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Study of Basic Physical Processes in Liquid Rocket Engines

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SUMMARY

Inconsistencies between analytical results and measurements for liquid rocket thrust chamber performance, which escape suitable explanations, have motivated the examination of the basic physical modeling formulations as to their unlimited application. The publication of Prof. D. Straub's book, "Thermofluid-dynamics of Optimized Rocket Propulsions", further stimulated the interest of understanding the gas dynamic relationships in chemically reacting mixtures. A review of other concepts proposed by Falk-Ruppel (Gibbsian Thermodynamics), Straub (Alternative Theory, AT), Prigogine (Non-Equilibrium Thermodynamics), Boltzmann (Kinetic Theory), and Truesdell (Rational Mechanism) has been made to obtain a better understanding of the Navier-Stokes equation, which is now used extensively for chemically reacting flow treatment in combustion chambers.

In addition to the study of the different concepts, two workshops were conducted to clarify some of the issues. The first workshop centered on Falk-Ruppel's new "dynamics" concept, while the second one concentrated on Straub's AT.

In this report brief summaries of the reviewed philosophies are presented and compared with the classical Navier-Stokes formulation in a tabular arrangement. Also the highlights of both workshops are addressed. End

The primary conclusions are as follows:

1. The new thermodynamics theory by Faulk-Ruppel provides an indepth approach to formulate thermo-fluid equations. However, the connection with the conventional Navier-Stokes equation is not apparent. Further investigation of this issue is necessary for the assessment of the governing equations in combustion chamber flows for CFD simulations.

2. Both, NASA's ODE program and the Munich Method Code for thermodynamic equilibrium calculations of rocket engines now carry an option to consider finite area combustion effects. The solution process in both approaches is based on the Lagrangian multiplier scheme. The results from these two programs are practically identical for two demonstrated sample cases. However, the ODE program contains many more chemical elements and species and is equipped with several practical calculation options.

3. The derivation of a new "Navier-Saint Venant" equation as a result of Prof. Straub's "Alternative Theory" was not presented. Hence, the equation was not accepted as a preferred scheme over the Navier-Stokes Equation at this time. Some interesting results should be surveyed.

4. The comparison of Navier-Stokes equation with other formulations from Boltzmann, Prigogine, and Truesdell have

revealed certain limitations, when this equation is used for combustion chamber flow modeling.

5. This review process is an initial attempt to establish a sound foundation for the analytical simulation of rocket engine flow processes. Further re-evaluations are in order and should be supported by a group of experts from the academic profession to assist the engineering community in solving their problems with a high degree of confidence.

I. INTRODUCTION

Since the introduction of the maximization of entropy for equilibrium in rocket engine combustion processes by Prozan [1] in 1969, this scheme has induced considerable different opinions in the JANNAF community. In 1982, NASA/MSFC awarded a contract (NAS8-34946) to Continuum Inc. to program this entropy maximization concept and provide quantitative evidence. The results led to a workshop at Continuum Inc., where Prozan's proposed concept was reviewed and debated. In the meantime, some new developments appeared in Europe. The introduction of a "Dynamics" concept by Falk and Ruppel [2,3] forms the basis for a new look at the currently used thermodynamic and fluid dynamic laws. Building on their concept, Prof. Straub formulated an "Alternative Theory (AT)" which is characterized in a recently published book entitled "Thermofluid-Dynamics of Optimized Rocket Propulsions". The contents of the book became strongly controversial. To gain further understanding of these differences, MSFC awarded a contract to The University of Alabama in Huntsville (UAH) to investigate the fundamental analytical formulations, which are currently used to simulate the physical processes in liquid rocket combustion chambers and nozzles.

To accomplish these goals, two workshops were organized, and their proceedings have been published [4,5]. Brief information about both workshops and the conclusions are included in Appendix I and II of this report. The foundation of the "Gibbsian Thermodynamics" and one important application is described in Section II. Information about Prof. Straub's (AT) is included in Section III. Section IV discusses the derivation of conservation laws via Boltzmann equations, and the ones based on Prigogine's non-equilibrium thermodynamics are presented in Section V. Truesdell's rational mechanics theory is displayed in Section VI. A comparison of these concepts and theories with concluding remarks are presented in Section VII.

The motivation to select the classical theorems (Gibbsian, Boltzmann, Prigogine and Truesdell)-to be included in this study is because in one way or another they attempt to formulate the non-equilibrium chemically and radiatively acting flow. These are being compared with the current Navier Stokes Equation used in the present Computational Fluid Dynamics (CFD) for the combustion chamber flow simulation.

II. GIBBSIAN THERMODYNAMICS

Professors Gottfried Falk and Wolfgang Ruppel are the originators of a new concept, called "Gibbsian Thermodynamics", which is presented in the following two books [2,3], written in German and printed by the Springer Publishing Company:

1. Mechnik, Relativität, Gravitation - (1977)
2. Energie und Entropie - (1976)

Some important chapters of these books have been summarized and translated, and they are included as Appendix C in [4]. This section provides only excerpts from [4], relating to the justification of the new concept and one notable application. A comprehensive document showing the derivation of the novel equation and its advantage should be prepared in English to assure proper attention and relevant studies.

In the book "Energy and Entropy" the mass character of energy, the various forms in which energy is exchanged, energy fluxes, and the spatial distribution of energy or energy flux concentration are addressed. The mass character of energy permits the summation of all energy forms. The energy which is connected with an energy transport during a process appears in specific energy forms. Please note that only the transported energy relates to an energy form and not the stored energy. Energy forms are: energy of rotation, energy of motion, energy of compression, surface energy, chemical energy, heat energy, and others. All energy forms can be represented with the following mathematical description $\zeta\, dX$, where X is the extensive variable specifying the energy form and ζ is the intensive variable, identifying the quantity of energy which is exchanged in this form.

$$\text{Energy Form} = (\text{intensive variable } \zeta) \cdot d(\text{extensive variable } X)$$

There are as many different energy-forms as there are extensive variables, however, they do not have to be independent of each other. The number of independent energy forms reflect the number of degrees of freedom in a system. The general validity of this energy form convention cannot be proven, like no assertion about nature can be confirmed.

One of the great achievements in physics has been the identification of "standard variables", which permit the description of an untold number of processes in nature. A special simple treatment of such processes can be accomplished with variables which satisfy conservation laws. They are especially favored as standard variables.

Since energy is a mass quantity, which is distributed in space and can flow, the following Gibbs Fundamental Form is introduced. The terminology "form" is used because the equation is composed of differentials of the first order (linear), also known as Pfaff's form.

$$dE = \zeta_1 dX_1 + \zeta_2 dX_2 + \ldots + \zeta_n dX_n \qquad \text{(II.1)}$$

Distinct energy forms are presented below with bold letters identifying vector quantities:

Energy of:

ROTATION:	ΩdL	(Angular Velocity) * L (Rot. Momentum)
TRANSLATION:	$-Fdr$	(-Force) * **r** (Position Vector)
MOTION:	vdP	(Velocity) * P (Momentum)
COMPRESSION:	$-pdV$	(-Pressure) * V (Volume)
SURFACE:	σdA	(Surface Tension) * A (Surface Area)
ELECTRICAL:	ϕdQ	(Electrical Potential) * Q (Charge)
CHEMICAL:	μdN	(Chemical Potential) * N (Partical No.)
HEAT:	TdS	(Temperature) * S (Entropy)
POLARIZATION:	$Ed\gamma$	(El. Field Strength) * γ (Dipole Moment)
MAGNETISM:	Hdm	(Mag. Field Strength) * **m** (Dipole Moment)

Gibbs Fundamental Form

$$dE = \Sigma \zeta_n dX_n \qquad \text{(II.2)}$$

In this equation dE is the received or produced energy. It is important that each energy form is independent of the other ones, which means that the energy flux of each energy form must be possible regardless of the other fluxes.

If all extensive variables have a constant value, then all differentials are zero, which in turn requires $dE = 0$ or $E =$ constant. The corresponding Gibbs Function reads:

$$E = f\,(P, r, L, S, V, A, N) \qquad \text{(II.3)}$$

(The electrical, polarization, and magnetic energy forms are not considered here)

This function describes systems which are physically equal when the same extensive variables are involved. However, they do not need to be the same in reality.

Gibbs functions are also called Thermodynamic Potentials.

Statement

The identification of the energy E of a system as a function of the independent extensive variables is a very difficult task, which can only be solved by approximations in the end. Large disciplines of physics, such as statistical mechanics, are used primarily to find these functions.

The intensive variables are obtained by differentiating the Gibbs function E = E (.....) with respect to the extensive variables.

$$dE = \frac{\partial E}{\partial P} dP - \frac{\partial E}{\partial r} dr + \frac{\partial E}{\partial S} dS + \frac{\partial E}{\partial V} dV + \frac{\partial E}{\partial N} dN \qquad (II.4)$$

where the partial derivatives represent the velocity $v = \partial E/\partial P$, the force $F = \partial E/\partial r$, the temperature $T = \partial E/\partial S$, the pressure $-p = \partial E/\partial V$, and the chemical potential $\mu = \partial E/\partial N$ respectively. These results give

$$dE = vdP + Fdr + TdS + pdV + \mu dN \qquad (II.5)$$

The specific features of this equation are:

- o The fundamental equation reflects an energy change and not its conservation.
- o All energy terms are portrayed by the same mathematical structure.
- o All terms have quantity character and become additive.
- o Each term represents a specific energy form.
- o Each energy form is presented by two conjugate physical parameters of an intensive and extensive variable.
- o Each variable can appear in the equation only once.
- o A system can be subdivided if the variables in one subsystem do not affect the variables in the other one.

