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Technical Note

Comments on ''critical view on new results in micro-fluid mechanics''

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In two recent papers [1,2], Drs. H. Herwig and O. Hausner dismiss ''almost all'' recent studies that claim special effects for flow and heat transfer through microdevices. They find the approach in those studies misleading and argue that existing observations in microdevices can be explained by merely rescaling the traditional models routinely used for macrodevices. Herwig and Hausner suggest that the same equations, properly non-dimensionalized, should be used for both micro and macrosystems. In Ref. [2], Professor Herwig states emphatically and in capital letters, ''IN A NONDI-MENSIONAL FORM ALL SPECIAL ''MICRO-EF-FECTS'' WILL TURN OUT TO BE SCALING EFFECTS WITHIN A CONTINUUM THEORY EQUALLY VALID FOR MACRO AND MICRO PROBLEMS.''

In this Technical Note, we argue that traditional treatments of transport phenomena may not be appropriate for certain situations involving microdevices. The simplistic dimensional analysis approach advocated in [1,2], though not incorrect, does miss important physics and is therefore misleading. We first start by defining microdevices and what we mean by traditional modeling of mass, momentum and heat transfer in or around conventional devices. We then describe the conditions under which non-traditional modeling of transport phenomena may be needed. Finally, we list the available alternative modeling tools. The focus here will be on fluid transport, but similar arguments can be made for solid transport, for example heat conduction through solid media.

Microelectromechanical systems (MEMS) refer to devices that have characteristic length of less than 1 mm but more than $1 \mu m$, that combine electrical and me-

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chanical components, and that are fabricated using integrated circuit batch-processing techniques. The crucial issue here is the small length scale of microdevices and what that might imply about modeling transport phenomena.

Fluid and heat flows in conventional macrodevices is traditionally modeled using the principles of conservation of mass, momentum (Newton's second law), and energy (first law of thermodynamics). Additionally, all processes are constrained by the second law of thermodynamics. Those principles are typically expressed in the form of partial differential field equations, where the macroscopic quantities of interest such as velocity, temperature, pressure, etc., depend on a continuum space and time. The first principles, as expressed to describe fluid-transport phenomena in conventional devices, are collectively called the Navier–Stokes equations, a system of non-linear partial differential equations subject to a sufficient number of initial and boundary conditions, the latter is typically in the form of no velocity slip and no temperature jump at a fluid–solid interface.

There are three fundamental assumptions that must be satisfied in order for the Navier–Stokes equations to be valid:

- The Newtonian framework of mechanics—which specifies that mass and energy are conserved separately and that, in an inertial frame of reference, the sum of all forces is equal to the rate of change of momentum––is valid.
- The continuum approximation—which assumes that space and time are indefinitely divisible continuum–– is applicable.
- Thermodynamic equilibrium or at least quasi-equilibrium––which permits linear relations between stress and rate of strain and between heat flux and temperature gradient—is assumed.

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Fluid isotropy and stress tensor symmetry are also typically, albeit not always, assumed. Violation of any one of the three assumptions listed above invalidates the Navier–Stokes equations and alternative modeling is then called for. We elaborate on the three assumptions in turn.

Newtonian framework: The fluid motions under consideration are assumed non-relativistic, i.e. their characteristic velocities are far below the speed of light. Thus, mass and energy are not interchangeable and each is separately conserved. As long as we are not dealing with atomic or subatomic particles or, at the other extreme of length scale, with stars and galaxies, the Newtonian framework is an excellent modeling tool for most problems in mechanics including those dealing with microelectromechanical systems. Quantum and relativistic mechanics are clearly beyond the scope of the present paper. Therefore, the Newtonian assumption is one that we no longer have to revisit for the rest of this Technical Note.

Continuum model: In both solid and fluid mechanics, the continuum approximation implies that the spatial and temporal derivatives of all the macroscopic dependent variables exist in some reasonable sense. In other words, local properties such as density, velocity, stress and heat flux are defined as averages over elements sufficiently large compared with the microscopic structure in order to guarantee a sufficiently large number of molecules inside each fluid element and thus to effect molecular chaos, but small enough in comparison with the scale of the macroscopic phenomena to permit the use of differential calculus to describe those properties. The continuum approximation is almost always met, but exceptions do exist. The resulting equations therefore cover a very broad range of situations, the exception being flows with spatial scales which are not much larger than the mean distance between the fluid molecules, as for example in the case of rarefied gas dynamics, shock waves that are thin relative to the molecular distances, and some flows in micro and nanodevices. We will describe later the conditions under which the continuum approximation fails for certain minute devices.

It should be emphasized that the continuum approximation in and by itself leads to an indeterminate set of equations, i.e. more unknowns than equations [3]. To close the resulting system of partial differential equations, relations between the stress and rate of strain and between the heat flux and temperature gradient are needed. At least for compressible flows, two equations of state, relating density and internal energy each to pressure and temperature, are also required. The fact that the continuum approximation does not necessarily lead to the Navier–Stokes equations is a subtle point that is often confused in the literature including Refs. [1,2].

