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# A New Near-Equilibrium Breakdown Parameter Based on the Rayleigh-Onsager Dissipation Function

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**Abstract.** The near-equilibrium breakdown parameter is essential in quantifying the gas flow regions in which the linear Navier-Stokes-Fourier hypothesis is no longer valid. It plays a significant role in the development of a hybrid continuum/DSMC method in which computational domains need to be identified as either rarefied or continuum. There were several breakdown parameters appearing in the literature such as a semi-empirical parameter based on the spatial derivative of flow properties and a parameter based on the maximum gradient-length local Knudsen number. In this study, we present a new near-equilibrium breakdown parameter based on the degree of thermal nonequilibrium and the Rayleigh-Onsager dissipation function related to the calortropy production arising from the irreversible process in the system. The property of the new breakdown parameter is investigated by numerically solving hypersonic rarefied and low Mach microscale gas flows around a cylinder.

**Keywords:** Kinetic theory, non-classical constitutive laws.

**PACS:** 47.45.Ab, 47.10.ab.

## INTRODUCTION

The continuum (or near-equilibrium) breakdown parameter is essential in quantifying the gas flow regions in which the linear Navier-Stokes-Fourier hypothesis is no longer valid. There were several breakdown parameters appearing in the literature. Bird [1] first proposed a semi-empirical parameter based on the spatial derivative of flow properties such as density, pressure, temperature or velocity magnitude, for steady state expanding flows. Boyd et al. [2] derived a parameter based on the gradient-length local Knudsen number in which the derivative is taken in the direction of the maximum gradient. It turned out to resolve a problem in the Bird approach that the parameter becomes zero near stagnation points. It was generally assumed that continuum breakdown occurs whenever the gradient-length Knudsen number is greater than 0.05. The breakdown parameter also plays a significant role in the development of a hybrid continuum/DSMC method in which regions in a flow need to be identified as either rarefied or continuum [3]. In other words, a criterion is required for the placement of the interfaces between the continuum and rarefied domains.

The breakdown parameter is directly related to how to define the degree of thermal nonequilibrium. Traditionally, the Knudsen number was considered the sole parameter for measuring the degree of thermal nonequilibrium, since the ratio of the collision term to the kinematic term in the Boltzmann equation is nothing but the Knudsen number. However, owing to the statistical average introduced from the kinetic Boltzmann equation to the continuum conservation laws, there are three, instead of two, terms in the conservation law of momentum: convective, pressure, and viscous terms. Therefore the degree of thermal nonequilibrium in thermodynamic space can be best represented by the composite number  $Kn \cdot M$ , not the Knudsen number alone, since it represents the ratio of the viscous force to the thermodynamic pressure and the viscous force is a direct consequence of the thermal nonequilibrium effect.

This observation indicates that the near-equilibrium breakdown parameter can be derived based on the new understanding of the degree of thermal nonequilibrium. That is, a parameter based on the ratio of the viscous force to the thermodynamic pressure can be developed. Indeed, in order to identify what regions are expected to deviate significantly from near-local-equilibrium assumption, a new parameter, which is basically Rayleigh-Onsager dissipation function [4], can be defined.

In this study, we present the new near-equilibrium breakdown parameter and its distribution in hypersonic rarefied and low Mach microscale gas flows around a cylinder. The flow field is numerically solved using a recent triangular discontinuous Galerkin method for non-Newtonian implicit constitutive models [5-8]. Special emphasis is

given to how the new parameter depicts various flow features such as the compressive shock region, the boundary layer near the wall, and rapidly expanding region at the rear part of cylinder.

## PREVIOUS BREAKDOWN PARAMETERS

A semi-empirical parameter based on the spatial derivative of flow properties was proposed by Bird [1] as follows:

$$P = M \sqrt{\frac{\gamma\pi}{8}} \frac{\lambda}{\rho} \left| \frac{d\rho}{ds} \right|, \quad (1)$$

where  $M, \rho$  are the *local* Mach number and density. Here  $\lambda$  denotes the local mean free path and can be defined by

$$\lambda = \frac{k_B T}{\sqrt{2} \pi d^2 p}, \quad (2)$$

where  $d$  is the gas molecular diameter and  $T, p$  are the temperature and the pressure. The spatial gradient along the streamline,  $d\rho/ds$ , can be calculated in Cartesian coordinates as follows:

