LE MATEMATICHE
Vol. LX (2005) – Fasc. I, pp. 181–188

A KINETIC TYPE EXTENDED MODEL FOR DENSE GASES AND MACROMOLECULAR FLUIDS

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Extended thermodynamics is an important theory which is appreciated from mathematicians and physicists. Following its ideas and considering the macroscopic approach with suggestions from the kinetic one, we find in this paper, the solution of an interesting model: the model for dense gases and macromolecular fluids.

1. Introduction.

As usual in extended thermodynamics [1], we adopt a model which takes, as independent variables, the mass density F, momentum density F_i, momentum flux density F_{ij} and the energy flux density $\frac{1}{2}F_{ill}$. For their determination, the following field equations have to be considered

$$
\begin{aligned}
&\partial_t F + \partial_k F_k = 0,\\
&\partial_t F_i + \partial_k G_{ik} = 0,\\
&\partial_t F_{ij} + \partial_k G_{ijk} = P_{<ij>},\\
&\partial_t F_{ill} + \partial_k G_{illk} = P_{ill},
\end{aligned}
\tag{1}
$$

with $F_{ij} = F_{ji}$, $G_{ijk} = G_{jik}$, $P_{<ij>} = P_{<ji>}$, and this last tensor, with P_{ill} are the production terms. In ideal gases, we have also the conditions $G_{ik} = F_{ik}$,

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Entrato in redazione il 23 Novembre 2004.

$G_{ill} = F_{ill}$; and for this particular case an elegant solution of the entropy and objectivity conditions have been found by T. Ruggeri and G. Boillat and is known as the "kinetic approach" to these conditions. But this case isn't applicable to all materials; so we have chosen here the less restrictive model. In any case, we accept suggestions from the kinetic approach also for our less restrictive case and for this reason we call the present one as of "kinetic type". On the other hand, we aim to produce a model which may constitute the "ground zero" upon which to built other significant physical applications. To this end, simplicity will be pursued. A first application of these results has already been used in a model for magnetizable and polarizable fluids (see [2]).

Coming to the point, we want that our system (1) be a symmetric hyperbolic system, with all the consequent nice mathematical properties. To this end we impose now that every solution of eqs. (1) satisfies a supplementary conservation law $\partial_t h + \partial_k \phi_k = \sigma \geq 0$. This amounts in assuming the existence of Lagrange multipliers λ, λ_i, λ_{ij}, λ_{ill} such that

$$\begin{aligned} dh &= \lambda dF + \lambda_i dF_i + \lambda_{ij} dF^{ij} + \lambda_{ill} dF^{ill}, \\ d\phi_k &= \lambda dF_k + \lambda_i dG_{ik} + \lambda_{ij} dG_{ijk} + \lambda_{ill} dG_{illk}, \end{aligned} \tag{2}$$

besides a residual inequality which we leave out for the sake of brevity.

By taking λ, λ_i, λ_{ij}, λ_{ill} as independent variables, and defining

$$\begin{aligned} \tilde{h} &= \lambda F + \lambda_i F^i + \lambda_{ij} F^{ij} + \lambda_{ill} F^{ill} - h, \\ \tilde{\phi}_k &= \lambda F_k + \lambda_i G_{ik} + \lambda_{ij} G_{ijk} + \lambda_{ill} G_{illk} - \phi_k, \end{aligned} \tag{3}$$

the eqs.(2) become

$$F = \frac{\partial \tilde{h}}{\partial \lambda}, \quad F^i = \frac{\partial \tilde{h}}{\partial \lambda_i}, \quad F^{ij} = \frac{\partial \tilde{h}}{\partial \lambda_{ij}}, \quad F^{ill} = \frac{\partial \tilde{h}}{\partial \lambda_{ill}}, \tag{4}$$

$$\frac{\partial \tilde{\phi}_k}{\partial \lambda} = \frac{\partial \tilde{h}}{\partial \lambda^k}, \quad G_{ik} = \frac{\partial \tilde{\phi}_k}{\partial \lambda_i}, \quad G_{ijk} = \frac{\partial \tilde{\phi}_k}{\partial \lambda_{ij}}, \quad G_{illk} = \frac{\partial \tilde{\phi}_k}{\partial \lambda_{ill}}. \tag{5}$$

These are the equations of the extended approach to dense gases and macromolecular fluid. In the next section we will see also the implications of the indifference frame principle. Finally, in the section 3 all these conditions will be exploited and solved.