The identified "Gibbs Fundamental Form" and its identified features form the basis of Gibbsian Thermodynamics. In order to show the connection with the classical mechanics (i.e. Newton's Second Law) we shall discuss the derivation of Newton's Second Law from the Gibbs Fundamental Equation. Recall the Gibbs fundamental equation.

$$dE = \Sigma \zeta_i dX_i$$
$$E = E(\mathbf{L},\mathbf{r},P,V,A,Q,N_i,S,\gamma,m) \qquad \text{(II.6)}$$

Separating the energy into two parts which represent the motion and the internal character, neglecting the energy forms of **polarization** and **magnetism** results in:

$$E(\mathbf{P},\mathbf{r},\mathbf{L},S,V,A,N_i) = E_1(\mathbf{P},\mathbf{r}) + E_0(\mathbf{L},S,V,A,N_i) \qquad \text{(II.7)}$$

Reducing this equation to hold only the energy of motion (**vdP**) and energy of translation (**Fdr**) requires that the dynamic variables of the internal energy subsystem have: (1) constant values and, therefore, their differentials are zero, (2) their differentials are not zero, but the summation of the associated energy forms are zero, (3) the independent variables representing the internal energy have no influence, or perhaps only a weak one on the other subsystem.

$$\zeta_1 dX_1 = vdP;\ \text{Velocity} \cdot d\ \text{(Impulse)}$$
$$\zeta_2 dX_2 = Fdr;\ \text{-Force} \cdot d\ \text{(Position)} \qquad \text{(II.8)}$$

With a further assumption that the system does not exchange energy with another system finally results in the equation:

$$dE = \mathbf{vdP} - \mathbf{Fdr} = 0$$

or (II.9)

$$E = E(\mathbf{P},\mathbf{r}) = \text{const.}$$

In a static field where the force is only a function of the position, $\mathbf{F} = F(\mathbf{r})$, which postulates that the velocity is only a function of the impulse, $v = v(\mathbf{P})$, the differentials of the extensive variables become total differentials. The energy of motion is now representing the kinetic energy, and the energy of translation the potential energy.

If the system is subject to a change in time and postulating that P and **r** are functions of time, then differentiation with respect to time yields:

$$v\frac{dP}{dt} - F\frac{dr}{dt} = 0 \qquad \text{(II.10)}$$

Recognizing that the change of position with time is equivalent to the kinematic velocity, v = dr/dt, which can be equated for point particle motion with the dynamic velocity $\mathbf{v} = \partial E/\partial \mathbf{P}$, and substituting the proper term in the equation leads to:

$$\mathbf{v}\frac{d\mathbf{P}}{dt} - \mathbf{F}\mathbf{v} = 0$$

$$\mathbf{v}\left(\frac{d\mathbf{P}}{dt} - \mathbf{F}\right) = 0 \qquad \text{(II.11)}$$

This equation is satisfied when

$$\mathbf{v} = 0$$

$$\left(\frac{d\mathbf{P}}{dt} - \mathbf{F}\right) = 0$$

and the scalar vector product is Zero.

The second requirement leads to the equation below

$$\frac{d\mathbf{P}}{dt} = \mathbf{F} \qquad \text{(II.12)}$$

Please note that there are two equations of motion which are valid in general when only the energy of motion and energy of translation are present, where $\mathbf{F} = \mathbf{F}(\mathbf{P},\mathbf{r})$ and $\mathbf{v} = \mathbf{v}(\mathbf{P},\mathbf{r})$. Separation into two independent subsystems requires that they cannot share independent variables, and total derivatives can be used.

$$\frac{d\mathbf{P}}{dt} = \mathbf{F}$$

$$\frac{d\mathbf{r}}{dt} = \mathbf{v} \qquad \text{(II.13)}$$

Now, the intensive variables **F** and **v** are only functions of either **P** and **r** respectively.

For Newton's condition (v << c) the two equations translate into a better known form. With the assumption that a field of the first type is present, the force **F** is only a function of **r**, which requires that the velocity **v** is only a function of **P**. The latter condition can be obtained in the following approach. In Einstein's important relationship the impulse is related to the energy in the following way:

$$\mathbf{P} = \frac{E}{c^2}\mathbf{v} \qquad \text{(II.14)}$$

In this equation E represents the total transport energy which itself depends on **v** and increases with growing velocity. For transport velocities **v** → 0 the energy approaches a finite value which is known as the internal energy $E_0 = M c^2$. Substituting this term in the previous equation results in

$$\mathbf{P} = M\mathbf{v} \tag{II.15}$$

This is just the relationship we are looking for, where **v** is a function of **P**. In this equation M represents the inert mass, which is normally a function of the velocity, but here M is equivalent to the velocity independent rest energy or internal energy E_0 for **v** = 0 and **P** = 0.

Substituting the impulse value for Newton's condition (v << c) in the bracket term (II.11), and taking M out of the differential expression, since it is a constant and therefore independent of time, yields the following equation:

$$\begin{aligned} \frac{d\mathbf{P}}{dt} &= \mathbf{F} \\ \frac{d(M\mathbf{v})}{dt} &= \mathbf{F} \\ M\frac{d\mathbf{v}}{dt} &= \mathbf{F} \\ M\frac{d^2\mathbf{r}}{dt^2} &= \mathbf{F} \end{aligned} \tag{II.16}$$

The last equation is Newton's famous law:

MASS * ACCELERATION = FORCE

During this derivation the following assumptions have been made:

- The motion of the system is virtually independent of the internal energy of the system with v << c or $c|\mathbf{P}| \ll E$.
- The energy of motion and translation of a system remain when:

  (1) The fixed values of the extensive variables L (Rotational Momentum), S (Entropy), V (Volume), N (Particle Numbers) and therefore, also their conjugated intensive variables Ω (Angular Velocity), T (Temperature), p (Pressure), μ (Chemical Potential), state that the internal energy does not change. This relates to the motion of rigid

bodies or mass particles.

(2) The sum of the energy forms representing the internal energy is zero, but the individual terms are not. Here the motion is independent of the internal energy.

(3) The independent variables portraying the internal energy do not affect the other subsystem or have only a weak impact on it.

- The mass M is independent of time.
- Only two forms of energy are considered which are independent of each other.
- The transitional energy **F**d**r** is restricted even to a static field, where **F** = F(**r**) and not of **v**.

Please note: If fields of the second type (non-conservative fields) with **F** = F(**P**,**r**) and **v** = v(**P**,**r**) are present, the relationship **P** = M**v** is not possible. Therefore, equation (II.16) cannot result for such a condition.

III. ALTERNATIVE THEORY: STRAUB METHOD*

Straub has deduced his so-called "Alternative Theory" (AT), [6], on the basis of the 'dynamics' theory by Falk and Ruppel, [2,3], combined with Progogine's new micro-theory [7]. The Navier-Saint Venant equation is a principle result of the AT and leads to a confrontation with the Navier-Stokes equation of motion. Subsequently, Straub's description of the AT from [6] is presented.

III.1. The Navier-Saint Venant Equation of Motion

In order to offer a quantitative presentation of the numerous important results of the AT, the equation of motion of a compressible multicomponent single-phase fluid mixture is compared to the Navier-Stokes equation of motion. The basic relationship representing the momentum conservation law is a Cauchy-type equation of motion.

$$\rho D\mathbf{v} = \rho \mathbf{f} - \nabla \cdot \dot{\pi} + 1/2\ \partial_t \rho \phi, \qquad \text{(III.1)}$$

whereas D is a differential operator called the substantial or material time derivative

$$D: = \partial_t + \mathbf{v} \cdot \nabla \qquad \text{(III.2)}$$

in this definition ∂_t denotes the partial time derivatives and ∇ is the gradient vector operator (nabla-operator).

The local flow velocity **v** involved has a double definition: the original 'dynamic' establishment

$$\mathbf{v} = \frac{\partial E(P,r,s,V,N_k)}{\partial P} \qquad \text{(III.3)}$$

is obtained with the Gibbs Fundamental Equation [6] of the multicomponent single-phase fluid mixture. Identification of **v** with the kinematic velocity $\mathbf{v}_*: = dr/dt$ guarantees conservation of the particle number of all baryons. This invariance generalizes the Newtonian mechanics of finite systems of mass-points, called 'bodies'. At every given instant the body is located at some place and assigned real numbers denoting the properties of state. In field theories the continuity equation controls the time behavior of such a body by considering the baryons constancy (see Straub 1988, pp. 53 f).

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*The content of this section is directly transposed form ref.[6].

The properties $\dot{\pi}$ and ϕ appearing in equation (III.1) along with mass density ρ and the specific field force f (for example, gravity), are defined as follows in the AT:

$$\dot{\pi} := p\delta - \tau \quad \text{pressure tensor} \tag{III.4}$$

$$\phi := v - i \quad \text{dissipation velocity} \tag{III.5}$$

Here δ stands for the unity tensor and p is the thermodynamic pressure established with the equation for the hypothetical state of rest [6]. This pressure is permitted to be calculated only with the thermal equation of state

$$p = R\,T\,\rho\,Z \tag{III.6}$$

where ρ denotes the density and T is the temperature defined for a hypothetical state of rest [6]; the compressibility factor Z = $Z(T,\rho)$ is identical to one only with ideal gases.

The viscous stress tensor τ typical for individual classes of flowing fluids is related to the AT's characteristic dissipation velocity through the dyadic product

$$\tau := 1/2\ \rho v \phi \quad \text{viscous stress tensor} \tag{III.7}$$

The quantity ϕ equals the vector difference between the local flow velocity v and the specific (linear) impulse i; the limiting case

$$\lim_{\sigma \to 0} \phi = 0 \tag{III.8}$$

disappears only for vanishing dissipation, expressed by the local values of the entropy production density σ.

For $\phi = \hat{\phi}(\sigma \neq 0) \equiv 0$, equation (III.1) formally corresponds to the classical Cauchy equation of motion.

The following Navier-Saint Venant equation of motion for a defined class of compressible fluids and their mixture is taken from the AT and is comprised of equations (III.1) and (III.4). For the viscous stress tensor τ the expression

$$\left.\begin{aligned}\tau = {} & t_\tau \, Z^{-1} \, p \, \frac{s}{R} \left\{ D - \frac{1}{2} (\nabla \cdot v) \, \delta \right\} - \\ & - \frac{1}{2} \, t_\tau \, T(\partial_t s + \nabla \cdot j_s) \; \delta - \\ & - \, t_\tau \, (ZR)^{-1} \, p \left\{ \nabla s v - \frac{1}{2} (\nabla \cdot s v) \; \delta \right\} \\ & - \, t_\tau \, (ZR)^{-1} \, p \left\{ [\nabla s \times v] \times \delta \right\} \end{aligned}\right\} \qquad \text{(III.9)}$$

is theoretically derived.

For simplification, the abbreviation

$$t_\tau \, \rho T s : = 2\beta = t_\tau \, Z^{-1} \, p \, \frac{s}{R} \qquad \text{(III.10)}$$

is introduced.

Before equation (III.9) is discussed in greater detail, its corresponding traditional continuum mechanics relationship should be offered for comparison. These Navier-Stokes equations, as generalized notations of the set of field equations for $v(\mathbf{r},t)$, $T(\mathbf{r},t)$, $p(\mathbf{r},t)$ and $\rho(\mathbf{r},t)$, are defined by its viscous stress tensor:

$$\tau : = 2\mu D + \left(\eta_v - \frac{2}{3} \mu \right) \delta \; \nabla \cdot v \qquad \text{(III.11)}$$

Perhaps the clearest interpretation of this equation is found in Truesdell (1984, pp. 426-427 & 409-410). In this case, D is the deviator which is the symmetrical share of the (tensorial) velocity gradient ∇v in symmetrical stress tensors; μ and η_v are the fluid's shear or volume viscosity respectively. C. Truesdell offers convincing reasons why the known Stokes relation (i.e. $\eta_v \equiv 0$) is valid.