$$\frac{d\rho}{ds} = \frac{d\rho}{dx} \frac{u}{\sqrt{u^2 + v^2}} + \frac{d\rho}{dy} \frac{v}{\sqrt{u^2 + v^2}}, \quad (3)$$

where  $u$  and  $v$  represent the  $x$  and  $y$  directional velocities, respectively. Moreover, if other flow properties  $Q$ , like the temperature and the velocity, are introduced in order to take both viscous effect and heat transfer into account, the following breakdown parameters  $P_Q$  (e.g.  $P_D, P_T$ , and  $P_V$ ) can be obtained:

$$P_Q = M \sqrt{\frac{\gamma\pi}{8}} \frac{\lambda}{Q} \left| \frac{dQ}{ds} \right|. \quad (4)$$

Then, by considering all the parameters, a breakdown parameter  $P_{\max}$  can be defined by

$$P_{\max} \equiv \max(P_D, P_T, P_V). \quad (5)$$

In case of steady expanding flows, it was known that the value of  $P$  of about 0.05 is a good criterion for identifying the near-equilibrium breakdown.

However, it was soon recognized that there may be a problem when the Mach number approaches to zero at stagnation points. Boyd *et al.* [2] carried out an extensive numerical investigation of one-dimensional normal shock waves and two-dimensional bow shocks using DSMC and CFD results in order to determine an appropriate breakdown parameter. The gradient length local (GLL) Knudsen number,

$$\text{Kn}_{\text{GLL}} = \frac{\lambda}{Q} \left| \frac{dQ}{dl} \right|, \quad (6)$$

where  $l$  is some distance between two points in flow field, was introduced and demonstrated to provide a better indication of continuum breakdown than  $P$  for compression-dominated hypersonic flows. The distance  $l$  was taken approximately along the line of the steepest gradients in the flow properties. For simplicity,  $dQ/dl$  was evaluated by  $\nabla Q$ . Then, the parameter is reduced into

$$\text{Kn}_Q = \frac{\lambda}{Q} |\nabla Q| = \frac{\lambda}{Q} \sqrt{\left( \frac{\partial Q}{\partial x} \right)^2 + \left( \frac{\partial Q}{\partial y} \right)^2}. \quad (7)$$

Also, by considering all the flow properties, the following breakdown parameter  $\text{Kn}_{\max}$  can be derived:

$$\text{Kn}_{\max} \equiv \max(\text{Kn}_D, \text{Kn}_T, \text{Kn}_V). \quad (8)$$

It is apparent that there is a direct relationship between equations (4) and (7);

$$P_Q = M \sqrt{\frac{\gamma\pi}{8}} \cos \theta \text{Kn}_Q, \quad (9)$$

where  $\theta$  is the angle between gradient  $\nabla Q$  and the flow direction.

## BREAKDOWN PARAMETER BASED ON THE RAYLEIGH-ONSAGER DISSIPATION FUNCTION AND CONSTITUTIVE RELATIONS

The primary objective of the near-equilibrium breakdown parameter is to quantify the gas flow regions according to the breakdown of the linear hypothesis in the Navier-Stokes-Fourier constitutive relation. Therefore, the problem of finding such a parameter is essentially related to the knowledge of when the (first-order) Newtonian hypothesis breaks down, which in turn demands the derivation of the (second-order) non-Newtonian constitutive relation.

A systematic method to derive the higher-order non-Newtonian constitutive relation from the kinetic Boltzmann equation was recently developed by Myong [6]. The kinetic Boltzmann equation can be transformed into the continuum constitutive equations by introducing the statistical average; after some manipulation, the following exact constitutive equation of the shear stress tensor  $\Pi \equiv \langle m[\mathbf{c}\mathbf{c}]^{(2)} f \rangle$  can be derived

$$\rho \frac{d(\Pi / \rho)}{dt} + \nabla \cdot \Psi^{(\Pi)} + 2[\Pi \cdot \nabla \mathbf{u}]^{(2)} + 2p[\nabla \mathbf{u}]^{(2)} = \Lambda^{(\Pi)} \left( \equiv \langle m[\mathbf{c}\mathbf{c}]^{(2)} C[f, f_2] \rangle \right), \quad (10)$$

$$\Psi^{(\Pi)} \equiv \langle m\mathbf{c}\mathbf{c}\mathbf{c}f \rangle - \langle m\text{Tr}(\mathbf{c}\mathbf{c})f \rangle \mathbf{I} / 3.$$

The symbols  $m, \mathbf{c}, \mathbf{u}, \langle \rangle, [ ]^{(2)}$  denote the mass of gas molecule, the peculiar velocity, the average velocity, the integral in velocity space, and the traceless symmetric part, respectively.