2. Implications arising from the galilean relativity principle..

We report now briefly how this principle is imposed in literature (see [1], [4] for example), in order to investigate its consequences in the subsequent considerations. Firstly, the following change of independent variables is considered

$$\begin{aligned} F &= m \quad F_i = mv_i, \quad F_{ij} = mv_i v_j + m_{ij}, \\ F_{ill} &= \quad m_{ill} + m_{ll} v_i + 2m_{il} v_l + mv^2 v_i \end{aligned} \tag{6}$$

and of constitutive functions

$$\begin{aligned} &G_{ik} = mv_i v_k + M_{ik}, \\ &G_{ijk} = F_{ij} v_k + 2v_{(i} M_{j)k} + M_{ijk}, \\ &G_{illk} = F_{ill} v_k + v^2 M_{ik} + 2v_i v_l M_{lk} + v_i M_{llk} + 2v_l M_{lik} + M_{illk}. \end{aligned} \tag{7}$$

The galilean relativity principle imposes that h, $\phi_k - hv_k$, M_{ik}, M_{ijk}, M_{illk}, M_i don't depend on v_i. Imposing this condition for h and $\phi_k - hv_k$ we obtain

$$\begin{aligned} 0 =& F\lambda_a + 2\lambda_{ia} F_i + \lambda_{ill}(F_{ll}\delta_{ia} + 2F_{ia}), \\ 0 =& F_k\lambda_a + 2\lambda_{ia} G_{ik} + \lambda_{ill}(G_{llk}\delta_{ia} + 2G_{iak}) + \\ &+(\lambda F + \lambda_i F_i + \lambda_{ij} F_{ij} + \lambda_{ill} F_{ill} - h)\delta_{ka}; \end{aligned} \tag{8}$$

where eqs (2) have been used. The independence of M_{ik}, M_{ijk}, M_{illk}, M_i on v_i follows as consequence. In fact, eqs. (2) now become

$$\begin{aligned} dh &= \lambda^I dm + \lambda^I_{ij} dm_{ij} + \lambda^I_{ill} dm_{ill} \\ d(\phi_k - hv_k) &= \lambda^I_i dM_{ik} + \lambda^I_{ij} dM_{ijk} + \lambda^I_{ill} dM_{illk} \end{aligned} \tag{9}$$

with

$$\begin{aligned} \lambda^I &= \lambda + \lambda_i v_i + \lambda_{ij} v_i v_j + \lambda_{ill} v_i v^2, \\ \lambda^I_i &= \lambda_i + 2\lambda_{ai} v_a + \lambda_{ill} v^2 + 2\lambda_{all} v_a v_i, \\ \lambda^I_{ij} &= \lambda_{ij} + \lambda_{all} v_a \delta_{ij} + 2\lambda_{ll(i} v_{j)}, \\ \lambda^I_{ill} &= \lambda_{ill}. \end{aligned}$$

From eq. $(9)_1$ we see that λ^I, λ^I_{ij}, λ^I_{ill} don't depend on v_i (because $\frac{\partial h}{\partial m} = \lambda^I$ but h and m don't depend on v_i, similarly for λ^I_{ij}, λ^I_{ill}; but eq. $(8)_1$ can be written also as

$$0 = m\lambda^I_a + \lambda^I_{ill}(m_{ll}\delta_{ia} + 2m_{ia}), \tag{10}$$

so that also λ^I_i doesn't depend on v_i. By defining h' and ϕ'_k from

$$\begin{aligned} h &= \lambda^I m + \lambda^I_{ij} m_{ij} + \lambda^I_{ill} m_{ill} - h' \\ \phi_k - h v_k &= \lambda^I_i M_{ik} + \lambda^I_{ij} M_{ijk} + \lambda^I_{ill} M_{illk} - \phi'_k \end{aligned}$$

the eqs. (9) become

$$\begin{aligned} dh' &= m d\lambda^I + m_{ij} d\lambda^I_{ij} + m_{ill} d\lambda^I_{ill} \\ d\phi'_k &= M_{rk} d\lambda^I_r + M_{ijk} d\lambda^I_{ij} + M_{illk} d\lambda^I_{ill} \end{aligned}$$

from which by taking λ^I, λ^I_{ij}, λ^I_{ill} as independent variables, it follows