At first glance one notes that the expression (III.9) for the compressible fluid's viscous stress tensor τ is considerably more complicated than the formulation - equation (III.11) - for a Navier-Stokes fluid. The structure of equation (III.9), with its characteristic Nabla operators (which have multiple effects on the local specific entropy s of the fluid), contains the asymptotic limiting case

$$\lim_{\sigma \to 0} \tau = 0 \qquad \text{(III.12)}$$

allowing a physially satisfactory transition from friction-affected motion to a dissipation-free Euler flow. A serious and historically explicable defect of the Navier-Stokes equation of motion is its lack of this limit for each infinitesimal local entropy production density σ. The demand for such an asymptotic behaviour is closely related to Maxwell's principle of kinetic equilibrium. On the level of the Maxwell-Boltzmann gas kinetics, a flow field with gradients results as a solution to the Boltzmann equation when the collision operator disappears identically for all r and t. This case of kinetic equilibrium is asymptotically possible only for reversible processes in which all transfer current densities equal zero (see Truesdell, (ed.), p. 414).

Equation (III.9) contains not only one term (which cannot be generally neglected: see Straub, 1988, p. 123) for the unsteady changes of the specific entropy s. In addition, the divergence of the entropy flow vector j_s also appears, which through

$$j_s = T^{-1} \dot{q} + \sum_k s_k j_k - (RZ\rho)v \qquad \text{(III.13)}$$

is related not only to the heat flow density $\dot{q}$ and a convective term, but to the diffusion flow density j_k as well. The latter is weighted by the partial specific entropy s_k of all the polynary single-phase system's components. This divergence term in an expression for a second order tensor τ apparently contradicts the Curie principle. It is a constitutive part of the linear Irreversible Thermodynamics and postulates without proof: even and odd order tensors may not appear together in an equation for continuum mechanics. C. Truesdell vehemently polemicized against this "principle" (Truesdell, 1984, pp 387-391). He not only traced its rather dubious origin, but criticized above all its mathematical ambiguity. Equation (III.9) offers an example of the problems encountered with the principle: from divergence of vectors $\dot{q}$ and j_k ($k = 1(1)K$) follow two scalars. They are tensors of even order zero, whose occurrence together with the viscous stress tensor by no means contradicts the Curie principle. Otherwise the coupling of all transfer processes conforms with all physical experiences; this is not reflected, however, in the Navier-Stokes equation of motion (see Moore, 1964, p. 192).

This is probably because its "deduction" fails to take simultaneously occuring transfer processes into consideration. Such a restriction is consequent, however, for an artificial construction such as an incompressible model fluid. If one accepts the known incompatibility of this theoretical fluid with the thermodynamics of real materials, one is compelled to acknowledge that concepts such as temperature, entropy, heat flow density, etc. are not, strictly speaking, compatible. Taking this circumstance into consideration and assuming $\beta = \mu$ for the shear viscosity μ, it is notable that the Navier-Saint Venant motion equation (III.9) for an incompressible model fluid ($\nabla \cdot \mathbf{v} \equiv 0$) contains the Navier-Stokes motion equation as a "pathological" limiting case (see Straub, 1988, pp. 141-144).

Seen from the standpoint of the AT, a notable conclusion can be made: for an incompressible fluid with constant shear viscosity μ, the Navier-Stokes equation of motion, together with the incompressibility condition

$$\nabla \cdot \mathbf{v} \equiv 0 \qquad \text{(III.14)}$$

and the compatible initial boundary constraints, represent a complete set of equations. The solution - flow velocity **v** and pressure p dependent on location **r** and time t - is parametrically dependent only on the kinematic viscosity $\nu = \mu/\rho$ = constant (and, additionally, on the parameters fixed by the initial and boundary constraints); to a certain extent individualizes the incompressible fluid with a number for comparison.

In reality things look completely different: for all compressible fluids the new quantity β (a physically corresponding function of μ) - equation (III.10) - is normally a function of state, provided the proportionality coefficient t_τ is either a constant or a known function of the density ρ, the mass fraction ω_k and temperature T. In the latter case this characteristic time t_τ is a property of state like the pressure p, the compressibility factor Z and the absolute specific entropy s of the polynary single-phase system.

Even simple examples, however, lead one to expect that this coefficient β is more likely to be dependent on the class of given flows (for example, a shear flow under certain constraints such as constant shear and isothermal fluid) than on the material properties (see Straub 1988, section 5.2). It is evident that this difficulty raises questions about conventional viscosity concepts. This is not the place, however to present an answer to this problem, particularly since other authors have already made some pertinent attempts (see, for example, Nettleton 1987). If necessary, there are no theoretical objections against accepting t_τ as an empirical coefficient for the present.

Generally speaking, one arrives at an interesting conclusion: **the Navier-Stokes equation of motion can be substantiated only for incompressible model fluids; for real compressible materials, one can only define it as addressed by Truesdell [9].**

It is understandable that the Navier-Saint Venant equation of motion at present cannot be used for actual projects.

Currently available numerical procedures and computers are still too inefficient to handle the work. Therefore it is appropriate to search for a first non-trivial approximation of equation (III.9). The answer naturally depends on which approximations one can agree upon.

The gas kinetics fundamentals of non-uniform and thermally-perfect gases lead one to the conclusion that the most important prerequisite for a decisive simplification of the problem, the inequation

$$\nabla T/T \ll 1, \qquad \text{(III.15)}$$

may be valid for the profiles of local temperatures. In equation (III.15) ∇T relates to the absolute value of the local temperature gradients. If one ignores extreme cases, the condition (III.15) is still fulfilled within the linear dimensions of the order of magnitude $(V_m/N_A)^{1/3} \simeq 33$ Å [6]. This means that in most practical cases there are no relevant limitations.

In these cases, both Navier-Saint Venant equation of motion (III.9) and the energy field equation can be simplified further in the form:

$$c_v \rho DT = -p\nabla \cdot v - \nabla \cdot \dot{q}_F + 1/2\, \mu_M (\nabla \cdot v)^2 \qquad \text{(III.16)}$$

$$\rho D\mathbf{v} = \rho f - \nabla p_v \qquad \text{(III.17)}$$

$$p_v :\,= p - 1/2\mu_M\, \nabla \cdot v \qquad \text{(III.18)}$$

$$\mu_M :\,= t_\tau p \qquad \text{(III.19)}$$

$$p = RT\rho \qquad \text{(III.20)}$$

The same can be done with the field equations of the mass fractions not shown here.

Equation (III.17) agrees formally with the Euler equation of motion. Yet the pressure p_v by no means corresponds with the thermodynamic pressure p according to equation (III.20). Equation (III.17) describes dissipative processes and can, like the Navier-Stokes equation of motion, fulfill no-slip boundary conditions. Analogies due to numerical viscosity effects obviously are the reason why the Euler equations of motions have recently been so successfully applied in industry for simulating real flows.

An equation of motion of the Euler type (and not the Navier Stokes equation of motion!) is thus a first step toward describing real flow fields of compressible fluids. All field properties such as velocity v, specific field force f, mass density ρ, pressure p, and temperature T are clearly defined by the Gibbs Fundamental Equation and related to one another.

If one accepts for $\dot{q}_F$ the known proportionality to ∇T according to the First law of Fourier

$$\dot{q}_F := -\lambda \nabla T = -\nabla \cdot [c_v \mu_M f \nabla T]. \qquad (III.21)$$

that is equivalent to assume steady transfer processes (see Straub et al. 1987) in connection with the Fourier heat flow vector $\dot{q}_F$. The coupling of heat conductivity λ with the Maxwell viscosity (analog to the known gas kinetic relationship $\lambda = f c_v \eta$ between λ and the dynamic viscosity η of non-uniform gases [6] allows further simplification of equations (III.16) and (III.17), assuming continued constant material data. If one adds the well-known relations

$$c_v/R = (\kappa - 1)^{-1}; \ \Omega := p/\rho = RT \qquad (III.22)$$

for perfect gases and ignores the quadratic $\nabla \cdot v$ term in equation (III.16) as well as the field force term in equation (III.17), then these two equations are immediately transformed - taking equation (III.15) into account (see Straub, 1988, p.148) - into the forms

$$D\Omega = -(\kappa - 1)\ [\Omega\ \nabla \cdot v - 1/2 \nu_M\ \nabla \cdot \nabla\ \Omega]\ \ \kappa := c_p/c_v \qquad (III.23)$$

$$D_{\mathbf{v}} = -\nabla\Omega + 1/2\ \nu_M\ \nabla(\nabla \cdot v)\ ;\ \ \nu_M := \mu_M/\rho\ . \qquad (III.24)$$

They are of particular interest because they contain only two dependent variables - flow velocity **v** and the scalar potential Ω, which with constant material data can also be easily connected with the special enthalpy of a perfect gas - as well as two parameters κ and ν_M. To solve them, one needs suitable initial and boundary conditions, but not the continuity equations: the latter can subsequently be used, when fields $\Omega(\mathbf{r}, t)$ and $\mathbf{v}(\mathbf{r},t)$ are established to calculate the density field $\rho(\mathbf{r},t)$.

IV. DERIVATION OF EQUIVALENT NAVIER-STOKES EQUATION ON THE BASIS OF THE BOLTZMANN EQUATION

In this section, we shall summarize the classical kinetic theory of transport properties developed by Chapman and Enskog [8]. Particularly, we shall demonstrate that the first order approximation is equivalent to the Navier-Stokes equation of fluid flow as well as gasdynamics.