It can be easily noted that there are two places for closure (or approximation) in the exact moment equation (10); the high order term  $\nabla \cdot (\langle m\mathbf{c}\mathbf{c}\mathbf{c}f \rangle - \langle m\text{Tr}(\mathbf{c}\mathbf{c})f \rangle \mathbf{I} / 3)$  and the dissipation term  $\langle m[\mathbf{c}\mathbf{c}]^{(2)} C[f, f_2] \rangle$ , which are the only terms in the constitutive equation that are directly connected to next level high order moments and the explicit form of the distribution function or the collision integral. Then it is natural to impose the same level of approximations on both places so that the resulting constitutive equation may remain balanced even in high nonequilibrium. For the general type of molecules, equation (10) can be written

$$\rho \frac{d(\Pi / \rho)}{dt} + \nabla \cdot \Psi^{(\Pi)} + 2[\Pi \cdot \nabla \mathbf{u}]^{(2)} + 2p[\nabla \mathbf{u}]^{(2)} = -\frac{p}{\mu_{NS}} \Pi F(p, T, \Pi, \mathbf{Q}, \dots). \quad (11)$$

In case of the Maxwellian molecules,  $F = 1$ , irrespective of the degree of thermal nonequilibrium. If the positive nonlinear scalar function  $F$  reduces to 1 near thermal equilibrium and its exact form is determined by the Boltzmann equation, then (11) is still exact to the original Boltzmann equation. Then the key step is to find a proper form of the nonlinear viscosity factor  $F_{approx}$  corresponding to the next level approximation of closure for the high order term, for example,  $\nabla \cdot \Psi^{(\Pi)} = 0$ ;

$$\rho \frac{d(\Pi / \rho)}{dt} + 2[\Pi \cdot \nabla \mathbf{u}]^{(2)} + 2p[\nabla \mathbf{u}]^{(2)} = -\frac{p}{\mu_{NS}} \Pi F_{approx}(p, T, \Pi, \mathbf{Q}, \dots). \quad (12)$$

Notice that equation (12) is also applicable to the Maxwellian molecules since the closure of the open high order term can be incorporated into the nonlinear factor  $F_{approx}$  in the dissipation term by applying a closure

$\nabla \cdot \Psi^{(\Pi)} = -p\Pi(1 - F_{approx}) / \mu_{NS}$  to the equation of Maxwellian molecules. Therefore all types of molecules can be treated within a single framework (12).

A proper form of the nonlinear factor in the dissipation term has been derived by considering the Boltzmann entropy balance equation consistent with the second law of thermodynamics in Eu's work [4]. After introducing the following canonical distribution function in exponential form,

$$f^c = \exp \left[ -\beta \left( \frac{1}{2} mc^2 + \sum_{n=1}^{\infty} X^{(n)} h^{(n)} - N \right) \right], \quad (13)$$

$$\exp(-\beta N) = \frac{1}{n_d} \left\langle \exp \left[ -\beta \left( \frac{1}{2} mc^2 + \sum_{n=1}^{\infty} X^{(n)} h^{(n)} \right) \right] \right\rangle, \quad \beta \equiv \frac{1}{k_B T},$$

and applying the cumulant expansion to the explicit calculation of the dissipation term  $\Lambda^{(n)}$ , a natural platform suitable for the balanced closure and consistent with the second law of thermodynamics can be derived:

$$\rho \frac{d(\Pi / \rho)}{dt} + \nabla \cdot \Psi^{(\Pi)} + 2[\Pi \cdot \nabla \mathbf{u}]^{(2)} + 2p[\nabla \mathbf{u}]^{(2)} = \frac{1}{\beta g} \sum_{l=1}^{\infty} R_{12}^{(2l)} X_2^{(l)} q(\kappa_1^{(\pm)}, \kappa_2^{(\pm)}, \dots), \quad (14)$$

where  $g = \frac{1}{n^2 d^2} \sqrt{\frac{m}{2k_B T}}$ .

