Reply I to "Comments on nonlinear viscosity and Grad's moment method"

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We show that the comments given by Santos [preceding paper, Phys. Rev. E **67**, 053201 (2003)] to our work do not hold since he failed to notice the difference between an approximation and an exact result. We also follow his line of thought for the Navier-Stokes equations showing that although his assumptions lead to specific conclusions, they are totally unrelated with those which he takes as the basis of his comment. Several other aspects of the problem are also mentioned.

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In his Comment to our work, Santos [1] asserts that a steady unidirectional flow, which was studied by us [2] and later subject to a discussion about its contents [3], is inconsistent with the exact macroscopic conservation laws under the assumptions stated by clauses (a), (c), (d′), and (e) adopted by the author. Following those assumptions Santos is essentially correct although his arguments are completely foreign to the work we have done.

In order to sustain our assertion we follow the commentator and start with the conservation equations for a dilute monatomic gas (Eqs. (1)–(3) in Ref. [1]), namely,

$$D_t n + n\nabla\cdot\mathbf{u} = 0, \tag{1}$$

$$D_t\mathbf{u} + \frac{1}{mn}\nabla\cdot\mathbf{P} = \mathbf{0}, \tag{2}$$

$$D_t T + \frac{2}{3nk_B}(\nabla\cdot\mathbf{q} + \mathbf{P}:\nabla\mathbf{u}) = 0. \tag{3}$$

The five conservation equations, Eqs. (1)–(3), do not form a complete set as they contain more than five unknowns. Therefore, it is necesary to provide constitutive equations (as in the Chapman-Enskog method) or additional equations for $\mathbf{P}$ and $\mathbf{q}$ (as in Grad's method). One of the motivations for our previous work [2] was to see if Grad's method could provide such constitutive equations beyond the Navier-Stokes regime. Before considering the more general setting we decided to see if the more restrictive situation of considering ten moments could give us sensible results as were obtained by the successful approach of Gorban and Karlin [4] and Karlin *et al.* [5]. Also, we decided to leave out the heat flux, by taking $\mathbf{q}=\mathbf{0}$, a condition certainly not physically sound so that physically unsound results could be expected. In fact, Karlin and Gorban [6] were able to include the heat flux, however, while we used explicity $\mathbf{q}=\mathbf{0}$, our results remain the same if a constant heat flux is considered, at least when a linearized collision operator is used. Therefore, we will include the heat flux and in order to keep the discussion on the same basis as Santos [1] and ours [2], we shall here assume that $\mathbf{q}(\mathbf{r},t)=q(x,t)\mathbf{i}$. In this respect it is interesting to notice that the energy conservation equation, see Eq. (3), gives rise to the same equation whether $\mathbf{q}=\mathbf{0}$ or $\nabla\cdot\mathbf{q}=0$. We also wish to stress at this stage that in our original work [2] the conservation equations were never considered, since its aim was precisely to provide for a constitutive equation for the stress tensor. Clauses (d) and (d′) of Santos were never used. It is worth emphasizing that although the condition of zero heat flux can be replaced with a constant one without altering the results in Ref. [2], the argumentation of including such a variable is strongly related with Grad's moment method which seems to be subjected to deep objections [7]. We shall leave this question for future debate. Furthermore, we considered unidirectional flow of the form $\mathbf{u}(\mathbf{r},t)=u(x,t)\mathbf{i}$ and for the pressure tensor we used $\mathbf{P}(\mathbf{r},t)=\mathbf{P}(x,t)$, together with $\mathbf{P}_{xy}=\mathbf{P}_{xz}$ and $\mathbf{P}_{yy}=\mathbf{P}_{zz}$. We also regarded the flow as stationary, meaning that the time derivatives are zero, a restriction which we shall not introduce for the time being. Then under the conditions just given, Eqs. (1) and (3) read

$$\partial_t n + \partial_x(nu) = 0, \tag{4}$$

$$\partial_t u + u\,\partial_x u + \frac{1}{mn}\partial_x\mathbf{P}_{xx} = 0, \tag{5}$$

$$\partial_x\mathbf{P}_{xy}(x,t) = 0, \tag{6}$$

$$\partial_x\mathbf{P}_{xz}(x,t) = 0, \tag{7}$$

$$D_t T + \frac{2}{3nk_B}(\mathbf{P}_{xx}\partial_x u + \partial_x q) = 0. \tag{8}$$

We now use the results obtained in Ref. [2] to discuss the nature of the conserved variables that follow from Eqs. (4)–(8) for the stationary case. For this case they reduce to

$$\frac{d}{dx}(nu) = 0, \tag{9}$$

$$mn(x)u(x)u'(x) + \frac{d\mathbf{P}_{xx}}{dx} = 0, \tag{10}$$

$$\tfrac{3}{2}n(x)k_B u(x)T'(x) + \mathbf{P}_{xx}u'(x) + q'(x) = 0, \tag{11}$$

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where the prime denotes derivative with respect to x and Eqs. (6) and (7) have been omitted.