IV.1. The Boltzmann Equation and the Equation of Transport

Let us define the local distribution function for the gas, $f(\vec{v},\vec{r},t)$, such that

$$f(\vec{v},\vec{r},t)\, d\vec{v}\, d\vec{r} \tag{IV.1}$$

represents the number of particles having velocity $\vec{v}$, $\vec{v} + d\vec{v}$ at position $\vec{r}$, $\vec{r} + d\vec{r}$ at time t. The local distribution function is a function of the macroscopic properties such as number density, mean velocity and temperature. Thus, the rate of change of the distribution function $f(\vec{v},\vec{r},t)$ at a specific position $\vec{r}$ and time t by considering a gas is subject to an external force $m\vec{F}$, which may be a function of $\vec{r}$ and t but not of $\vec{v}$. Between the time t and t + dt, the velocity $\vec{v}$ of any molecule which does not collide with another, changes to $\vec{v} + \vec{F}dt$, and its position-vector $\vec{r}$ will change to $\vec{r} + \vec{v}dt$. There are $f(\vec{v},\vec{r},t)d\vec{v}d\vec{r}$ molecules which at time t lie in the volume-element $\vec{r}, d\vec{r}$, and have velocities in the range $\vec{v}$, $d\vec{v}$. After the interval dt, if the effect of collisions could be neglected, the same molecules, and no others, would compose the set that occupy the volume $\vec{r} + \vec{v}dt$, $d\vec{r}$, and have velocities in the range $\vec{v} + \vec{F}dt$, $d\vec{v}$, the number in this set is:

$$f(\vec{v} + \vec{F}dt,\ \vec{r} + \vec{v}dt,\ t + dt)\ d\vec{v}d\vec{r}.$$

On dividing by $d\vec{v}d\vec{r}dt$, and making dt tend to zero, Boltzmann's equation for the distribution function f is obtained.

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \frac{\partial f}{\partial \vec{r}} + \vec{F} \cdot \frac{\partial f}{\partial \vec{v}} = \frac{\partial_e f}{\partial t} \tag{IV.2}$$

The quantitiy of $\frac{\partial_e f}{\partial t}$ defined above is equal to the rate of the change, owing to encounters in the velocity-distribution function of f at a fixed point. It will appear that $\frac{\partial f_e}{\partial t}$ is expressible as an integral involving the unknown function f:

$$\left(\frac{\partial_e f_1}{\partial t}\right)_2 = \iint \left(f'_1 \; f'_2 - f_1 f_2\right) k_{12} d\vec{k} \; d\vec{v}_2 \tag{IV.3}$$

with $k_{12}d\vec{k}$ the collision parameters.

Another important equation may be derived from Boltzmann's equation which give the connection between the molecular velocity distribution and conservation laws of fluid dynamic equations.

Let ϕ be any molecular property as defined by:

$$\bar{\phi} = \frac{1}{n} \int \phi f d\vec{v} \tag{IV.4}$$

with n being the number density of molecules and mass the density given by nm, with m being the mass of a molecule.

Multiply Boltzmann's equation by $\phi d\vec{v}$ and integrate throughout velocity-space; it is assumed that all the integrals obtained are convergent, and that products such as ϕf tend to be zero and v tends to infinity in any direction (i.e., $-\infty$, $+\infty$). The result may be written as,

$$\int_{-\infty}^{\infty} \phi \left(\frac{\partial f}{\partial t} + \vec{v} \cdot \frac{\partial f}{\partial \vec{r}} + \vec{F} \cdot \frac{\partial f}{\partial \vec{v}}\right) d\vec{v} = n\Delta\bar{\phi} \tag{IV.5}$$

where

$$n\Delta\bar{\phi} \equiv \int \phi \frac{\partial_e f}{\partial t} d\vec{v} \tag{IV.6}$$

and the integration limits are from $-\infty$ to $+\infty$. The physical significance of $\Delta\phi$ is the measure of the rate of change in the molecular property with velocities in the range of $\vec{v}$, $d\vec{v}$ per unit volume at $\vec{r}$, t, owing to encounters.

From Eq. (IV.5), we obtain

$$\int \phi \frac{\partial f}{\partial t} d\vec{v} = \frac{\partial}{\partial t} \int \phi d d\vec{v} - \int f \frac{\partial \phi}{\partial t} d\vec{v} = \frac{\partial n\bar{\phi}}{\partial t} - n \overline{\frac{\partial \phi}{\partial t}} \tag{IV.7}$$

$$\int \phi\vec{v} \cdot \frac{\partial f}{\partial \vec{r}} = \frac{\partial}{\partial \vec{r}} \cdot \int \phi\vec{v} f d\vec{v} - \int f\vec{v} \cdot \frac{\partial \phi}{\partial \vec{r}} d\vec{v} = \frac{\partial}{\partial \vec{r}} \cdot \overline{n\phi\vec{v}} - n\vec{v} \cdot \frac{\partial \phi}{\partial \vec{r}} \tag{IV.8}$$

$$\int \phi \frac{\partial f}{\partial \dot{v}}\, d\dot{v} = \iint [\phi f]_{u=-\infty}^{u=\infty}\, dvdw - \int f \frac{\partial \phi}{\partial \dot{v}}\, d\dot{v} = -n \frac{\ddot{\partial}\dot{\phi}}{\partial \dot{v}} \qquad \text{(IV.9)}$$

Substituting these results into Eq. (IV.5) we obtain the transport equation:

$$\frac{\partial n\ddot{\phi}}{\partial t} + \frac{\partial}{\partial \dot{r}} \cdot \overline{n\ddot{\phi}\dot{v}} - n \left\{ \frac{\ddot{\partial}\ddot{\phi}}{\partial t} + \dot{v} \cdot \frac{\partial \phi}{\partial \dot{r}} + \dot{F} \cdot \frac{\ddot{\partial}\ddot{\phi}}{\partial \dot{v}} \right\} = n \triangle \phi \qquad \text{(IV.10)}$$

This equation could be expressed in terms of a peculiar velocity, $\dot{C} = \dot{v} - \dot{c}_0$, with $\dot{c}_0$ being the center of mass velocity. With proper mathematical manipulation, we obtain the transport equation in terms of the peculiar velocity:

$$\frac{D}{Dt} n\ddot{\phi} + n\ddot{\phi} \frac{\partial}{\partial \dot{r}} \cdot \dot{c}_0 + \frac{\partial}{\partial \dot{r}} \cdot \overline{n\phi\dot{c}} - n \left\{ \frac{\ddot{D}\ddot{\phi}}{Dt} + \dot{c} \frac{\ddot{\partial}\ddot{\phi}}{\partial \dot{r}} + \left(\dot{F} - \frac{D\dot{c}_0}{Dt} \right) \cdot \frac{\ddot{\partial}\ddot{\phi}}{\partial \dot{c}} \right.$$

$$\left. - \frac{\ddot{\partial}\ddot{\phi}}{\partial \dot{c}} \dot{c} \quad \frac{\partial}{\partial r} \dot{c}_0 \right\} = n \triangle \ddot{\phi} \qquad \text{(IV.11)}$$

with $\frac{D}{Dt}$ being the substantial derivative, which is given by

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \dot{c}_0 \cdot \frac{\partial}{\partial \dot{r}} \qquad \text{(IV.12)}$$

The transport equation (IV.11) is used for the bridge to connect the microscopic theory to the continuum (fluid) theory.

IV.2. Conservation Laws of Fluid Flow: Special Forms of the Equation of Change of Molecular Properties.

The conventional form of the governing equations of fluid flow could be obtained from the transport equation by assigning the proper form of the molecular property ϕ.

Case I. Let $\phi = 1$, $\phi\dot{c} = 0$, $\frac{\partial \phi}{\partial \dot{c}} = 0$, $\frac{D\phi}{Dt} = 0$, $\frac{\partial \phi}{\partial \dot{r}} = 0$, $\triangle\ddot{\phi} = 0$.

Thus Eq. (IV.11) becomes

$$\frac{Dn}{Dt} + n \frac{\partial}{\partial \dot{r}} \cdot \dot{c}_0 = 0, \qquad \text{(IV.13)}$$

This is the equation of continuity.

Case II. Let $\phi \equiv m\vec{C}$; then $\overline{\phi} = 0$, $\overline{n\phi\vec{c}} = \overline{n\vec{c}\vec{c}} = \Pi$ (i.e. pressure tensor), $\dfrac{\partial\phi}{\partial\vec{r}} = 0$, $\dfrac{D\phi}{Dt} = 0$, $\dfrac{\partial\phi}{\partial\vec{c}} = (m)$, $\dfrac{\partial\phi}{\partial\vec{c}} = 0$, $\Delta\overline{\phi} = 0$.

Hence, Eq. (IV.11) becomes

$$\rho \frac{D\vec{c}_0}{Dt} = \frac{\partial}{\partial\vec{r}} \cdot \Pi - \delta\vec{F}, \ldots \qquad \text{(IV.14)}$$

This momentum equation at the lowest order corresponds to the Maxwellian distribution function which will lead to the momentum equation for inviscid flow. The next higher order will lead to the Navier-Stokes equation for both compressible and incompressible flow.

Case III. Let $\phi = E = \frac{1}{2} m\vec{C}^2$, then $\overline{\phi} = \frac{3}{2} nkT$, $\overline{n\phi\vec{c}} = \vec{q}$ (i.e. heat flux), $\dfrac{\partial\phi}{\partial\vec{r}} = 0$, $\dfrac{D\phi}{Dt} = 0$ and, since E depends on $\vec{c}$ only through the contribution of the kinetic energy of translation, $\dfrac{\partial\phi}{\partial\vec{c}} = m\vec{c}$; thus $\dfrac{\partial\phi}{\partial\vec{c}} = 0$, and $n \dfrac{\partial\phi}{\partial\vec{c}} \vec{c} = \overline{\rho\vec{c}\vec{c}} = \Pi$. Since $\Delta\overline{\phi} = 0$, the transport equation becomes,

$$\frac{DT}{Dt} = -\frac{2}{3nk} \left\{ \Pi \, \frac{\partial}{\partial\vec{r}} \vec{c}_0 + \frac{\partial}{\partial\vec{r}} \cdot \vec{q} \right\}, \qquad \text{(IV.15)}$$

this is the energy equation.