$$(11) \qquad m = \frac{\partial h'}{\partial \lambda^I}, \quad m_{ij} = \frac{\partial h'}{\partial \lambda^I_{ij}}, \quad m_{ill} = \frac{\partial h'}{\partial \lambda^I_{ill}},$$

$$\frac{\partial \phi'_k}{\partial \lambda^I} = M_{rk} \frac{\partial \lambda^I_r}{\partial \lambda^I}, \quad \frac{\partial \phi'_k}{\partial \lambda^I_{ij}} = M_{rk} \frac{\partial \lambda^I_r}{\partial \lambda^I_{ij}} + M_{ijk}, \quad \frac{\partial \phi'_k}{\partial \lambda^I_{ill}} = M_{rk} \frac{\partial \lambda^I_r}{\partial \lambda^I_{ill}} + M_{illk}.$$

Moreover, the sum of eq. $(8)_1$, pre-multiplied by $-v_k$, and of eq. $(8)_2$ becomes

$$(12) \qquad 0 = 2\lambda^I_{ia} M_{ik} + \lambda^I_{ill}(M_{llk}\delta_{ia} + 2M_{iak}) + h'\delta_{ka},$$

or, by using $(11)_{4,6}$,

$$(13) \qquad 0 = \left[2\lambda^I_{ra} - \lambda^I_{all} \frac{\partial \lambda^I_r}{\partial \lambda^I_{ij}} \delta_{ij} - 2\lambda^I_{ill} \frac{\partial \lambda^I_r}{\partial \lambda^I_{ia}} \right] M_{rk} + \\ + \lambda^I_{all} \frac{\partial \phi'_k}{\partial \lambda^I_{ij}} \delta_{ij} + 2\lambda^I_{ill} \frac{\partial \phi'_k}{\partial \lambda^I_{ia}} + h'\delta_{ka}.$$

From this relation we see that M_{rk} doesn't depend on v_i; let us prove this by the iterative procedure on the order respect to the state with $\lambda^I_{ra} = \frac{1}{3}\lambda^I_{ll}\delta_{ra}$, , $\lambda^I_{<ra>} = 0$, $\lambda^I_{all} = 0$. Equation (13) at the order N gives

$$\frac{2}{3}\lambda^I_{ll}(M_{ak})^N + \sum_{q=0}^{N-1} (M_{rk})^q \left[2\lambda^I_{ra} - \lambda^I_{all} \frac{\partial \lambda^I_r}{\partial \lambda^I_{ij}} \delta_{ij} - 2\lambda^I_{ill} \frac{\partial \lambda^I_r}{\partial \lambda^I_{ia}} \right]^{N-q}$$

as a function of quantities not depending on v_i. (here $(\cdots)^q$ denotes the expression of $(\cdots)$ at the order q). For example, for $N = 0$, we obtain that M^0_{ak} doesn't depend on v_i; by assuming, via the iterative procedure, that also $(M_{ak})^q$ satisfies this property for $q \leq N-1$, it follows that also $(M_{ak})^N$ satisfies it. After that, $(11)_{6,7,8}$ show that also M_{ijk}, M_{illk} and M_j don't depend on v_i. In this way we have proved that entropy principle and the principle of galilean relativity amount simply to conditions $(11)_4$, (10) and (12).

In the next section the equations (10)-(12) will be solved.

3. Exploitation of the entropy principle and of galilean relativity..

In order to solve the conditions (10)-(12), let us firstly consider another mathematical problem: we look for two functions $h^*(\lambda^I,\ \lambda^I_i,\ \lambda^I_{ij},\ \lambda^I_{ill})$ and $\phi^*_k(\lambda^I,\ \lambda^I_i,\ \lambda^I_{ij},\ \lambda^I_{ill})$ that satisfy the sequents

$$(14) \qquad m = \frac{\partial h^*}{\partial \lambda^I}, \quad m_{ij} = \frac{\partial h^*}{\partial \lambda^I_{ij}}, \quad m_{ill} = \frac{\partial h^*}{\partial \lambda^I_{ill}},$$

$$(15) \qquad \frac{\partial \phi^*_k}{\partial \lambda^I} = \frac{\partial h^*}{\partial \lambda^I_k}, \quad \frac{\partial \phi^*_k}{\partial \lambda^I_i} = M_{ik}, \quad \frac{\partial \phi^*_k}{\partial \lambda^I_{ij}} = M_{ijk}, \quad \frac{\partial \phi^*_k}{\partial \lambda^I_{ill}} = M_{illk},$$