Here  $R_{12}^{(2l)}, X_2^{(l)}, \kappa_{1,2}^{(\pm)}, \dots$  are scalar coefficients made up of collision bracket integrals, the conjugate variables to the molecular expressions for moment  $h^{(n)}$ , and cumulants, respectively. In particular, the first reduced collision integral  $\kappa_1$  can be expressed as a quadratic form

$$\kappa_1^2 = \sum_{n,l=1}^{\infty} X^{(n)} R_{12}^{(nl)} X_2^{(l)}, \quad (15)$$

where  $R_{12}^{(nl)}$  are scalar coefficients made up of collision bracket integrals of the molecular expressions for moment  $h^{(n)}$  and  $h_2^{(l)}$  for an isotropic system of dilute gases. It must be emphasized that the constitutive equation (14) for general type of molecules is still exact to the original Boltzmann equation. Then the simplest approximation in next level to the linear Navier-Stokes in the left-hand side would be  $\nabla \cdot \Psi^{(\Pi)} = 0$ , while the leading order approximation of the dissipation term in the right-hand side would be  $R_{12}^{(21)} X_2^{(1)} q(\kappa_1^{(\pm)})$ . Then, after the Chapman-Enskog collision integral approximation and the first order cumulant expansion  $q(\kappa_1^{(\pm)})$  are applied ( $\kappa_1^+ = \kappa_1^- \equiv \kappa_1$ ), the resulting second-order constitutive relation from  $F_{approx} = q(\kappa_1)$  can be summarized in steady-state case as follows;

$$2[\Pi \cdot \nabla \mathbf{u}]^{(2)} + 2p[\nabla \mathbf{u}]^{(2)} = -\frac{p}{\mu_{NS}} \Pi q(\kappa_1), \quad (16)$$

where  $q(\kappa_1) = \frac{\sinh \kappa_1}{\kappa_1}$ ,  $\kappa_1 = \frac{(mk_B)^{1/4}}{\sqrt{2}d} \frac{T^{1/4}}{p} \left( \frac{\Pi : \Pi}{\mu_{NS}} + \frac{\mathbf{Q} \cdot \mathbf{Q}}{k_{NS}} \right)^{1/2}$ .

Notice that the first-order cumulant expansion takes a form of hyperbolic sine function whose argument is given in terms of basically a quadratic function. Then the function  $\kappa_1$  can be shown nothing but the Rayleigh-Onsager dissipation function  $\hat{R}$  and is readily used to identify what regions are expected to deviate significantly from near-local-equilibrium assumption since it measures the level of calortropy production in irreversible process;

$$\hat{R} = \frac{N_{\delta}}{p} \left( \Pi : \Pi + \frac{2\varepsilon}{T} \mathbf{Q} \cdot \mathbf{Q} \right)^{1/2} \quad (17)$$

where  $N_{\delta} = \sqrt{\frac{2\gamma}{\pi}} MKn$ ,  $\varepsilon = \frac{1}{Ec Pr} \left| \frac{T_w}{T_r} - 1 \right|$ ,  $Ec = \frac{(\gamma-1)M^2}{|T_w/T_r - 1|}$ .

Here  $N_{\delta}, \varepsilon$  are the reference values, while  $p, T, \Pi, \mathbf{Q}$  are local cell values.

The non-Newtonian constitutive relations (16) can then be reduced into two distinctive cases; compression (or expansion) and velocity shear. In steady-state condition of one-dimensional compression (and expansion), (16) reduces to ( $\hat{\Pi} \equiv \Pi / p$ )

$$-\hat{\Pi} \hat{\Pi}_{NS} - \hat{\Pi}_{NS} = -\hat{\Pi} q(c|\hat{\Pi}|) \left( -\hat{\Pi} - \frac{1}{3!} \hat{\Pi} (c\hat{\Pi})^2 - \frac{1}{5!} \hat{\Pi} (c\hat{\Pi})^4 - \dots \right). \quad (18)$$

Here the coefficient  $c$  is a positive value, close to 1, dependent on the type of gas molecules; for example, it is 1.0138, and 1.1908 for Maxwellian and hard sphere molecules, respectively [5]. On the other hand, the nonlinear viscosity factor  $F_{approx}$  turns out to play a negligible role in the velocity shear case due to its cancellation under the constraint of the free-molecular asymptotic behavior. The solution of the constitutive equation in this case can be written as

$$\hat{\Pi}_{xy} = \frac{3\hat{\Pi}_{xyNS}}{3q(c|\hat{R}|) + 2\hat{\Pi}_{xyNS}^2 / q(c|\hat{R}|)} \quad \text{where } \hat{R}^2 \equiv 2\hat{\Pi}_{yy}(\hat{\Pi}_{yy} - 1), \quad \hat{\Pi}_{xy}^2 = -\frac{3}{2}(1 + \hat{\Pi}_{yy})\hat{\Pi}_{yy}. \quad (19)$$

These highly nonlinear algebraic equations of stresses (18) and (19) can be solved by the method of iterations.