IV.3. Maxwellian Velocity Distribution

Consider a simple gas whose molecules are spherical, possesses only energy of translation, and is subject to no external forces. If its state is uniform:

$$\frac{\delta f}{\delta t} = 0 = \iint (f'f_1 - ff_1)\ k_1 d\vec{k} d\vec{c}_1$$

$f'f_1 = ff_1$ Detailed balancing (i.e. at statistical equilibrium)

$$\log f' + \log f_1' = \log f + \log f_1$$

This shows that log f is a summational invariant for encounters. Thus, it must be a linear combination of the three summational invariants (conservation laws):

$$\log f = \Sigma\, \alpha^{(i)}\, \psi^{(i)}$$
$$= \alpha^{(1)} + \alpha^{(2)} \cdot m\vec{c} - \alpha^{(3)} \frac{1}{2} mc^2 .$$

The form of the Maxwellian distribution is

$$f = \alpha^{(0)}\, e^{-\alpha^{(3)} 1/2\ mc^2},$$

$$\log f = \alpha^{(1)} + m\left(\alpha_x^{(2)} u + \alpha_y^{(2)} v + \alpha_z^{(2)} w\right) - \frac{\alpha^{(3)}}{2} m(u^2+v^2+w^2)$$

$$= \log\alpha^{(0)} - \alpha^{(3)} \left\{ \underbrace{\left(u - \frac{\alpha_x^{(2)}}{\alpha^{(3)}}\right)}_{c_x'} + \underbrace{\left(v - \frac{\alpha_y^{(2)}}{\alpha^{(3)}}\right)}_{c_y'} + \underbrace{\left(w - \frac{\alpha_z^{(2)}}{\alpha^{(3)}}\right)^2}_{c_z'} \right\}$$

$$c' = c - \frac{\alpha^{(2)}}{\alpha^{(3)}}$$

By definition

$$n = \int f d\vec{c} = \alpha^{(0)} \int e^{-\alpha^{(3)} 1/2\ mc^{2\prime}}$$

$$= \alpha^{(0)} \int_0^\infty c^{2\prime} e^{-\alpha^{(3)} 1/2\ mc^{2\prime}} dc' \int_0^\pi \sin\theta d\theta \int_0^2 d\phi\ .$$

$$= \alpha^{(0)} \left(\frac{2\pi}{m\alpha^{(3)}}\right)^{3/2}$$

$$n\dot{c}_0 = \int \dot{c} f d\dot{c}$$

$$= \int \left(\frac{\alpha^{(2)}}{\alpha^{(3)}} + \dot{c}'\right) f \; d\dot{c}'$$

$$= n \frac{\dot{\alpha}^{(2)}}{\alpha^{(3)}} + \alpha^{(0)} \underbrace{\int e^{-\alpha^{(3)} 1/2mc'^2} \dot{c}' d\dot{c}'}_{0}$$

$$\dot{c}_0 = \frac{\dot{\alpha}^{(2)}}{\alpha^{(3)}}$$

$$f = \alpha^{(0)} e^{-\alpha^{(3)} 1/2mc^2} = n \left(\frac{m\alpha^{(3)}}{2\pi}\right)^{3/2} e^{-\alpha^{(3)} 1/2mc} \qquad \text{(IV.16)}$$

Using,

$$\frac{3}{2} kT = \frac{1}{2} \overline{mc^2} = \frac{m}{2n} \int c^2 f d\dot{c}$$

$$= \frac{m}{2} \left(\frac{m\alpha^{(3)}}{2\pi}\right) \int c^2 \; e^{-\alpha^{(3)} 1/2mc'^2} \; d\dot{c}$$

$$= \frac{3}{2\alpha^{(3)}}$$

we obtained $\alpha^{(3)} = \frac{1}{kT}$, thus Eq (IV.16) becomes

$$f = n \left(\frac{m}{2\pi kT}\right)^{3/2} e^{-\frac{mc^2}{2kT}}$$

This is the Maxwellian distribution. It is well-known [10,11] that gas has Maxwellian distribution, it corresponds to a non-dissipative state which is equivalent to the Euler equation of motion of fluid dynamics.

IV.4. Remarks

It should be noted that this formalism for the derivation of conservation laws is only valid for the dilute gas, because of the limited treatment of the Boltzmann collisional integral, in which only the binary collisions are considered. However, this formalism does not give us a clear track to chase these physical processes as expressed in kinetic theory. For example, the gas behavior follows a Maxwellian distribution; with it lowest order it leads to the Euler equation of motion, whereas the next higher order behavior of the gas leads to the Navier-Stokes equation of motion. A summary of these comments is depicted in the Table below.

Parallelism Between Gasdynamical and Radiative Aspects Under Various Approximations

Order of Approximation	Description	Distribution function f		Equation for the Description		Mechanism
		Gasdynamics	Radiative Problem	Gasdynamics	Radiative Problem	
Zeroth	At complete thermodynamic equilibrium. System is steady homogeneous.	Maxwellian with T = const. $f^{(o)}$	Boltzmann distribution for internal levels and Saha distribution ionization state	No motion	Constant flux	Collison dominant $S_\nu = B_\nu(T)$
First	Local-Thermodynamic-Equilibrium	Local Maxwellian where $T = T(r,t)$ $n = n(r,t)$ $u - u(r,t)$	Local Boltzmann and Saha distribution Radiation field is planck	Euler's Equation	Finite flux	Collision dominant $S_\nu = B_\nu\,[T(\dot{r},t)]$
Second	Non-LTE	$f = f^{(o)}(1+\Phi)$	Boltzmann and Saha distribution is no longer valid	Navier-Stoke's Equation	Radiative Transfer Equation Equation	Collision dominant $S_\nu = B_\nu\,[T_e(\dot{r},t)]$
Higher Order Approximation	Multicomponent gas mixture at Non-LTE	$f_s' = f_s^{(o)}(1+\Phi_s)$	Should calculate the population of levels by rate equation	Modified Navier-Stoke's Equation	Radiative Transfer Equation with $S_\nu = \frac{\epsilon_\nu}{K_\nu}$ $= \frac{\text{Emissivity}}{\text{Absortivity}}$	

V. PRIGOGINE'S NON-EQUILIBRIUM THERMODYNAMICS: CONSERVATION LAWS*

It has been understood that the description of a "mechanical system" is in terms of the coordinates and momenta of the molecules, or in terms of its wave function. However, such a description, when applied to systems of interests in chemical physics and fluid dynamics such as combustion chamber flow, leads to great practical and conceptual difficulties, because it is impossible to say 10^{23} molecules in a macroscopic system. In order to remedy these difficulties, the combined thermodynamic and fluid dynamic methods are used to provide us with a "reduced description," as pointed out by Prigogine, "simplified language" with which to describe macroscopic systems. In this chapter, we shall briefly summarize Prigogine's concept through the derivation of conservation laws and balance equations which are equivalent to the equation of motion of combustion chamber flows being used for current CFD simulation.

Let us consider a system of volume V limited by the surface Ω. We wish to follow the time change of the intergral

$$I(t) = \int f dV \qquad (V.1)$$

This intergral is extended over the volume V of the system we are interested in. The surface Ω is assumed to be at rest. In the terminology usually adopted in thermodynamics, I(t) is an extensive quantity. For instance, it may be the mass or the energy of the system. On the contrary, f(x, y, z, t)is an intensive quantity, which does not depend on the system as a whole. It corresponds to the volume density associated to I and may be represented by the functional derivative

$$f \equiv \frac{\delta I}{\delta V} \qquad (V.2)$$

The change can be expressed by

$$\frac{\partial I}{\partial t} = P[I] + \phi[I] \qquad (V.3)$$

---

*The materials presented in this chapter are based on a text book entitled <u>Thermodynamic Theory of Structure, Stability and Fluctuations</u>, by P. Glansdorff and I. Prigogine; Wiley-Interscience, 1971.

The first term on the r.h.s. corresponds to the production per unit time of the quanity I inside the volume V. It can be written as a volume intergral

$$P[I] = \int \sigma[I]dV \tag{V.4}$$

where $\sigma[I]$ denotes the source of I per unit time and unit volume.

The second term in the r.h.s. of (V.3) represents the flow of the quantity I through the boundary surface Ω. It can be written as a surface intergral

$$\Phi[I] = \int j_n[I]d\Omega \tag{V.5}$$

This formula introduces the density of flow $j[I]$ associcated with I; $j_n[I]$ is its projection along the inside normal to the surface. For simplicity, we shall also use the term flow instead of density flow (or current, or flux). From equations (V.4) and (V.5) we obtain the so-called balance equation corresponding to the extensive variable I as:

$$\frac{\partial I}{\partial t} = \int \sigma[I]dV + \int j_n[I]d\Omega \tag{V.6}$$

It is sometimes useful to write the balance equation (V.3) or (V.6) in the symbolic form

$$dI = d_iI + d_eI \tag{V.7}$$

where d_iI represents the source term and d_eI the flow term. One may write as well

$$d_iI = dI + (-d_eI) \tag{V.8}$$

In this form, we see that the source d_iI contributes on one side to the time change of I and on the other to the flow from the system to the outside world $(-d_eI)$. It must be emphasized that only dI is in general a total differential of the state variables.

Equality (V.6) has to be valid whatever the volume V. Therefore, the application of Green's formula gives us directly the balance equation in local form

$$\frac{\partial f}{\partial t} = \sigma[I] - \operatorname{div} j[I] \tag{V.9}$$

One of the advantages of this formulation is that all conservation equations can be expressed by the statement that the source term corresponding to a conserved quanity vanishes. For example, if I represents the total mass system on has

$$I = M$$

f becomes the mass density ρ

$$f = \rho$$

and conservation of mass is expressed by the relation

$$\sigma[M] = 0 \tag{V.10}$$

The time change of the density ρ is then, apart from the sign, equal to the divergence of the mass flow. Moreover, the mass flow is clearly

$$j[M] = \rho v \tag{V.11}$$

where v is the velocity of matter. Using (V.10) and (V.11), we therefore obtain the classical continuity equation

$$\frac{\partial \rho}{\partial t} + \operatorname{div} \rho v = 0 \tag{V.12}$$

Likewise, conservation of total energy U (first law of thermodynamics), and of total momentum Q (in the absence of external forces), may be expressed as

$$\sigma[U] = 0; \ \sigma[Q] = 0 \tag{V.13}$$

The source term for entropy S plays a special role as the second principle of thermodydnamics and postulates the inequality:

$$\sigma[S] \geq 0 \tag{V.14}$$

Entropy is not a conserved quanity, but increases as the result of irreversible processes included in the source term. It is only for reversible processes that the change of entropy is entirely due to entropy exchanges with the outside world.

Let us go back to the density of flow j[I] in the balance equation (V.9). In general, we are concerned not only with a convection flow such as (V.11) but also with a conduction flow j_{cond} (say), which occurs even in a system at rest. We have therefore

$$j = j_{cond} + j_{conv} = j_{cond} + fv \tag{V.15}$$

For example, the heat flow **W** is the conduction current associated with internal energy. We shall consider other examples later on in this chapter.

In many cases, it is useful to introduce the so-called substantial or hydrodynamic derivative

$$\frac{d}{dt} \equiv \frac{\partial}{\partial t} + \sum_i v_i \frac{\partial}{\partial x_i} \qquad (V.16)$$

The continuity equation (1.12) leads then to the equalities:

$$\rho \frac{d\phi}{dt} = \rho \frac{\partial \phi}{\partial t} + \sum_i \rho V_i \frac{\partial \phi}{\partial x_i} = \frac{\partial (\rho\phi)}{\partial t} + \sum_i \frac{\partial}{\partial x_i} (\rho V_i \phi) \qquad (V.17)$$

This relation may be applied to an arbitrary intensive variable $\phi(x,y,z,t) \equiv \phi(x_1,x_2,x_3,t)$.

