ON THE NAVIER-STOKES EQUATIONS FOR WATER

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In general, the existence of entropy imposes restrictions on the constitutive functions in the Navier–Stokes equations. In this paper, it is shown that if the energy per unit mass is a function of the temperature T only, then the pressure p is an arbitrary function of the density ρ multiplied by the temperature T.

However, for many fluids with the properties radically different than ideal gases (the best example here is water) the pressure as a function of ρ and T is not of the form $p_0(\rho)T$. Therefore the energy density per unit mass in the Navier–Stokes equations for water should depend also on the mass density and the explicit form of this dependence requires further discussion.

Key words: Gibbs identity, thermodynamics, constitutive functions for water.

1. Introduction

In acoustics, especially hydroacoustics (both "linear" and "nonlinear"), the Navier– Stokes equations for water are of a crucial importance. In order to formulate mathematical models of sound propagation and the related transport processes in water (or other fluids with properties radically different than ideal gases), the engineer or modeller must understand the mathematical and physical processes involved. The equation of state for liquid water given in [1, 7] defines the pressure as a function of the mass density and the temperature. However, the explicit form of the Navier–Stokes equations depends also on the expression for the energy density per unit mass, given as a function of the temperature T and the mass density ρ . In this paper, it is shown that if the energy per unit mass is a function of temperature T only, then the pressure p is an arbitrary function of the density ρ (which can be denoted $p_0(\rho)$), multiplied by the temperature T. However, for many fluids with the properties radically different than ideal gases (the best example here is water) the pressure as a function of ρ and T is not of the form $p_0(\rho) T$. Therefore the energy density per unit mass in the Navier–Stokes equations for water should depend also on the mass density. This problem concerns the whole class of real fluids but water is the best one investigated. The explicit calculations are in the second chapter and the conclusions are given in the last chapter of the paper.

2. The basic equations

The symmetric Cauchy stress tensor can be written as a sum of two terms; the first term is the product of pressure p and the identity tensor (taken with the minus sign) and the second one is the "dissipative part of the stress tensor":

$$t_{ij} = -p\left(\rho, T\right)\delta_{ij} + t'_{ij}.$$
(1)

In the above formula δ_{ij} denotes the identity tensor, t_{ij} and t'_{ij} are the symmetric Euclidean tensors of rank two, ρ denotes the mass density and T denotes the temperature.

The mass density balance has the form

$$\frac{\mathrm{D}}{\mathrm{D}t}\rho + \rho \frac{\partial u^i}{\partial x^i} = 0, \tag{2}$$

where u^i denotes velocity field and D/Dt is the substantial derivative

$$\frac{\mathrm{D}}{\mathrm{D}t} = \frac{\partial}{\partial t} + u^{i} \frac{\partial}{\partial x^{i}} \tag{3}$$

with $\partial/\partial t$ and $\partial/\partial x^i$ being the time derivative and the "spatial" derivative, correspondingly.

The momentum balance is of the form

$$\rho \frac{\mathrm{D}}{\mathrm{D}t} u^{i} = \frac{\partial}{\partial x^{j}} t_{ij} = \frac{\partial}{\partial x^{j}} \left[-p\left(\rho, T\right) \delta_{ij} + t'_{ij} \right], \tag{4}$$

and the energy balance reads

$$\rho \frac{\mathrm{D}}{\mathrm{D}t} E = t_{ij} \frac{\partial u^i}{\partial x^j} - \frac{\partial q^i}{\partial x^i},\tag{5}$$

where q^i is the heat flux. The explicit form of the "dissipative part of the stress tensor" for the Navier–Stokes equations is [3]

$$t_{ij}^{\prime} = \left[\eta\left(\rho, T\right) - \zeta\left(\rho, T\right)\right] \delta_{ij} \frac{\partial u^{k}}{\partial x^{k}} + \zeta\left(\rho, T\right) \left[\frac{\partial u^{i}}{\partial x^{j}} - \frac{\partial u^{j}}{\partial x^{i}}\right],$$

where $\zeta(\rho,T)$ is the shear viscosity coefficient while $\eta(\rho,T)$ is the bulk viscosity coefficient.