## COMPARISON OF BREAKDOWN PARAMETERS

The new near-equilibrium breakdown parameter (17) is shown to avoid the problem in the Bird's parameter that the Mach number approaches to zero at stagnation points. Further, it takes both viscous stress and heat transfer into account within a single framework.

Before comparing three parameters  $P_{\max}$ ,  $Kn_{\max}$ ,  $\hat{R}$  in detail, the second-order non-Newtonian implicit constitutive relations in one-dimensional  $u_x$ -only problem are plotted in Fig. 1. The figures show in concise manner how the first-order and second-order constitutive relations begin to deviate from near-local-equilibrium assumption. In order to compare the deviation using a single reference, the values of  $\hat{\Pi} \equiv \Pi / p$  corresponding to 20 percent of  $(\hat{\Pi} - \hat{\Pi}_{\text{NSF}}) / \hat{\Pi}_{\text{NSF}}$  are evaluated. It turns out that, for compression, expansion, and velocity shear, they are 0.18, -0.24, 0.53, respectively. Thus a criterion with the value of 0.18 may be used as a near-equilibrium breakdown parameter for 20 percent deviation from the linear Navier-Stokes-Fourier hypothesis.

Finally, distributions of the near-equilibrium breakdown parameters in multi-dimensional hypersonic rarefied and microscale gas flows around a cylinder are calculated. The flow field is numerically solved using a recent triangular discontinuous Galerkin method [8] for the conservation laws in conjunction with the non-Newtonian implicit constitutive model. Working gas is assumed argon for both cases with  $Pr = 2/3$ ,  $c = 1.0179$  and  $s = 0.75$  for all cases.

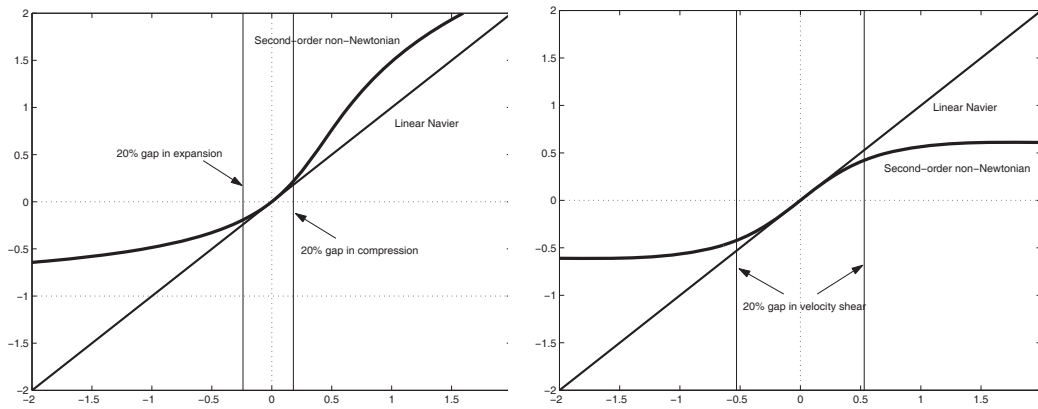


FIGURE 1. The second-order non-Newtonian implicit constitutive relations and 20 percent deviation criteria. Left – compression and expansion, right – velocity shear.