$$(16) \qquad \begin{aligned} 0 &= \tfrac{\partial h^*}{\partial \lambda^I}\lambda^I_a + 2\tfrac{\partial h^*}{\partial \lambda^I_i}\lambda^I_{ia} + \lambda^I_{ill}(\tfrac{\partial h^*}{\partial \lambda^I_{rs}}\delta_{rs}\delta_{ia} + 2\tfrac{\partial h^*}{\partial \lambda^I_{ia}}), \\ 0 &= \tfrac{\partial \phi^*_k}{\partial \lambda^I}\lambda^I_a + 2\tfrac{\partial \phi^*_k}{\partial \lambda^I_i}\lambda^I_{ia} + \lambda^I_{ill}(\tfrac{\partial \phi^*_k}{\partial \lambda^I_{rs}}\delta_{rs}\delta_{ia} + 2\tfrac{\partial \phi^*_k}{\partial \lambda^I_{ia}}) + h^*\delta_{ka}. \end{aligned}$$

After that, we consider λ^I_i implicitly defined by the equation $0 = \frac{\partial h^*}{\partial \lambda^I_i}$. Well, h^* and ϕ^*_k calculated in this value of λ^I_i are exactly the functions h' and ϕ'_k (respectively) satisfying the eqs. (10)-(12). So let us begin with the mathematical problem (14)-(16).

3.1 Resolution of conditions $(15)_1$ and (16).

We look for a solution, of the conditions $(15)_1$-(16), of the type

$$(17) \qquad h^* = h^0 \quad , \quad \phi^*_k = \phi^0_k + \phi^*_{0k}(\lambda^I_i, \lambda^I_{ij}, \lambda^I_{ill}),$$

where h^0 and ϕ^0_k are the expressions of h^* and ϕ^*_k in the case of the macroscopic approach with the further conditions $G_{ik} = F_{ik}$, $G_{ill} = F_{ill}$. They can be found in ref. [5]; more restrictive results can be obtained in the following way. Consider the kinetic approach with 14 moments, i.e.,

$$(18) \qquad \begin{aligned} h^0 &= \int f(\lambda^I + \lambda^I_i c_i + \lambda^I_{ij} c_i c_j + \lambda^I_{ill} c_i c^2 + \lambda^I_{llnn} c^4)\, d\underline{c}, \\ \phi^0_k &= \int f(\cdots) c_k\, d\underline{c}, \end{aligned}$$

where c_i are the integration variables in the phase-space and f is related to the distribution function. After that, one can consider the expansions of h^0 and ϕ^0_k

around thermodynamical equilibrium and adopt the results for the macroscopic approach to the model with 14 moments. Consider, finally, the subsistem (see ref. [1]) of this one obtained simply by putting $\lambda^I_{llnn} = 0$ and recover, in this way the macroscopic approach with 13 moments. Also for this reason we call (17) with $\phi^*_{0k} \neq 0$ a "kinetic type" solution. In other words, the kinetic approach is here used only as a mathematical tool to obtain a particularly simple solution of the macroscopic approach; starting from it, a more significative solution will be found in the next passages. Obviously, the kinetic approach with 13 moments hasn't been used, to avoid integrability problems.

It is easy to see (17) satisfy $(15)_1$ $\forall \phi^*_{0k}$, due to the fact that $\forall \phi^*_{0k}$ doesn't depend on λ^I.

In this way all relations are certainly satisfied if $\phi^{0*}_{0k} = 0$, so that for the general case it remains to impose that eqs. (17) satisfy the conditions $(16)_2$ i.e.,

$$0 = 2\frac{\partial\phi^*_{0k}}{\partial\lambda^I_i}\lambda^I_{ia} + \left(2\frac{\partial\phi^*_{0k}}{\partial\lambda^I_{ia}} + \frac{\partial\phi^*_{0k}}{\partial\lambda^I_{rs}}\delta_{rs}\delta_{ia}\right)\lambda^I_{ill}\;; \tag{19}$$

let us impose this with an expansion with respect to the state s where $\lambda^I_i = 0$, $\lambda^I_{<ia>} = 0$, $\lambda^I_{ill} = 0$. The symbol ϕ^{N*}_{0k} denotes the expression of ϕ^*_{0k} of order N with respect to this state. Obviously, we have $\phi^{0*}_{0k} = 0$ because at the order 0, ϕ^*_{0k} may depend only on λ^I_{ll}. We shall see that, by imposing eq. (19) at order N, we find ϕ^{N+1*}_{0k} except for terms not depending on λ^I_i which, on the other hand, can be also found with the representation theorems [6], [7]. In fact, eq. (19) at the order zero gives