Thermodynamic equilibrium: Thermodynamic equilibrium implies that the macroscopic quantities have sufficient time to adjust to their changing surroundings. In motion, exact thermodynamic equilibrium is impossible as each fluid particle is continuously having volume, momentum or energy added or removed, and so in fluid dynamics and heat transfer we speak of quasiequilibrium. The second law of thermodynamics imposes a tendency to revert to an equilibrium state, and the defining issue here is whether or not the flow quantities are adjusting fast enough. The reversion rate will be very high if the molecular time and length scales are very small as compared to the corresponding macroscopic-flow scales. This will guarantee that numerous molecular collisions will occur in sufficiently short time to equilibrate fluid particles whose properties vary little over distances comparable to the molecular length scales. The characteristic length for molecular collision is the mean free path, \mathcal{L} , the average distance traveled by a molecule before colliding with another. When $\mathscr L$ is, say, one order of magnitude smaller than the flow length scale, macroscopic quantities such as velocity and temperature will have nearly linear gradients over molecular distances, and it is on these gradients alone that departure from equilibrium will depend. Therefore, the quasiequilibrium assumption signifies that the stress is linearly related to the rate of strain (Newtonian fluids) and the heat flux is linearly related to the temperature gradient (Fourier fluids). Thermodynamic equilibrium additionally gives rise to the no-slip and no-temperature-jump boundary conditions [4,5].

As is the case with the continuum approximation, the quasi-equilibrium assumption can be violated under certain circumstances relevant to microdevices. In these cases, alternatives to the no-slip condition or even to the Navier–Stokes equations themselves must be sought.

We are now ready to quantify the conditions under which the continuum approximation or the quasi-equilibrium assumption can be made. The answer to both questions is well known from statistical thermodynamics particularly as was extensively applied to rarefied gas dynamics half a century ago [5,6]. For that reason we discuss gas flows first deferring the discussion of liquid flows to afterward.

The well-known chart reproduced in Fig. 1 clearly illustrates the answer we are seeking. All scales in this plot are logarithmic. The bottom abscissa represents the density normalized with a reference density, ρ/ρ_0 , or equivalently the normalized number density (number of molecules per unit volume), n/n_0 . The top abscissa is the average distance between molecules normalized with the molecular diameter, δ/σ . Clearly, the density ratio is proportional to the inverse cube of δ/σ . The left ordinate represents a characteristic flow dimension, L, in meter. This can be computed from a characteristic macroscopic property, such as density, divided by the absolute value of its gradient. The right ordinate is the length scale normalized with the molecular diameter,

Fig. 1. Effective limits of different flow models. Adapted from Bird [6].

 L/σ . The chart in Fig. 1 depicts a gas having a molecular diameter of $\sigma = 4 \times 10^{-10}$ m, which diameter very closely represents air modeled as rigid spheres. Similar charts can be drawn for other gases.

The vertical line inserted in Fig. 1 represents the boundary between dilute gas and dense one. Dilute gas is to the left of this line where $\delta/\sigma > 7$. For such gas, intermolecular forces play no role and the molecules spend most of their time in free flight between brief collisions at which instances the molecules' direction and speed abruptly change. Additionally, the probability of more than two molecules colliding is minuscule. We then speak of only binary collisions, and all the simplifications of the powerful kinetic theory of gases can be invoked when dealing with dilute gases. Dry air at standard conditions has a pressure of 1.01×10^5 N/m², temperature of 288 K, density ratio of 1, and $\delta/\sigma = 9$. Standard air is therefore a dilute, ideal gas, but barely.

The gently sloped line in Fig. 1 indicates the limit of molecular chaos. When averaging over many molecules to compute macroscopic quantities, insignificant statistical fluctuations occur when there is at least 100 molecules to the side ($L/\delta > 100$), in other words when at least 1 million molecules reside inside the smallest macroscopic fluid volume of interest. Therefore, the continuum approximation is valid only on top of that line.

The steeper line in Fig. 1 indicates the boundary of validity of the quasi-equilibrium assumption. This limit is governed by the Knudsen number, $Kn \equiv \mathcal{L}/L$, which

is the ratio of the mean free path to the characteristic macroscopic length. Navier–Stokes equations are valid only if $Kn < 0.1$, although the no-slip condition demands the stricter limit of $Kn < 0.001$. The mean free path is proportional to n^{-1} , and therefore the slope of the quasi-equilibrium line, in the logarithmic plot, is three times steeper than that of the molecular chaos line. Much of that has been known since the classical experiments conducted by Knudsen [7]. These experiments have been recently repeated with great precision at the US National Institute of Standards and Technology [8].

How does all that relate to microdevices? As density is reduced, the gas changes from dense to dilute. As size shrinks for a low-density gas, the Navier–Stokes equation fails first followed by a failure of the continuum approximation. For a dense gas, a reverse trend is observed as L is reduced: the continuum approximation fails first followed by a failure of the quasi-equilibrium assumption. Clearly, the continuum approximation and the quasi-equilibrium assumption are two different things. The two lines in Fig. 1 describing the two respective limits meet only at a single point.