As noted by Santos [1] (see also Ref. [8]), Eqs. (9)–(11) can be integrated to give

$$n(x)u(x)=C_1, \tag{12}$$

$$\mathbf{P}_{xx}+mn(x)u^2(x)=C_2, \tag{13}$$

$$\left(\frac{3}{2}p(x)+\mathbf{P}_{xx}(x)+\frac{m}{2}n(x)u^2(x)\right)u(x)+q(x)=C_3, \tag{14}$$

where C_1, C_2, and C_3 are constants. Thus the problem is to solve Eqs. (4), (5), and (8) for n, u, and T (for an ideal gas we have that $p=nk_BT$) in the nonstationary case, or Eqs. (12)–(14) for the stationary case.

We notice that so far we do not know $\mathbf{P}_{xx}$ and therefore additional information is needed. Therefore, the main issue for the moment is how to find an expression for $\mathbf{P}_{xx}$ in terms of n, u, and T, or equivalently an additional equation for $\mathbf{P}_{xx}$. Such equation comes from Grad's method and reads, under the assumptions mentioned previously [9,10], as

$$\partial_t(\mathbf{P}_{xx}-p)+\partial_x[(\mathbf{P}_{xx}-p)u]+\frac{8}{15}\partial_x q+\frac{4}{3}(\mathbf{P}_{xx}-p)\partial_x u + \frac{4}{3}p\,\partial_x u+\frac{6}{m}B_1^{(2)}\rho(\mathbf{P}_{xx}-p)=0, \tag{15}$$

where ρ is the mass density and $B_1^{(2)}$ is a collision integral which has been evaluated by Grad [9] approximately for inverse power molecules (soft spheres), see Eq. (A3.50) in Ref. [9]. Furthermore, by considering special cases Grad was able to identify $B_1^{(2)}$ in terms of the viscosity η so that

$$B_1^{(2)}=\frac{k_BT}{6\eta}. \tag{16}$$

Then Eq. (15) can be written as

$$\partial_t(\mathbf{P}_{xx}-p)+\partial_x[(\mathbf{P}_{xx}-p)u]+\frac{8}{15}\partial_x q+\frac{4}{3}\mathbf{P}_{xx}\partial_x u = -\frac{p}{\eta}(\mathbf{P}_{xx}-p). \tag{17}$$

It is instructive at this moment to compare Eq. (17) with the equations that have been used by other authors. First of all since for the case considered here we have that $\mathbf{P}_{xx}-\mathbf{P}_{yy}=\frac{3}{2}(\mathbf{P}_{xx}-p)$ (see Eq. (20) in Ref. [2]), it can be shown that in the stationary case and for a constant heat flux (not only for zero heat flux as we mentioned [2]) Eq. (17) reduces precisely to Eq. (17) of Ref. [2]. On the other hand, Eq. (17) reduces [12] to Eq. (1d) in the work by Karlin *et al.* [5] for the case of a constant heat flux. Furthermore, it also reduces to Eq. (16) of Ref. [1]) when $\partial_x(\mathbf{P}_{xx}-p)=0$ (and for constant heat flux). Finally, in the stationary case Eq. (17) reduces to the one considered by Grad [11] in his study of the shock wave problem.

For constant heat flux, Eqs. (4), (5), (8), and (15) can in principle be solved for n, u, T, and $\mathbf{P}_{xx}$, if boundary and or intial conditions are given. We would like to stress the fact that in our previous work we dealt exclusively with Eq. (17) [10]. Our main aim was to obtain an explicit equation for $\mathbf{P}_{xx}$ which we obtained as follows.

(i) We considered the stationary case of Eq. (15) for a constant heat flux, that is,

$$\partial_x[(\mathbf{P}_{xx}-p)u]+\frac{4}{3}\mathbf{P}_{xx}\partial_x u=-\frac{p}{\eta}(\mathbf{P}_{xx}-p). \tag{18}$$

(ii) We used the approximation (see Eq. (27) in Ref. [2])

$$\|u(x)\partial_x(\mathbf{P}_{xx}-p)\|\ll\|(\mathbf{P}_{xx}-p)\partial_x u\| \tag{19}$$

in Eq. (18) [13].

The explicit expression that we obtained [2] is

$$\mathbf{P}_{xx}=p(x)\frac{3p(x)+3\eta u'(x)}{3p(x)+7\eta u'(x)}, \tag{20}$$

where u' denotes the derivative with respect to x. Equation (20) recovers the Navier-Stokes constitutive relation, and has physical meaning only if $u'>-p/3\eta$ [14,15]. Notice that the Navier-Stokes constitutive relation can be obtained from Eq. (17) by using $\mathbf{P}_{xx}=p$ and $q=0$ in the left hand side of this equation to obtain

$$\mathbf{P}_{xx}=p-\tfrac{4}{3}\eta\partial_x u, \tag{21}$$

an idea that goes back to Grad [9] (see p. 371), thus leaving the condition given by Eq. (19) or the condition $\partial_x(\mathbf{P}_{xx}-p)=0$ out of context.