After inserting (1) into (5) one obtains

$$\rho \frac{\mathrm{D}}{\mathrm{D}t} E = t_{ij} \frac{\partial u^i}{\partial x^j} - \frac{\partial q^i}{\partial x^i} = \left[-p\left(\rho, T\right) \delta_{ij} + t'_{ij} \right] \frac{\partial u^i}{\partial x^j} - \frac{\partial q^i}{\partial x^i}.$$
 (6)

The above formula can be written equivalently as

$$\rho \frac{\mathrm{D}}{\mathrm{D}t} E = -p\left(\rho, T\right) \frac{\partial u^k}{\partial x^k} + t'_{ij} \frac{\partial u^i}{\partial x^j} - \frac{\partial q^i}{\partial x^i}.$$
(7)

In order to eliminate $\partial u^k / \partial x^k$ from (7), one can determine $\partial u^k / \partial x^k$ from (2):

$$\frac{\partial u^k}{\partial x^k} = -\frac{1}{\rho} \frac{\mathrm{D}}{\mathrm{D}t} \rho \tag{8}$$

and insert (8) into (7), what gives

$$\rho \frac{\mathrm{D}}{\mathrm{D}t} E = -p\left(\rho, T\right) \left[-\frac{1}{\rho} \frac{\mathrm{D}}{\mathrm{D}t} \rho \right] + t'_{ij} \frac{\partial u^{i}}{\partial x^{j}} - \frac{\partial q^{i}}{\partial x^{i}} = \frac{p\left(\rho, T\right)}{\rho} \frac{\mathrm{D}}{\mathrm{D}t} \rho + t'_{ij} \frac{\partial u^{i}}{\partial x^{j}} - \frac{\partial q^{i}}{\partial x^{i}}.$$
 (9)

Now, (9) is equivalent to

$$\rho \left\{ \frac{\mathrm{D}}{\mathrm{D}t} E - \frac{p\left(\rho, T\right)}{\rho^2} \frac{\mathrm{D}}{\mathrm{D}t} \rho \right\} = t'_{ij} \frac{\partial u^i}{\partial x^j} - \frac{\partial q^i}{\partial x^i}.$$
 (10)

After introducing

$$\frac{\mathrm{D}}{\mathrm{D}t}\frac{1}{\rho} = -\frac{1}{\rho^2}\frac{\mathrm{D}}{\mathrm{D}t}\rho.$$
(11)

into (10), one obtains

$$\rho \left\{ \frac{\mathrm{D}}{\mathrm{D}t} E + p\left(\rho, T\right) \frac{\mathrm{D}}{\mathrm{D}t} \frac{1}{\rho} \right\} = t'_{ij} \frac{\partial u^{i}}{\partial x^{j}} - \frac{\partial q^{i}}{\partial x^{i}}.$$
 (12)

For the temperatures different from zero, the above equation can be multiplied by the inverse of the temperature

$$\rho \left\{ T^{-1} \frac{\mathrm{D}}{\mathrm{D}t} E + T^{-1} p\left(\rho, T\right) \frac{\mathrm{D}}{\mathrm{D}t} \frac{1}{\rho} \right\} = T^{-1} \left\{ t'_{ij} \frac{\partial u^{i}}{\partial x^{j}} - \frac{\partial q^{i}}{\partial x^{i}} \right\}.$$
 (13)