A summary of these results are shown in Table IV. Table IV also provides a comparison with solutions from Straub's AT method.

The details for the derivation of conservation laws can be found in the book entitled "Thermodynamic Theory of Structure, Stability and Fluctuation" by Glansdorff and Prigogine (1971)[7].

VI. TRUESDELL'S RATIONAL THERMODYNAMICS: A CLASSICAL REPROACH

The approach taken by rational thermodynamics researchers is to seek concepts and principles sufficient to describe and calculate temperature fields in bodies subject to deformation and heating. Rational thermodynamics has pointed its attention at a process occuring in time, as opposed to the classical approach of Gibbs who has sought in statistical mechanics and from it has constructed a rational foundation for the statics of hotness, heat, and equilibrated forces. Recent applications of rational thermodynamics were the propagation of stress waves, the effects of severe deformation upon a body's ability to conduct heat and of heating, upon a body's response to stress and strain, and the nature of energetic and diffusive transfer, incident upon change of shape. Because such effects notoriously differ in bodies of different materials, an adequate theory must distinguish materials by constitutive properties, openly and explicitly stated. The constitutive function of a body must make it impossible for that body ever to violate the fundamental axioms of thermodynamics. The fundamental theory of rational thermodynamics is to reproach that the concepts and assumptions of the pioneers such as Kelvin, Clausius and Gibbs, selected and refined and extended, can be made the basis of a treatment that reflects simply the physics of heat and work and is not only rigorous, but also broad enough to cover irreversible processes in deformable continua.

The treatment of dissipative phenomena highlights the spirit of rational thermodynamics of Truesdell. In terms of describing fluid flows, rational thermodynamics rests upon some prior concepts of mechanics which may mean the ordinary theory of a deformable body. The concepts of mechanics were further extended to allow for diffusion and chemical reactions as well.

In developing a thermodynamic theory for deformable bodies, Truesdell starts with the classical theory of continua. Let a body B occupy a domain of space at each time t. These domains are its configurations. The mapping of one such domain or reference configuration K onto the present configuration is called the motion of B with respect to that configuration:

$$x = x_{\kappa}(X, t), \qquad -\infty < t < \infty. \qquad \text{(VI.1)}$$

Here x_{κ} is the mapping that carries the place X in the reference configuration K into the place x at time t. The places X identify the particles; thus we may speak of "the particle X" without fear of confusion. The velocity $\dot{x}$ is the rate of change of position of a particle:

$$\dot{x} \equiv \partial_t x_{\kappa}(X,t) = \dot{x}(x,t). \qquad \text{(VI.2)}$$

A mass, which is a non-negative measure M, is defined once and for all over measurable subsets of the body and is also assumed to be an absolutely continuous function of volume. Hence a non-negative mass-density $\rho(\cdot)$ exists almost everywhere at each time, and at points where it and the velocity field $\dot{\mathbf{x}}(\cdot)$ are sufficiently smooth

$$\dot{\rho} + \rho \operatorname{div} \dot{\mathbf{x}} = 0. \tag{VI.3}$$

The linear momentum $\mathbf{m}$ and rotational momentum $\Omega_{\mathbf{x}_0}$ of B in its present configuration are defined by

$$\mathbf{m} \equiv \int_B \dot{\mathbf{x}}\, dM, \qquad \Omega_{\mathbf{x}_0} \equiv \int_B (\mathbf{x} - \mathbf{x}_0) \wedge \dot{\mathbf{x}}\, dM, \tag{VI.4}$$

where $\mathbf{x}_0$ is a fixed place and where the integration is based on mass. Euler's laws of mechanics assert that for every body the time rates of change $\dot{\mathbf{m}}$ and $\dot{\Omega}_{\mathbf{x}_0}$ of these quantities are equal to the total force f and total torque $F_{\mathbf{x}_0}$ acting upon that body in its present configuration:

$$\dot{\mathbf{m}} = f, \qquad \dot{\Omega}_{\mathbf{x}_0} = F_{\mathbf{x}_0}. \tag{VI.5}$$

In the simplest kind of continuum mechanics, the force f is assumed to be the sum of two forces of special kinds: the total body force f_b and the total contact force f_c. The total body force is an absolutely continuous function of mass, while the total contact force is an absolutely continuous function of surface area:

$$\begin{aligned} f &= f_c = f_b\, , \\ &= \int_{\partial B} \mathbf{t}\, dA + \int_B \mathbf{b}\, dM. \end{aligned} \tag{VI.6}$$

The field $\mathbf{b}$, defined in the interior of B, is the body force per unit mass; it represents forces acting at a distance, e.g., those of gravitation and electromagnetism. The traction $\mathbf{t}$ represents the action of neighboring parts of material upon one another, or any forces applied in any way to the boundary ∂B of the body B in its present configuration. According to a theorem of Cauchy, the traction is delivered by the stress tensor $\mathbf{T}$:

$$\mathbf{t} \equiv \mathbf{T}\mathbf{n}, \tag{VI.7}$$

$\mathbf{n}$ being the outward unit normal to ∂B. By combining (VI.4), (VI.5), (VI.6), and (VI.7), on the assumption that the various fields occurring in those equations must be sufficiently smooth , it is easy to derive a local equivalent to the principle of linear momentum for continua:

$$\text{div } T + \rho\mathbf{b} = \rho\ddot{\mathbf{x}}, \tag{VI.8}$$

called Cauchy's first law of motion.

If we restrict attention to the case when all torques are moments of forces, and so

$$\mathbf{F}_{x_0} = \int_{\partial B} (\mathbf{x} - \mathbf{x}_0) \wedge \mathbf{t}\, dA + \int_{\partial B} (\mathbf{x} - \mathbf{x}_0) \wedge \mathbf{b}\, dM, \tag{VI.9}$$

then another theorem of Cauchy asserts that the stress tensor T is symmetric:

$$T = T^T \tag{VI.10}$$

This is Cauchy's second law of motion.

The kinetic energy K of B in the present configuration is defined by

$$K \equiv \frac{1}{2} \int_B \dot{x}^2\, dM, \tag{VI.11}$$

while the power P is the rate of working of all the forces acting on B:

$$P \equiv \int_{\partial B} \mathbf{t} \cdot \dot{\mathbf{x}}\, dA + \int_B \mathbf{b} \cdot \dot{\mathbf{x}}\, dM. \tag{VI.12}$$

Now, according to a simple theorem first proved by Stokes, the net working W at a time T on the body B is given by the difference of P, the mechanical power, and K, the kinetic energy, thus:

$$\begin{aligned} W &\equiv P - K, \\ &= \int_B w\, dV, \end{aligned} \tag{VI.13}$$

where

$$w = T \cdot \text{grad } \dot{x}, \tag{VI.14}$$

the dot indicating the inner product in the vector space of second-order tensors ($X \cdot Y \equiv \text{tr } (XY^T)$). The scalar w is the net working per unit volume; it is often called the stress power.

These few formulae provide a specfic mechanical framework upon which a structure of thermodynamics may be raised. Here, of course, all quantities are given in terms of time-dependent spatial fields, not merely functions of time alone, and so we cannot blindly apply the results of Lecture 1, but we may proceed in a parallel way. A number of things I shall say will be valid equally in more general kinds of mechanics, where a result of the form (VI.13) holds with a density w which is given by an expression more complicated than (VI.14), allowing, for example, for the action of couple stresses, but, so as to have a fully definite and explicit mechanical background.

The first law of thermodynamics, expressing the balance of energy is [9]:

$$\dot{E} = W + Q$$

where E is the internal energy of a body, W is the net working on it, and Q is its heating. This axiom we now set alongside Euler's laws (VI.5) as basic for all theories relating forces and energies to motions. Just as we have specialized Euler's laws by assuming (VI.6) so as to obtain forms appropriate to continuum mechanics, so also we may specialize the principle of balance of energy in a corresponding way. First of all, we take the net working W to be that calculated according to continuum mechanics and hence given by (VI.13) as an absolutely continuous, additive set function with density (VI.14). Parallel to the assumptions (VI.6) and (VI.9) regarding the resultant force and resultant torque, we lay down the assumption that the heating Q is the sum of the two heatings of special kinds: the body heating Q_b and the contact heating Q_c; the former being an absolutely continuous funcntion of mass, and the latter, an absolutely continuous function of surface area:

$$\begin{aligned} Q &= Q_c + Q_b, \\ &= \int_{\partial B} q \, dA + \int_B s \, dM. \end{aligned} \qquad \text{(VI.15)}$$

The volume density s is called the heating supply; the surface density q, the influx of heating. The two kinds of heating, Q_c and Q_b, are often said to describe conduction and radiation, respectively, but no such specific connotation need be made in general. Finally, the internal energy is assumed to be an absolutely continuous, additive set function:

$$E = \int_B \epsilon \, dM, \qquad \text{(VI.16)}$$

the density ϵ being called the specific internal energy or, for short, the energetic.

Under the assumption (VI.16), from [9] and (VI.15) Stokes

derived by Cauchy's method a result inferred earlier in a major special case by Fourier, namely, the influx of heating is delivered by the heating-flux vector **h**:

$$q = \mathbf{h} \cdot \mathbf{n}, \tag{VI.17}$$

n being the outward unit normal to ∂B. For sufficiently smooth fields, by (VI.17), (VI.16), (VI.15), (VI.14), and [9] it is easy to show by use of the divergence theorem and (VI.10) and (VI.8) that

$$\rho\dot{\epsilon} = w + \operatorname{div} \mathbf{h} + \rho s. \tag{VI.18}$$

This differential equation is sometimes regarded as a local statement of the "first law of thermodynamics", although in fact it is a consequence of a rather subtle sequence of field definitions along with Cauchy's laws of motion (VI.8) and (VI.10) as well as the general balance of energy [9]. Major special cases of this differential equation were derived, under various special hypotheses, by Fourier, Kirchhoff, and C. Neumann.

