-1} \Theta_{11}^{-1} + \Theta_{12}^{-1} \Theta_{22}^{-1}) w_1 + (\Theta_{12}^{-1} \Theta_{12}^{-1} + \Theta_{22}^{-1} \Theta_{22}^{-1}) w_2] \right. \\ & \quad \left. + \frac{1}{60} \theta w_2 [(\Theta_{11}^{-1} \Theta_{11}^{-1} + \Theta_{12}^{-1} \Theta_{12}^{-1}) w_1^2 + (\Theta_{12}^{-1} \Theta_{12}^{-1} + \Theta_{22}^{-1} \Theta_{22}^{-1}) w_2^2 + (2\Theta_{11}^{-1} \Theta_{12}^{-1} + 2\Theta_{12}^{-1} \Theta_{22}^{-1}) w_1 w_2] \right\}. \end{aligned} \tag{A13}$$

3. Abbreviations

Here, we list the abbreviations used in Eq. (48)

$$\begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix} = \begin{bmatrix} \Theta_{12}\Theta_{11}^{-1} + \frac{1}{5}[(2w_1\Theta_{12} + w_2\Theta_{11})w_1\Theta_{11}^{-1}\Theta_{11}^{-1} \\ + (w_1\Theta_{22} + 2w_2\Theta_{12})w_1\Theta_{12}^{-1}\Theta_{11}^{-1} \\ + (2w_1\Theta_{12} + w_2\Theta_{11})w_2\Theta_{11}^{-1}\Theta_{12}^{-1} \\ + (w_1\Theta_{22} + 2w_2\Theta_{12})w_2\Theta_{12}^{-1}\Theta_{12}^{-1}] - \frac{\Theta_{12}}{3\theta - \Theta_{11} - \Theta_{22}} \\ \Theta_{22}\Theta_{11}^{-1} + \frac{1}{5}[(2w_2\Theta_{12} + 2w_1\Theta_{22})w_1\Theta_{11}^{-1}\Theta_{11}^{-1} \\ + (3w_2\Theta_{22})w_1\Theta_{12}^{-1}\Theta_{11}^{-1} \\ + (2w_2\Theta_{12} + w_1\Theta_{22})w_2\Theta_{11}^{-1}\Theta_{12}^{-1} \\ + (3w_2\Theta_{22})w_2\Theta_{12}^{-1}\Theta_{12}^{-1}] - \frac{\Theta_{22}}{3\theta - \Theta_{11} - \Theta_{22}} \end{bmatrix}, \tag{A14}$$

$$\begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} = \begin{bmatrix} 2 + 2\Theta_{12}\Theta_{12}^{-1} + \frac{1}{5}[(2w_1\Theta_{12} + w_2\Theta_{11})2w_1\Theta_{12}^{-1}\Theta_{11}^{-1} \\ + (w_1\Theta_{22} + 2w_2\Theta_{12})w_1\Theta_{22}^{-1}\Theta_{11}^{-1} \\ + (w_1\Theta_{22} + 2w_2\Theta_{12})w_1\Theta_{12}^{-1}\Theta_{12}^{-1} \\ + (2w_1\Theta_{12} + w_2\Theta_{11})w_2\Theta_{12}^{-1}\Theta_{12}^{-1} \\ + (w_1\Theta_{22} + 2w_2\Theta_{12})2w_2\Theta_{22}^{-1}\Theta_{12}^{-1} \\ + (2w_1\Theta_{12} + w_2\Theta_{11})w_2\Theta_{11}^{-1}\Theta_{22}^{-1}] \\ 2\Theta_{22}\Theta_{12}^{-1} + \frac{1}{5}[(2w_2\Theta_{12} + w_1\Theta_{22})2w_1\Theta_{12}^{-1}\Theta_{11}^{-1} \\ + (3w_2\Theta_{22})w_1\Theta_{22}^{-1}\Theta_{11}^{-1} \\ + (3w_2\Theta_{22})w_1\Theta_{12}^{-1}\Theta_{12}^{-1} \\ + (2w_2\Theta_{12} + w_1\Theta_{22})w_2\Theta_{12}^{-1}\Theta_{12}^{-1} \\ + (2w_2\Theta_{22})2w_2\Theta_{22}^{-1}\Theta_{12}^{-1} \\ + (2w_2\Theta_{12} + w_1\Theta_{22})w_2\Theta_{11}^{-1}\Theta_{22}^{-1}] \end{bmatrix}, \tag{A15}$$

$$\begin{bmatrix} \gamma_1 \\ \gamma_2 \end{bmatrix} = \begin{bmatrix} \Theta_{12}\Theta_{22}^{-1} + \frac{1}{5}[(2w_1\Theta_{12} + w_2\Theta_{11})w_1\Theta_{12}^{-1}\Theta_{12}^{-1} \\ + (w_1\Theta_{22} + 2w_2\Theta_{12})w_1\Theta_{22}^{-1}\Theta_{12}^{-1} \\ + (2w_1\Theta_{12} + w_2\Theta_{11})w_2\Theta_{12}^{-1}\Theta_{22}^{-1} \\ + (w_1\Theta_{22} + 2w_2\Theta_{12})w_2\Theta_{22}^{-1}\Theta_{22}^{-1}] - \frac{\Theta_{12}}{3\theta - \Theta_{11} - \Theta_{22}} \\ 2 + \Theta_{22}\Theta_{22}^{-1} + \frac{1}{5}[(2w_2\Theta_{12} + w_1\Theta_{22})w_1\Theta_{12}^{-1}\Theta_{12}^{-1} \\ + (3w_2\Theta_{22})w_1\Theta_{22}^{-1}\Theta_{12}^{-1} \\ + (2w_2\Theta_{12} + w_1\Theta_{22})w_2\Theta_{12}^{-1}\Theta_{22}^{-1} \\ + (3w_2\Theta_{22})w_2\Theta_{22}^{-1}\Theta_{22}^{-1}] - \frac{\Theta_{22}}{3\theta - \Theta_{11} - \Theta_{22}} \end{bmatrix}, \tag{A16}$$

$$\begin{bmatrix} \delta_1 \\ \delta_2 \end{bmatrix} = \begin{bmatrix} -\frac{4}{5}[(2w_1\Theta_{12} + w_2\Theta_{11})\Theta_{11}^{-1} \\ + (w_1\Theta_{22} + 2w_2\Theta_{12})\Theta_{12}^{-1}] \\ -\frac{4}{5}[(2w_2\Theta_{12} + w_1\Theta_{22})\Theta_{11}^{-1} \\ + (3w_2\Theta_{22})\Theta_{12}^{-1}] \end{bmatrix}, \tag{A17}$$

$$\begin{bmatrix} \epsilon_1 \\ \epsilon_2 \end{bmatrix} = \begin{bmatrix} -\frac{4}{5}[(2w_1\Theta_{12} + w_2\Theta_{11})\Theta_{12}^{-1} \\ + (w_1\Theta_{22} + 2w_2\Theta_{12})\Theta_{22}^{-1}] \\ -\frac{4}{5}[(2w_2\Theta_{12} + w_1\Theta_{22})\Theta_{12}^{-1} \\ + (3w_2\Theta_{22})\Theta_{22}^{-1}] \end{bmatrix}. \tag{A18}$$

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