To give a concrete example, for air at 1 atm, slip occurs if $L < 100 \mu m$, (stress)–(rate of strain) relation becomes non-linear if $L < 1 \mu m$, and the continuum approximation fails altogether if $L < 0.4$ µm. For air at 10^{-3} atm, slip occurs if $L < 100$ mm, (stress)–(rate of strain) relation becomes non-linear if $L < 1$ mm, and the continuum approximation fails if $L < 4$ µm. Light gases such as helium will reach those limits at considerably larger characteristic lengths. All of those conditions are well within the operating ranges of microdevices. Thus, there are circumstances when transport in microdevices should not be modeled using the traditional equations.

We now turn our attention to liquid flows. The incompressible Navier–Stokes equations describe such flows under most circumstances. Liquids, however, do not have a well advanced molecular-based theory as that for dilute gases. The concept of mean free path is not very useful for liquids whose molecules are always in a 'collision' state. Therefore, the conditions under which a liquid flow fails to be in quasi-equilibrium state, though not uncommon, are not well defined. There is no Knudsen number nor kinetic theory of liquids to guide us through the maze. We do not know, from first principles, the conditions under which the no-slip boundary condition becomes inaccurate, or the point at which the (stress)–(rate of strain) relation or the (heat flux)–(temperature gradient) relation fails to be linear. Having said that, numerous empirical observations indicate that those simple relations that we take for granted occasionally fail to accurately model liquid flows. For example, it has been shown in rheological studies [9] that non-Newtonian behavior commences when the strain rate, $\dot{\gamma}$, approximately exceeds twice the molecular frequency-scale

Fig. 2. Molecular and continuum flow models. From Ref. [10].

$$
\dot{\gamma} = \frac{\partial u}{\partial y} \ge 2\tau^{-1} \tag{1}
$$

where u is the longitudinal macroscopic velocity, v is the normal coordinate, and τ is the molecular time-scale given by

$$
\tau = \left[\frac{m\sigma^2}{\epsilon}\right]^{1/2} \tag{2}
$$

where *m* is the molecular mass, and σ and ϵ are respectively the characteristic length- and energy-scale for the molecules. For ordinary liquids, such as water, flowing in conventional devices, this time-scale is extremely small and the threshold shear rate for the onset of non-Newtonian behavior is therefore extraordinarily high. For high-molecular-weight polymers, on the other hand, m and σ are both several orders of magnitude higher than their respective values for water, and the linear stress–strain relation breaks down at realistic values of the shear rate. But even for ordinary liquids, several recent experiments and molecular dynamics simulations of channel flows in confined spaces indicate the presence of perceptible slip and therefore the absence of thermodynamic equilibrium [10].

The next step for both gas and liquid flows is to figure out what to do if conventional modeling fails. For gases at least, there are first-principles equations that give the precise amount of slip or temperature jump to include in case the Knudsen number exceeds the critical limit of 0.001. Higher-order equations such as those of Burnett can replace the Navier–Stokes equations when Kn exceeds 0.1. Finally, if the continuum approximation fails altogether, the fluid can be modeled as it really is, a collection of molecules. There, one can use molecular dynamics simulations (for liquids), Boltzmann equation (for dilute gases), or direct simulations Monte Carlo

(also for dilute gases). Subject to their own limitations, all the molecular-based models can also be used in lieu of higher-order momentum and energy equations, i.e. for non-equilibrium, continuum situations. All the strategies listed here are schematically depicted in Fig. 2, and discussed in greater details in Refs. [10–12], which in turn cite numerous original publications.

In closing, neither L/δ nor Kn appears as a natural dimensionless parameter in the Navier–Stokes equations. Validity of these equations or even their boundary conditions cannot therefore be ascertained from the dimensional analysis presented in [1,2]. The fallacy of that analysis is in using the Navier–Stokes system as a starting point and therefore providing a circular argument for their validity. Despite the number of case studies and non-dimensional parameters offered by Drs. Herwig and Hausner, the logic is faulty and the fact remains that the continuum approximation is invalid for L/δ < 100, the no-slip boundary condition is invalid for $Kn > 0.001$, and the Navier–Stokes system is invalid for $Kn > 0.1$. Those are real restrictions that can readily be encountered in real microdevices. To state that the 'same equations', properly non-dimensionalized, should be used for both micro and macrosystems is at a minimum erroneous. No amount of non-dimensionalization can change the fact that there are circumstances when the Navier–Stokes equations with no-slip/no-temperature-jump boundary conditions should not be used to describe transport phenomena in microdevices. And that is what physics teaches us.

Professor Herwig first published his results in Zeitschrift für Angewandte Mathematik und Mechanik $(ZAMM)$ [2], based on a plenary lecture he presented during the 79th Annual Congress of the International Association of Applied Mathematics and Mechanics (Gesellschaft für Angewandte Mathematik und Mechanik, GAMM), Zürich, Switzerland, 12-15 February 2001. His arguments were repeated in a paper co-authored with O. Hausner and published in International Journal of Heat and Mass Transfer [1]. I therefore felt compelled to rebut Professor Herwig's thesis in both journals. Additional to the present Technical Note, my comments are repeated in Ref. [13].

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