In the thermodynamics of homogeneous processes the axiom of irreversibility takes the form of the Clausius-Planck inequality [9]:

$$\theta H \geq Q,$$

where θ is the absolute temperature and H is the calory. We must now introduce the concepts of temperature and calory in continuum mechanics. The former offers no difficulty. The temperature θ is given by a positive-valued temperature field,

$$\theta = \theta(\mathbf{x},t) > 0, \tag{VI.19}$$

defined over the persent configuration of the body B. As in statistical mechanics, also in continuum mechanics the reciprocal of the temperature, which may be called the coldness J is often more convenient for the mathematical theory:

$$J \equiv \frac{1}{\theta}. \tag{VI.20}$$

It is natural to assume that the calory, like the internal energy, is an absolutely continuous function of mass:

$$H = \int_B \eta \, dM \qquad \text{(VI.21)}$$

The density η, which is usually called the specific entropy, I prefer to name the coloric. This name has the virtue of dragging a red herring across the path of those who lay down police-edicts concerning when and how "entropy" is to be "defined". As they back off in horror at revival of the long-dead caloric theory of heat, we can return to our concrete, mathematical theory, safe behind our two negations of authority.

Caloric is introduced to represent gross dissipation. While coloric may flow from place to place and thus increase or decrease locally, its total, the calory H, is subjected to a rule favoring increase. We may regard this vague statement as expressing the content of Clausius' assertion:

$$\dot{H} \geq 0 \quad \text{when} \quad Q = 0. \qquad \text{(VI.22)}$$

The pioneers of thermodynamics regarded this assertion as a general axiom, not restricted to any special type of body or process, but they were unable to implement it by mathematics such as to give it a concrete form. Their various "second laws" sound more like warnings or threats than principles of a rational science. In modern continuum mechanics, because (VI.15) holds, we may express Clausius' assertion thus: In a body B where conditions are so balanced that

$$\int_{\partial B} q \, dA + \int_B s \, dM = 0 , \qquad \text{(VI.23)}$$

the calory cannot decrease:

$$\int_B \dot{\eta} \, dM \geq 0. \qquad \text{(VI.24)}$$

(A body B is said to be in a "calorically isolated" or "insulated" configuration if $q = 0$ on ∂B while $s = 0$ in the interior of B. For such a body, of course, (VI.23) holds.) While this statement expresses some idea about irreversibility, it does not lead to a unique generalization of the Clausius-Planck inequality [9] to deformable bodies. In particular, since temperature does not appear in it, it affords no connection between the ideas of heat and temperature. In this lecture I shall motivate the principle now regarded by most of the presently productive theorists, though not by all, as being a correct dissipation inequality. To this end I shall present some simple aspects of dissipation in familiar examples.

The internal dissipation δ is defined as being the amount by which the increase of caloric multiplied by the temperature exceeds the local heating:

$$\delta \equiv \theta\dot{\eta} - \frac{1}{\rho}(\operatorname{div}\mathbf{h} + \rho s). \tag{VI.25}$$

While δ is defined in terms of the quantities associated with temperature and heat alone, the equation of energy balance (VI.18) permits us to interpret δ also as the amount by which the increase of caloric times temperature exceeds the increase of energetic not produced by working:

$$\delta = \theta\dot{\eta} - \left(\dot{\epsilon} - \frac{w}{\rho}\right). \tag{VI.26}$$

If we were to transfer to the local description the ideas that motivate the Clausius-Planck inequality [9], we should require that this increase be non-negative:

$$\delta \geq 0. \tag{VI.27}$$

We shall name (VI.27) the Planck inequality.[4] For reasons to appear later, we shall not impose it as an axiom. Instead, in the remainder of this report, we shall first calculate δ for the most familiar kinds of materials and then note some consequences that follow when indeed $\delta \geq 0$.

First, for the ideal gas of the Euler-Hadamard theory,

$$\mathbf{T} = -p\mathbf{1} \tag{VI.28}$$

and also [9],

$$\epsilon = \epsilon(v,\eta), \qquad p = -\partial_v\epsilon, \qquad \theta = \partial_\eta\epsilon,$$

where $v \equiv 1/\rho$. Hence by (VI.14) and (VI.3)

$$\frac{w}{\rho} = -\frac{p}{\rho}\operatorname{tr}(\operatorname{grad}\dot{\mathbf{x}}) = -p\dot{v}, \tag{VI.29}$$

and so by (VI.26)

$$\begin{aligned}\delta &= (\partial_\eta \epsilon)\dot{\eta} + (\partial_v \epsilon)\dot{v} - \dot{\epsilon},\\ &= 0. \end{aligned} \tag{VI.30}$$

Thus the internal dissipation of the ideal gas is always null. The same result holds for the general thermo-elastic material, which includes as a special case the ideal gas.

Consider now the linearly viscous fluid of the Navier-Stokes theory. For it, a viscous stress V is superposed on the Eulerian pressure:

$$T = -p1 + V. \tag{VI.31}$$

and this V is assumed to be a homogeneous, linear, isotropic function of the stretching D:

$$2D \equiv \operatorname{grad} \dot{x} + (\operatorname{grad} \dot{x})^T, \tag{VI.32}$$

and

$$V = \lambda(\mathrm{tr}D)1 + 2\mu D, \tag{VI.33}$$

the pressure p still being related to the internal energy by [9]. Hence by (VI.26)

$$\begin{aligned}\rho\delta &= V \cdot D,\\ &= \lambda(\mathrm{tr}D)^2 + 2\mu \,\mathrm{tr}\, D^2. \end{aligned} \tag{VI.34}$$

Thus the internal dissipation of the Navier-Stokes fluid is the working of the viscous stress **V**. The requirement $\delta \geq 0$ is standard in this theory. Moreover, it is imposed identically in D. That is, in the theory of viscous fluids we demand that the viscous stress shall never give out work in any motion we might imagine[5], but it may use up work, and generally it will. It is easy to show from (VI.34) that the condition $\delta \geq 0$ for all **D** is equivalent to the classical inequalities of Duhem and Stokes:

$$\mu \geq 0 \qquad 3\lambda + 2\mu \geq 0. \tag{VI.35}$$

The concept, described so far in Lecture 2 of [9] by Truesdell, contains the important aspects of rational thermodynamics and its application to fluid flows.

VII. Discussions and Concluding Remarks

In this study, we have surveyed a number of theories in connection to the description of combustion chamber flows. Particular attention was paid to the Falk-Ruppel theory of 'Gibbsian thermodynamics' and Straub's 'Alternative Theory' (AT) in addition to Prigogine's theory of 'Non-eqilibrium Thermodynamics', Truesdell's 'Rational Mechanics', and Boltzmann's 'Kinetic Equation'. Whenever possible, comparisons were made with the conventional Navier-Stokes equations and Straub's AT. Table I shows side by side the equations of motion from Navier-Stokes and Straub. Table II compares respective formulations of Falk-Ruppel and Straub. Wu's formalism, deduced from Boltzmann's kinetic equation, is compared with the classical Navier-Stokes equation in Table III. Finally, the comparison between Prigogine's non-equilibrium thermodynamics and Straub's AT is shown in Table IV.

A direct correspondence between Falk-Ruppel's theory and the Navier-Stokes equation could not be established at this time. However, Boltzmann's kinetic equation with certain constraints, extended by Wu's formalism, permitted the derivation of the classical Navier-Stokes equation.

During this investigation, no conclusive results could be established. However, some comments about the application of the classical Navier-Stokes equation to combustion chamber flows can be stated. Before addressing these comments, some important characteristics, which are fundamental in combustion chamber flows, are summarized below:

(i). Many species exist in the spray/combustion domain under wide ranging pressure and temperature conditions. These species could be present also in different phases. This identifies the combustion chamber flow as a multi-flow and multi-phase system.

(ii). During the combustion process the multi-species, multi-phase flows go through states of non-equilibrium thermodynamics, i.e. each species exhibits its own number density, temperature, and velocity.

(iii). Since the flow conditions follow non-equilibrium thermodynamic states, the associated chemical reactions will also observe non-equilibrium behavior.

With these specific flow characterisics in the combustion chamber, it is obvious that the classical Navier-Stokes equation becomes theoretically inadequate to describe the complex flow system. We realize that the modified Navier-Stokes equations are being used currently for combustion chamber flow simulations. But these modified equations have been derived on an 'ad hoc' basis. To illustrate the inadequacy of the present Navier-Stokes equation for combustion chamber flow modeling, we offer the following few comments without exhaustion:

(i). It is known that the Navier-Stokes (NS) equation is derived for a single-fluid flow. Although the NS equation has been extended to multi-fluids with multi-phases, the equation of state for ideal gases is used to describe this fluid system, which we all know is not the case.

(ii). As demonstrated by Wu [10, 11], the radiative gasdynamics flow under non-local thermodynamic equilibrium (non-LTE) conditions has led to a number of additional transport coeficients. These additional transport coefficients will have an effect on the momentum and energy transport. Such phenomena should be expected for combustion chamber flows.

(iii). If the momentum and energy transport were modified, the flow field will be changed also. Thus, it will affect the design and performance parameters of the combustion chamber.

From these remarks, it is obvious that the governing equations (usually called NS equations) deserve a great deal of attention to better understand and model the physics of the combustion chamber flow. Therefore, we conclude with the following recommendations:

(i). Investigate the potential connection between Falk-Ruppel's theory of Gibbsian thermodynamics and the Navier-Stokes equations.

(ii). Examine whether Straub's claim from his AT could contribute to the improvement of the modeling of combustion chamber flows.

(iii). Conduct a rigorous investigation for a conclusive comparison of the NS equations with the respective governing equations from the theories developed by Faulk-Ruppel, Straub, Prigogine, Truesdell and Boltzmann as extended and demonstrated by Wu [10, 11]. The outcome will establish a reliable foundation for the modeling of combustion chamber flows.