As it has been already mentioned in the Introduction, in our case the primitive fields are ρ and T and the internal energy per unit mass and the pressure are

$$E = E\left(\rho, T\right) \tag{14}$$

and

$$p = p\left(\rho, T\right),\tag{15}$$

correspondingly. Now one can ask about the existence of a function $\Gamma\left(\rho,T\right)$ that satisfies the equation

$$\frac{\mathrm{D}}{\mathrm{D}t}\Gamma\left(\rho,T\right) = T^{-1}\frac{\mathrm{D}}{\mathrm{D}t}E\left(\rho,T\right) + T^{-1}p\left(\rho,T\right)\frac{\mathrm{D}}{\mathrm{D}t}\frac{1}{\rho}.$$
(16)

A detailed discussion of this problem can be done in terms of the formalism introduced in [5], but in order to get the answer quickly we shall make use of a simpler approach, based on the differential forms defined on arithmetic spaces. Let us start with the observation that after taking (11) into account, (16) can be written in the form

$$\frac{\mathrm{D}}{\mathrm{D}t}\Gamma\left(\rho,T\right) = T^{-1}\frac{\mathrm{D}}{\mathrm{D}t}E\left(\rho,T\right) - \frac{p\left(\rho,T\right)}{T\rho^{2}}\frac{\mathrm{D}}{\mathrm{D}t}\rho.$$
(17)

Now, (17) can be expressed in terms of the substantial derivatives of the primitive fields:

$$\begin{split} \frac{\mathbf{D}}{\mathbf{D}t}\Gamma\left(\rho,T\right) &= \frac{\partial\Gamma\left(\rho,T\right)}{\partial\rho}\frac{\mathbf{D}}{\mathbf{D}t}\rho + \frac{\partial\Gamma\left(\rho,T\right)}{\partial T}\frac{\mathbf{D}}{\mathbf{D}t}T\\ &= T^{-1}\left[\frac{\partial E\left(\rho,T\right)}{\partial\rho}\frac{\mathbf{D}}{\mathbf{D}t}\rho + \frac{\partial E\left(\rho,T\right)}{\partial T}\frac{\mathbf{D}}{\mathbf{D}t}T\right] - \frac{p\left(\rho,T\right)}{T\rho^{2}}\frac{\mathbf{D}}{\mathbf{D}t}\rho\\ &= \left[T^{-1}\frac{\partial E\left(\rho,T\right)}{\partial\rho} - \frac{p\left(\rho,T\right)}{T\rho^{2}}\right]\frac{\mathbf{D}}{\mathbf{D}t}\rho + T^{-1}\frac{\partial E\left(\rho,T\right)}{\partial T}\frac{\mathbf{D}}{\mathbf{D}t}T. \end{split}$$
(18)

Since the substantial derivatives of the mass density $(D/Dt) \rho$ and of the temperature field (D/Dt)T are linearly independent, a single equation (18) is equivalent to the following pair of identities:

$$\frac{\partial \Gamma(\rho,T)}{\partial \rho} \frac{\mathrm{D}}{\mathrm{D}t} \rho = \left[T^{-1} \frac{\partial E(\rho,T)}{\partial \rho} - \frac{p(\rho,T)}{T\rho^2} \right] \frac{\mathrm{D}}{\mathrm{D}t} \rho$$
(19)

and

$$\frac{\partial \Gamma(\rho, T)}{\partial T} \frac{\mathrm{D}}{\mathrm{D}t} T = T^{-1} \frac{\partial E(\rho, T)}{\partial T} \frac{\mathrm{D}}{\mathrm{D}t} T.$$
(20)

In turn, (19) and (20) are equivalent to the "scalar" equations:

$$\frac{\partial \Gamma\left(\rho,T\right)}{\partial \rho} = T^{-1} \frac{\partial E\left(\rho,T\right)}{\partial \rho} - \frac{p\left(\rho,T\right)}{T\rho^{2}}$$
(21)

and

$$\frac{\partial \Gamma\left(\rho,T\right)}{\partial T} = T^{-1} \frac{\partial E\left(\rho,T\right)}{\partial T}.$$
(22)