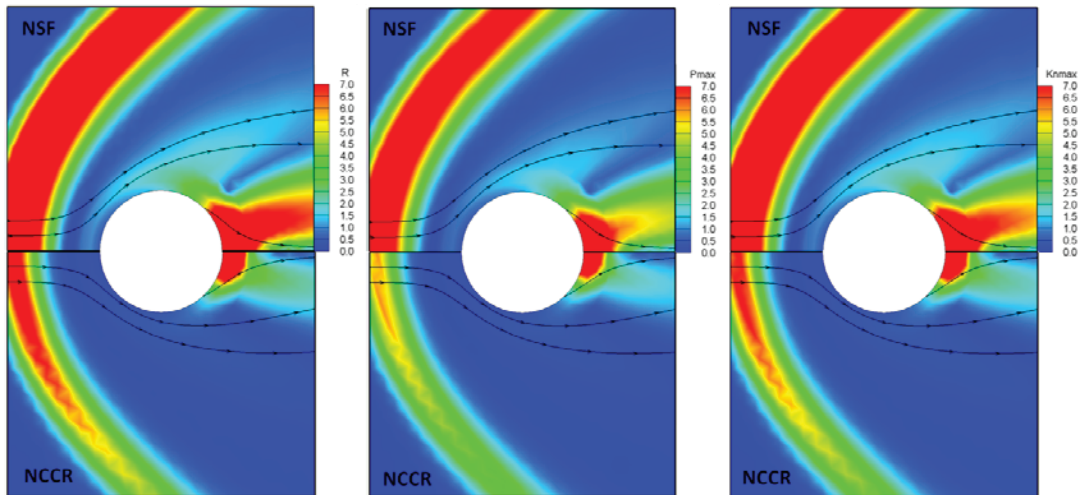
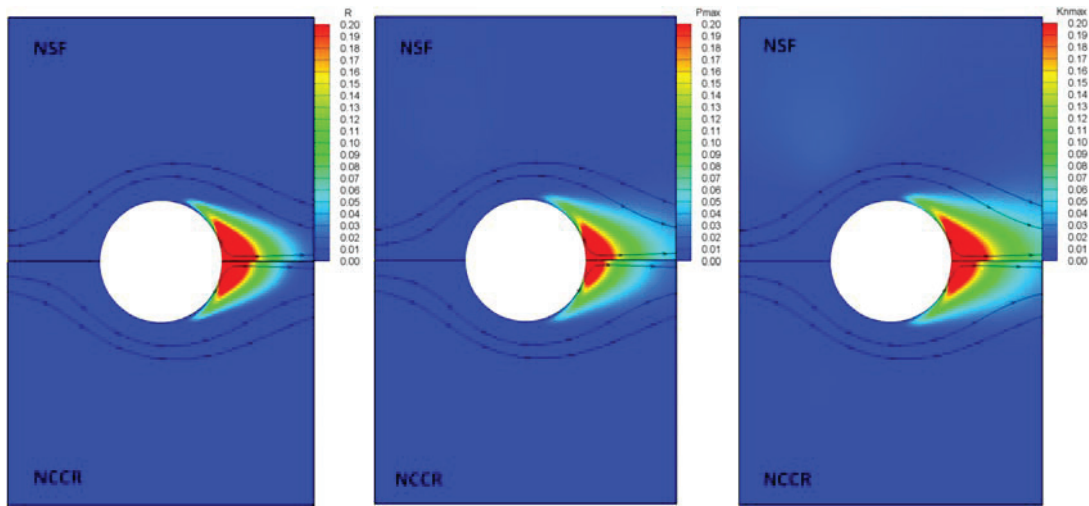


FIGURE 2. Comparison of the breakdown parameters in hypersonic rarefied gas flow ( $M=5.48$ ,  $Kn=0.5$ ).





**FIGURE 3.** Comparison of the breakdown parameters in low speed microscale gas flow ( $M=0.1$ ,  $Kn=0.1$ ).

Figures 2 and 3 compare the distributions of three near-equilibrium breakdown parameters for the NSF (Navier-Stoke -Fourier) and NCCR (nonlinear coupled constitutive relation) models. It can be noticed that 1) there exist two distinctive regions of gaseous compression and expansion in the frontal and rear parts of the cylinder, respectively; 2) the level of breakdown parameters is high at the bow shock structure and at the rear part of cylinder; and (3) the NSF model in general predicts high than the NCCR model in the level of parameters. In addition, it can be found that all three breakdown parameters produce qualitatively similar results, but new and Boyd's parameters predict more similar distributions.

## CONCLUSIONS

In this study, a new near-equilibrium breakdown parameter based on the Rayleigh-Onsager dissipation function related to the calortropy production arising from the irreversible process in the system is presented. It is shown to avoid the problem of the Mach number approaching to zero at stagnation points and, at the same time, to takes both viscous stress and heat transfer into account within a single framework. The property of the new breakdown parameter is investigated by numerically solving hypersonic rarefied and low Mach microscale gas flows around a cylinder. It is shown that the new breakdown parameter based theoretically on the calortropy production can serve as an alternative to the previous continuum breakdown parameters based empirically on the flow field characteristics.

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