Table I. Comparison Between Classical N-S and Straub's AT

	N-S	AT
1	Assuming start point is Newton's law $\bar{F} = \frac{d\bar{p}}{dt}$	Assuming start point is Newton's law $\bar{F} = \frac{d\bar{p}}{dt}$
2	$\bar{p} = m\bar{v}$ → momentum	$\bar{p} = m\vec{v} + m\vec{\phi}$
3	$\frac{\vec{F}}{V} = \rho\frac{d\vec{v}}{dt}$	$\frac{\vec{F}}{V} = \rho\frac{d\bar{v}}{dt} + \frac{d\vec{\phi}}{dt}$
4	$\frac{\bar{F}}{V} = -\nabla p + \nabla\cdot\bar{\tau} + \rho\bar{f}$	$\frac{\bar{F}}{V} = -\nabla p + \nabla\cdot\bar{\tau} + \rho\vec{f}$
5	$\rho\frac{d\bar{v}}{dt} = -\nabla p + \nabla\cdot\bar{\tau} + \rho\bar{f}$	$\rho\frac{d\bar{v}}{dt} = -\nabla p + \nabla\cdot\bar{\tau} + \rho\bar{f} - \rho\frac{d\vec{\phi}}{dt}$
6	No change	$\rho\frac{d\bar{\phi}}{dt} = \frac{\partial\rho\vec{\phi}}{\partial t} + \nabla\cdot\rho\vec{\phi}\vec{v}$
7	No change	$\rho\frac{d\bar{v}}{dt} = -\nabla p + \nabla\cdot\vec{\tau} + \rho\bar{f} - \frac{\partial\rho\vec{\phi}}{\partial t} - \nabla\cdot\rho\vec{\phi}\vec{v}$
8	No change	assuming $\vec{\phi} = 1/2\ (\vec{i} - \vec{v})$, $\vec{i}$: impulse $\rho\frac{D\bar{v}}{Dt} = -\nabla p + \nabla\cdot\bar{\tau} + \rho\bar{f} + \frac{1}{2}\frac{\partial}{\partial t}(\rho\bar{v} - \rho\vec{i})$ $+ \nabla\cdot\rho\frac{1}{2}(\vec{v} - \vec{i})\vec{v}$
9	result $\rho\frac{D\bar{v}}{Dt} = -\nabla p + \nabla\cdot\bar{\tau} + \rho\bar{f}$	result $\rho\frac{D\bar{v}}{Dt} = -\nabla p + \nabla\cdot\bar{\tau}_s + \rho\bar{f} + \frac{1}{2}\frac{\partial}{\partial t}(\rho\bar{v} - \rho\vec{i})$ here $\bar{\tau}_s = \bar{\tau} + \frac{1}{2}\rho\vec{v}(\vec{v} - \vec{i})$
10		Remarks: 1. What does $\bar{\tau}_s$ mean? 2. How does one derive the expression $\bar{\tau}_s$ in AT?

Table II. Comparison Between Falk-Ruppel and Straub

	Falk-Ruppel Theory	Straub
1	Gibbsian Thermodynamics	Alternative Theory (AT)
2	Momentum $p = m \bar{v}$	Momentum $p = m\bar{v} + m\phi\,(\bar{r},\ s,\ \rho,\ w_k)$
3	No difference with Newton's Equation of Motion under certain assumptions.	There are differences with Newton's Equation of Motion i.e. an extra term $\frac{\partial}{\partial t}(\rho\phi)$
4		He got his "AT" from Falk's dynamics.
5	Entropy production is the central problem	He dealt with AT using the entropy production
6	Reference G. Falk-W. Ruppel Energy and Entropy(1976) Mechanics, Relativity, Gravitation (1977)	Reference D. Straub (1989) Thermofluiddynamics of Optimized Rocket Propulsions

Table III-A. Comparison Between Wu's Formalism and Classical Navier-Stokes Equation

Wu's Formalism [11]	Classical Navier-Stokes Equation
Equation of Motion/ Equation (6.5) of Wu $\rho\frac{\partial C_0}{\partial t} + \partial C_0\cdot\frac{\partial C_0}{\partial \ddot{r}}\cdot\Pi = \ddot{F}_{\substack{body\\force}}$ (1)	Equation of Motion/N-S Eq $\rho\frac{\partial \ddot{u}}{\partial t} + \rho\ddot{u}\cdot\frac{\partial \ddot{u}}{\partial \ddot{r}} = \ddot{F} - \frac{\partial}{\partial \ddot{r}}\cdot\left\{\rho\underset{\sim}{U} - \mu\left[\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}(\nabla\cdot\ddot{u})\underset{\sim}{U}\right] - \mu'(\nabla\cdot\ddot{u})\underset{\sim}{U}\right\}$
From Equation (6.7) of Wu $\Pi = \sum_j \Pi_j = nkT_0\underset{\sim}{U} - \sum_j \mu_j \overleftrightarrow{\frac{\partial C_0}{\partial \ddot{r}}} - \sum\mu_j\left(\frac{\partial}{\partial \ddot{r}}\cdot C_0\right)\underset{\sim}{U}$, At LTE $\beta_j = 0 \Rightarrow C_0 = \ddot{u}$ $\overleftrightarrow{\frac{\partial C_0}{\partial \ddot{r}}} = \overleftrightarrow{\frac{\partial \ddot{u}}{\partial \ddot{r}}}$ is the rate of shear tensor $= \left(\frac{\partial u_j}{\partial x_j} + \frac{\partial u_j}{\partial x_j}\right) - \frac{2}{3}(\nabla\cdot\ddot{u})\underset{\sim}{U}$ Thus (1) becomes $\rho\frac{\partial \ddot{u}}{\partial t} + \rho\ddot{u}\cdot\frac{\partial \ddot{u}}{\partial \ddot{r}} = \ddot{F}_{body} - \frac{\partial}{\partial \ddot{r}}\cdot\left\{\rho\underset{\sim}{U} - (\Sigma\mu_j)\left[\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}(\nabla\cdot\ddot{u})\underset{\sim}{U}\right] - (\Sigma\mu_j')(\nabla\cdot\ddot{u})\underset{\sim}{U}\right\}$ $\mu = \Sigma\mu_j \ , \quad \mu' = \Sigma\mu_j'$	
$\rho\frac{\partial \ddot{u}}{\partial t} + \rho\ddot{u}\cdot\frac{\partial \ddot{u}}{\partial \ddot{r}} = \ddot{F}_{body} - \frac{\partial}{\partial \ddot{r}}\cdot\left\{\rho\underset{\sim}{U} - \mu\left[\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}(\nabla\cdot\ddot{u})\underset{\sim}{U}\right] - \mu'(\nabla\cdot\ddot{u})\underset{\sim}{U}\right\}$	Identical to N-S

Table III-B. Comparison Between Wu's Formalism and Classical Navier-Stokes Equation - Continuity

Wu's Formalism [10, 11]	Classical Navier-Stokes
Wu's Formalism on the Basis of the Boltzmann Equation	Classical N-S Equation
Continuity	Continuity
Equation (6.4) of Wu $\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial \ddot{r}} \cdot (\rho C_0) = 0$	$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial \ddot{r}} \cdot (\rho \ddot{u}) = 0.$
Eq. (2.22) $C_0 = \frac{1}{\rho} \sum_j \rho_j \ddot{u}_j$	
(2.24a) $\ddot{u}_j = C_0 + \beta_j$	
If all the species have the same velocity, namely at LTE.	
$\Rightarrow \beta_j = 0$	
$\ddot{u}_j = \ddot{C}_0$	
$\rho C_0 = \Sigma_j \rho_j \ddot{u}_j = (\Sigma \rho_j) \ddot{u} = \rho \ddot{u}$	
$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial \ddot{r}} \cdot (\rho \ddot{u}) = 0.$	$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial \ddot{\rho}} \cdot (\rho \ddot{u}) = 0.$

Table IV. Comparison Between Prigogine's Non-Equilibrium Thermodynamics and Straub's AT

	PRIGOGINE	STRAUB
1	$\rho \frac{D\dot{v}}{Dt} = \rho\dot{f} - \nabla (p\dot{s} - \dot{\tau})$	$\rho \frac{D\dot{v}}{Dt} = \rho\dot{f} - \nabla(p\dot{\delta}-\dot{\tau}) + \frac{1}{2}\frac{\partial}{\partial t}(\rho\dot{v}-\rho\dot{i})$
2	Micro theory (non-equilibrium statistical) (A) Starting at Liouville Equation (B) Parallel to quantum Mechanical method	AT is based on Prigogine's micro theory, but he referred only to Prigogine's book "Chemical Thermodynamics" in which the micro-theory was not involved.
3	What remains unclear in Boltzmann's derivation is the range of validity of his equation.	The macroscopic laws must be throroughly revised according to Prigogine's results. Justifying them with the Boltzmann equation is untenable.
4	In chemical thermodynamics, he described the entropy production.	He used the entropy products in his AT.
5	References: 1. Prigogine (1962) Non-equilibrium Statistical Mechanics 2. Prigogine (1964) Chemical Thermodynamics 3. Glansdorff and Prigogine (1971) Thermodynamic Theory of Structure, Stability and Fluxation	Reference: D. Straub (1989) Thermofluiddynamics of Optimized Rocket Propulsions

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APPENDIX I

Meeting Minutes

Gibbsian Thermodynamics

On January 9 to 14, 1991 Professor Wolfgang Ruppel from the University in Karlsruhe/Germany visited UAH and MSFC to present and discuss a new concept he defines as "Gibbsian Thermodynamics." This concept has been proposed in two books with Prof. Falk and Prof. Ruppel as authors, written in German and entitled Energy and Entropy and Mechanics, Relativity, Gravity.

Professor Ruppel familiarized us with the novel Gibbsian Concept, and he pointed out the simplicity of the new concept as well as many advantage associated with this approach.

The concept was accepted in its abstract formulation, but questions with respect to some applications were not resolved. Prof. Ruppel will give us his answer shortly, after he has looked at the problems from the different points of view presented at the meetings.

In general, the new concept appears to be superior to the classical thermodynamics approach. The presentations and discussions have only covered a limited number of topics due to the limited time available. It also takes time to comprehend this new approach. However, a dialog has been initiated and should be continued. A translation of the two books in question or a new report, which is oriented to the evaluation of existing equations of motion, will be of advantage.

APPENDIX II

Workshop Report

Thermo-Fluid-Dynamics Processes in Rocket Thrust Chambers

The workshop was held at the Mechanical Engineering Department of The University of Alabama in Huntsville from November 11 - 15, 1991 in Engineering Building Room 102. The principal investigator for the MSFC contract is Prof. S. T. Wu.

This workshop addressed two topics: (a) thermodynamic equilibrium calculation for rocket engines, and (b) critique of the Navier-Stokes equation, which are discussed in reference (6) by Prof. Straub.

(a) Both, the NASA ODE program and the Munich Method code carry now an option to consider finite area combustion effects. The solution process in both approaches is based on the identified Lagrange function, and the predictions are close. The claimed preference of the maximization of entropy over the minimization of energy was not accepted. Although comments in Ref. (6) relate to an earlier ODE program, documented in NASA SP 273, there are other specific harsh unjustified claims and erroneous results from an inadequate earlier Munich method program. To clear the ODE program from these allegations, the appropriate steps shall be initiated by Prof. Straub to correct this situation.

(b) Proof of a new 'Navier-Saint Venant' equation validity, resulting from Prof. Straub's proposed Alternative theory, was not presented and, therefore, the equation was not accepted as a preferred scheme over the Navier-Stokes equation at this time. Some interesting results, however, should be surveyed. A document, showing the derivation of the novel equation, should be prepared in English to assure attention and relevant studies.