It can be observed that (21) and (22) imply the existence of a potential to the 1-form

$$\left[T^{-1}\frac{\partial E\left(\rho,T\right)}{\partial\rho} - \frac{p\left(\rho,T\right)}{T\rho^{2}}\right]d\rho + T^{-1}\frac{\partial E\left(\rho,T\right)}{\partial T}dT$$
(23)

and the corresponding "integrability condition" is:

$$\frac{\partial}{\partial T} \left[T^{-1} \frac{\partial E\left(\rho, T\right)}{\partial \rho} - \frac{p\left(\rho, T\right)}{T\rho^2} \right] = \frac{\partial}{\partial \rho} \left[T^{-1} \frac{\partial E\left(\rho, T\right)}{\partial T} \right].$$
(24)

Often, the energy density per unit mass (14) does not depend on ρ , that is:

$$E = E(T), \qquad (25)$$

and for (25) the condition (24) simplifies to the form

$$\frac{\partial}{\partial T} \left[-\frac{p\left(\rho, T\right)}{T\rho^2} \right] = \frac{\partial}{\partial \rho} \left[T^{-1} \frac{\partial E\left(T\right)}{\partial T} \right].$$
(26)

The r.h.s. of (26) is identically equal to zero

$$\frac{\partial}{\partial\rho} \left[T^{-1} \frac{\partial E\left(T\right)}{\partial T} \right] = 0$$
(27)

and therefore also the l.h.s. of (26) is equal to zero

$$\frac{\partial}{\partial T} \left[-\frac{p\left(\rho, T\right)}{T\rho^2} \right] = 0.$$
(28)

In turn, (28) is satisfied under the condition that the pressure is a linear function of temperature, that is

$$p(\rho, T) = p_0(\rho) T.$$
⁽²⁹⁾

After inserting (29) and (25) into (23) one arrives at

$$\left[-\frac{p_0(\rho)T}{T\rho^2}\right]d\rho + T^{-1}\frac{\partial E(T)}{\partial T}dT = -\frac{p_0(\rho)}{\rho^2}d\rho + \frac{1}{T}\frac{\partial E(T)}{\partial T}dT.$$
 (30)

After inserting (11) into (30) one obtains

$$\frac{p_0(\rho)T}{T}d\left[\frac{1}{\rho}\right] + \frac{1}{T}\frac{\partial E(T)}{\partial T}dT.$$
(31)

From the form of the expression (31) it can be observed that it is equal to the product of inverse of temperature 1/T and the 1-form

$$p_0(\rho) T d\left[\frac{1}{\rho}\right] + \frac{\partial E(T)}{\partial T} dT = p_0(\rho) T d\left[\frac{1}{\rho}\right] + dE(T).$$
(32)

In a particular case of an ideal gas law

$$p = R\rho T, \tag{33}$$

where R is a constant, our expression (32) reduces to

$$R\rho T d\left[\frac{1}{\rho}\right] + dE\left(T\right) \tag{34}$$

and the product of (34) and 1/T reduces to the case discussed by WHITHAM ([3], p.152):

$$dS = \frac{dE(T)}{T} - d(R\ln\rho).$$
(35)

It is worth to mension that Whitham uses a different choice of primitive fields. Namely, we take (ρ, T) as the primitive fields while Whitham writes on p. 152:

..."In the equations of motion it is convenient to express E as a function of p and ρ . We see that for an ideal gas E is a function of p/ρ . The form of this function could be left open but in fact, a rather simple formula covers a wide range of phenomena in gas dynamics"...