$$0 = \frac{2}{3}\lambda^I_{ll}\frac{\partial\phi^{1*}_{0k}}{\partial\lambda^I_a}$$

from which ϕ^{1*}_{0k} doesn't depend on λ^I_a. But we have already seen that $\phi^{0*}_{0k} = 0$ so that up to the order 1, we have that ϕ^*_{0k} is given by

$$\phi^{1*}_{0k} = f_1(\lambda^I_{ll})\lambda^I_{kll}, \tag{20}$$

with f_1 arbitrary function. Eq. (19) at the order 1 is

$$0 = \frac{2}{3}\lambda^I_{ll}\frac{\partial\phi^{2*}_{0k}}{\partial\lambda^I_a} + 2\lambda^I_{<ia>}\frac{\partial\phi^{1*}_{0k}}{\partial\lambda^I_i} + \left(2\frac{\partial\phi^{1*}_{0k}}{\partial\lambda^I_{<rs>}}\delta^r_{<i}\delta^s_{a>} + 5\frac{\partial\phi^{0*}_{0k}}{\partial\lambda^I_{ll}}\delta_{ia}\right)\lambda^I_{ill}$$

from which

$$\phi^{2*}_{0k} = f_2(\lambda^I_{ll})\lambda^I_{<ki>}\lambda^I_{ill}, \tag{21}$$

with f_2 arbitrary function. Eq. (19) at the order 2 is

$$0 = \frac{2}{3}\lambda^I_{ll}\frac{\partial\phi^{3*}_{0k}}{\partial\lambda^I_a} + 2\lambda^I_{<ia>}\frac{\partial\phi^{2*}_{0k}}{\partial\lambda^I_i} + \left(2\frac{\partial\phi^{2*}_{0k}}{\partial\lambda^I_{<rs>}}\delta^r_{<i}\delta^s_{a>} + 5\frac{\partial\phi^{1*}_{0k}}{\partial\lambda^I_{ll}}\delta_{ia}\right)\lambda^I_{ill}$$

from which

$$\begin{aligned}\phi^{3*}_{0k} = &-\frac{3}{2}f_2(\lambda^I_{ll})^{-1}(\lambda^I_{rll}\lambda^I_{rll})\lambda^I_k - \frac{1}{2}(f_2 + 15f_1')(\lambda^I_{ll})^{-1}(\lambda^I_r\lambda^I_{rll})\lambda^I_{kll} + \\ &+ \left[f_3(\lambda^I_{ll})(\lambda^I_{rll}\lambda^I_{rll}) + f_4(\lambda^I_{ll})(tr(\lambda^I_{<rs>})^2)\right]\lambda^I_{kll} + f_5(\lambda^I_{ll})(\lambda^I_{<kr>})^2\lambda^I_{rll};\end{aligned} \tag{22}$$

with f_3, f_4, f_5 arbitrary function. Eq. (19) at the order 3 gives

$$\begin{aligned}\phi^{4*}_{0k} = &-\frac{3}{2}f_5(\lambda^I_{ll})^{-1}(\lambda^I_{<rs>}\lambda^I_{rll}\lambda^I_{sll})\lambda^I_k + \\ &+ \frac{3}{2}\left[f_2 + 15f_1')(\lambda^I_{ll})^{-2} - (4f_4 + f_5)(\lambda^I_{ll})^{-1}\right]\cdot(\lambda^I_{<rs>}\lambda^I_r\lambda^I_{sll})\lambda^I_{kll} \\ &+ \frac{3}{2}(\lambda^I_{ll})^{-2}(3f_2 - f_5\lambda^I_{ll})(\lambda^I_{rll}\lambda^I_{rll})\lambda^I_{<ka>}\lambda^I_a + \\ &+ \frac{1}{2}(f_5 - 15f_2')(\lambda^I_{ll})^{-1}(\lambda^I_r\lambda^I_{rll})\lambda^I_{<ks>}\lambda^I_{sll} + \\ &+ \text{ terms not depending on } \lambda_i\end{aligned} \tag{23}$$

and so on.

Acknowledgment. We thank an anonymous referee, for suggestions which helped in improving the quality of the article.

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