So far, except for our explicit evaluation of $\mathbf{P}_{xx}$, we have proceeded along the lines adopted by Santos. The crucial step is that Santos [1] used $\partial_x(p_{xx}-p)=0$ in Eqs. (12)–(14) to conclude that $u(x)=\text{const}$ is the only physical solution implying that his clauses (a), (c), (d′) and (e) are inconsistent with the conservation equations [16]. In our analysis, however, we must use the expression obtained for $\mathbf{P}_{xx}$, Eq. (20) [17], to obtain from Eqs. (12)–(14) that

$$p(x)\frac{3p(x)+3\eta u'(x)}{3p(x)+7\eta u'(x)}+mC_1u(x)=C_2, \tag{22}$$

$$\left(\frac{3}{2}p(x)+p(x)\frac{3p(x)+3\eta u'(x)}{3p(x)+7\eta u'(x)}+\frac{m}{2}C_1u(x)\right)u(x)=C_4, \tag{23}$$

where $C_4=C_3-q_0$ with q_0 the constant heat flux, after Eq. (12) was used to eliminate $n(x)$. If the viscosity is a function of the temperature only it can always be expressed in terms of p and u. Equations (22) and (23) represent two first-order differential equations for $u(x)$. They can be solved for u' to yield

$$u'(x)=-\frac{3p^2(x)+3mC_1u(x)p(x)-3C_2p(x)}{3p(x)\eta+7mu(x)\eta-7C_2\eta}, \tag{24}$$

$$u'(x) = -\frac{15u(x)p^2(x) + 3mC_1u^2(x)p(x) - 6C_4p(x)}{27p(x)\eta + 7mu^2(x)\eta - 14C_4\eta}. \quad (25)$$

Mathematical consistency requires that the right-hand sides of Eqs. (24) and (25) should be equal. This gives a third-order polynomial for $p(x)$, two of the solutions are $p(x) = 0$ which we will ignore, the other one is given by

$$p(x) = \frac{1}{3}\frac{mC_1u^2(x) + 2C_4 - 2C_2u(x)}{u(x)}. \quad (26)$$

Substitution of Eq. (26) in the right hand of Eq. (24), or in the right hand of Eq. (25), leads finally to the result that

$$u'(x) = F(u(x)) \equiv -\frac{P(u(x))}{Q(u(x))}, \quad (27)$$

where

$$P(u(x)) = 4m^2C_1^2u^4(x) + 10mC_1u^2(x)C_4 - 13mC_1u^3(x)C_2 + 4C_4^3 - 14C_2u(x)C_4 + 10C_2^2u^2(x), \quad (28)$$

and

$$Q(u(x)) = 3\eta[8mC_1u^2(x) + 2C_4 - 9C_2u(x)]u(x). \quad (29)$$

Equation (27) can in principle be solved for the initial condition $u(0)$ (provided the constants C_1, C_2, and C_4 are given), if the viscosity η is known. For example, for soft spheres we have that $\eta = CT^\gamma$, with C a constant, and thus the temperature can be expressed only in terms of u by using Eq. (26). Notice that F in Eq. (27) is a meromorphic function for soft spheres and the local uniqueness theorem for differential equations holds [18]. Thus, the solution to Eq. (27) is hardly only a constant function and therefore the remark by Santos is not generally true for our approach. The question is if a nonconstant heat flux can be included in our approach and what can be said. Actually, the procedure given here can be carried out in principle including the heat flux. However, recently Velasco *et al.* [7] noted a mathematical inconsistency in the moments method—a problem which has been detailed for shock waves [19]—and at this moment it seems better to properly understand this finding before considering this question.

Summarizing, Santos [1] has analyzed a problem which has an interest of its own although his argumentation and results are hardly related to the work he comments about. In fact we have been interested in deviations from equilibrium, as exemplified by the Navier-Stokes equations, but the exact solutions considered by Santos [1,14] either blow up in a finite time or when the limit for large times exists, they yield an unphysical zero number density. This means that in practice, his exact solutions do not reach equilibrium and therefore he is considering an entirely different problem than ours [2].

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[12] Actually, Karlin *et al.* [5] used another system of units and therefore the equation obtained from Eq. (17) for constant heat flux and Eq. (1d) in Ref. [5] are not strictly the same, but they are equivalent. The comparison with Eq. (1d) in Ref. [5] can be most easily done by noting that they used $\sigma = \mathbf{P}_{xx} - p$.
[13] Actually our results remain the same if one of the following conditions: $\|u\partial_x(\mathbf{P}_{xx} - p)\| \ll \|\frac{4}{3}\mathbf{P}_{xx}\partial_x u\|$ or $\|u\partial_x(\mathbf{P}_{xx} - p)\| \ll \|(p/\eta)(\mathbf{P}_{xx} - p)\|$ holds.
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[16] The word inconsistent is used by Santos in what we think is a loose way, but we will not comment further on this.
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