However, the pressure in water, expressed as a function of ρ and T, is not of the form (29); on p. 24 of [1]) it is written:

..."In 1999 year, C. A. Jeffery and P. H. Austin proposed an analytical equation of state for liquid water [7] that was a modification of the Song–Mason–Ihm equation but for the polar fluid, with taking into considerations the hydrogen bonds effect, such in POOLE *et al.* paper [8]. In that approach the equation of state has the form:

$$\frac{p}{\rho RT} = 1 - b_0 \rho - \frac{a\rho}{RT} + \frac{a\rho}{1 - \lambda b\rho}$$
(36)

where ρ is expressed in mol/m³ unit and function b(T) has the form

$$b(T) = \nu_B \left(0.25e^{1/2.3T/T_B + 0.5} - b_l e^{2.3T/T_B} + b_2 \right)$$

= $\nu_B \left(e^{T_1(T)} - b_l e^{T_2(T)} + b_2 \right)$
 $T_1(T) = -\ln 4 + \left(2.3\frac{T}{T_B} + 0.5 \right)^{-1},$
 $T_2(T) = 2.3\frac{T}{T_B}.$ (37)

The constants in the equation have the following values: $a = a_{VDW} = 0.5542$ Pa m⁶/mol²; $\lambda = 0.3159 \nu_B$; $b_0 = 1.0823 \nu_B$; $b_l = 0.02774$; $b_2 = 0.23578$, Boyle volume: $\nu_B = 4.1782 \cdot 10^{-5}$ m³/mol; Boyle temperature $T_B = 1408.4$ K, R – universal gas constant."

For the pressure different from (29) and the energy density of the form (25), the potential $\Gamma(\rho, T)$ does not exist.

3. Conclusions

In the second chapter it has been shown that the Gibbs identities are satisfied under the conditions that the pressure p is a product of the temperature T and a function of the density $p_0(\rho)$ and the energy density per unit mass given by a function of the temperature E = E(T). However, the analytical equation of state, described in [1,7] and given explicitly as (36), is not consistent with these conditions. It follows that the energy density per unit mass should depend not only on the temperature but also on the mass density. The explicit expression for this function is not known. This problem requires further discussion and it seems that in order to understand the behaviour of the "dense fluids", one should analyse perturbational approaches. However, such approaches are outside the scope of the present paper. Obviously, the final criterion here should be the experiment.

This problem is "of a general nature" in the sense that it does not depend on particular forms of the heat flux and the viscosity coefficients. Obviously, in the limit of "ideal gases without dissipation" our equations reduce to the field equations given by PERADZYŃSKI on p. 78 of [4].

It seems worth to mention that the results of this paper can be obtained in a more rigorous manner by means of the approach described in [5]. In future, we hope to use the formalism proposed in [5] in order to make a detailed comparison between our approach and that of WHITHAM [3].

In this paper, we discussed only the "smooth" solutions (which do not depend on the explicit form of the field equations). The cases of "singular" solutions are more complicated but they are outside the scope of this paper (see [2, 3]).

References

- [1] LEBLE S., KUŚMIREK-OCHRYMIUK M., Liquid water. Analytical equation of state and acoustic parameters evaluation., Hydroacoustics, **5/6**, p.23, Gdynia 2002/2003.
- [2] KOSIŃSKI W., *Field singularities and wave analysis in continuum mechanics*, PWN, Warszawa, Ellis Horwood Limited, Chichester 1986.
- [3] WHITHAM G. B., *Linear and nonlinear waves*, Wiley Interscience Publication. John Wiley & Sons, New York 1974.
- [4] PERADZYŃSKI Z., *Geometry of nonlinear interactions in partial differential equations* [in Polish], Habilitation Thesis, IFTR Reports, Warszawa 1981.
- [5] PIEKARSKI S., On the invariant formulation of fluid mechanics, http://xxx.lanl.gov/ftp/physics/ papers/0411/0411154.pdf.
- [6] WALSKI T. M. et al., Advanced water distribution modelling and management, Haestad Press, Waterbury 2003.
- [7] JEFFERY C. A., AUSTIN P. H., A new analytical equation of state for liquid water, J. Chem. Phys., 110, 1, 484–496 (1999).
- [8] POOLE P. H., SCIORTINO F., GRANDE T., STANLEY H. E., ANGELL C. A., Phys. Rev. Letters, 73, 12, 1632–1635 (1994).