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Model of the ideal fluid with scalar microstructure. An application to flashing flow of water

1   Introduction

1.1   Description of the growth, evolution and decay of microstructure in terms of a hidden variable

Ideal fluids, both compressible and incompressible exhibit a lack of thermal conductivity and viscous diffusion of momentum and mass. These fluids accumulate energy in a recoverable way and do not exhibit energy dissipation. It is a quite different phenomenon when, under the influence of a sudden pressure drop, a stress induced phase transition takes place. In spite of the fact that a new phase is strongly dispersed in the initial stages of the phase change, it is treated as an ideal fluid, and the resulting mixture of these ideal fluids is a recoverable-dissipative system. This new property of dissipation arises due to the existence in the transforming fluid of a large number of interfacial surfaces or interfacial zones. The interfaces, which are the places of strong gradients of density, pressure, velocity, and chemical potential, are practically the only sources of irreversibility in the mixture of these ideal phases.

Associated with and perhaps crucial for interfacial properties are the so-called fluid microstructures. Since nuclei of a new phase have negligible dimensions in comparison with the macroscopic characteristic dimension of a channel, they can be described as a phenomenon entirely evaluated at micro- or nano-level. Therefore, by the fluid microstructure we shall understand the microscopic region of medium where densities, fractions, compositions, etc. vary appreciably over a

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distance of the order of magnitude of the range of molecular forces.

The main question arising in mathematical modelling of the microstructure is whether there exists a simple and physically justified macroscopic field which would be relevant for complete description of the morfology of the microstructure. Independently of numerous achievements in this field, it seems to us that the understanding of the behaviour of first order phase transitions in terms of microstructural fluids[2] still forms an exciting and developing subject.

The simplest mathematical model capable of describing a phenomenological microstructure created by the interfacial surfaces is a model in where the whole microstructure is described by a single scalar parameter $\xi(\mathbf{x}, t)$[3] only. In such a model only one order parameter, being a function of space and time, describes deviation of a system from the thermodynamic equilibrium as well as from 'ideality' of the fluid. Physically, the parameter ξ is a fraction of phase transition and therefore it varies in the range $0 < \xi < 1$. For instance, in flashing water at ordinary temperature this parameter is identified as a dryness fraction. For condensing supercooled vapour it is defined as wetness fraction. It also appears that the deviation of the system from thermodynamic equilibrium can be expressed by a simple difference of the order parameter and its equilibrium value, i.e. $\xi - \xi_0$.

Although the parameter ξ does not directly describe the area and mean curvature of interfacial surfaces, its spatial gradient $\nabla \xi$ provides proper information on the additional contributions to internal energy and dissipation.[4]

It has been shown by several authors[5] that $\nabla \xi$ is responsible for small but essential contribution of recoverable energy to the specific internal energy, i.e. $\epsilon = \epsilon(\eta, v, \xi, \nabla \xi)$. This contribution follows from the interfacial tension σ defined for moving immaterial interfacial surfaces of changing topology. On the other hand, however, any interfacial zone is also a localized domain of strong gradients of density, temperature, velocity, chemical potential and other sources of irreversibility. It appears, therefore, that apart from recoverable properties, it reveals dissipation as a dominating feature.

Speaking in the language of fluid microstructure, it is important to establish

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[2]The microstructure can also be observed in a wide spectrum of technological and natural processes, such as products of the emollient, detergent, separation and reaction processes, pollution control and water treatment industry. The concept of microstructure is useful for the description of gels, films, foams, microporous media, emulsions, liquid crystals, bilayers in cellular biological systems, etc.

[3]There are a lot of names for ξ which are to be found in the literature. Among the most popular are: internal variable, hidden parameter, order parameter.

[4]Gradient theory has at first been initiated for inhomogeneous fluids with strong gradients of density by van der Waals (1893), Fuchs (1888), Rayleigh (1892) and Korteweg (1901). It has more recently been developed by Landau&Ginzburg (1950), Cahan&Hilliard (1958), Hart (1959) and many others for the description of systems undergoing first order phase transition.

[5]Landau&Teller (1936), Cahn&Hilliard (1958), van der Waals (1893), Hart (1959).

a model describing the kinetics of the microstructure, which would be capable of predicting real nucleation and growth of a new phase. Therefore, the main goal of our research is to anticipate proper and sufficient rules for describing the evolution of the microstructure in terms of $\xi, \nabla\xi$ and $\partial_t\xi$. In analogy to the nomenclature introduced by veterans of the theory of phase transitions,[6] we prefer the notion *kinetics of phase transition*, even though inertial effects are accounted for. For the same reason we prefer to speak of equations which govern the behavior of our microstructure as *evolution equations*.

Usually, the evolution of the microstructure is physically interpreted as a process of relaxation of ξ towards ξ_0. Generally, the kinetics of the relaxation towards equilibrium should be described both by the relaxation of irreversible parts of mass, momentum and energy fluxes and by the relaxation of the microstructure. However, the latter contribution can not be expressed by means of an appropriate flux, but is modeled with the aid of the pertinent order parameter ξ. In this paper we shall mainly concentrate on mathematical constituencies of the microstructure and, therefore, we will omit the class of problems which are related to the relaxation of the fluxes.[7] There is common agreement in the literature of the subject that the relxation mode frequently dominates in the kinetics of approaching thermodynamic equilibrium.

Nevertheless, for a system that undergoes first order phase transition (flashing of water, spontaneous condensation of vapor), there are also another important mechanisms of departure and arrival to equilibrium. We mean here both diffusion- and viscous-controlled phase transitions. It appears, that in both these cases the equations governing the evolution of the microstructure must be supplemented by the essential part containing the divergence of some microscopic flux of the order of the parameter ξ. Thus, in both cases, the evolution equation should take the form of equation similar to a conservation one. Therefore, we frequently speak of a microstructure with conserved order parameter.[8]

On the contrary, for diffusionless and inviscid phase transformations, the relaxational mode of ξ plays a dominant role. Then, the evolution equation takes a much simpler form.[9] This is the case for a type of systems where the mass fraction or concentration can be regarded as order parameters and the condition of local conservation need not to be imposed. There is a tendency in the literature

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[6]see, for instance, historical comments in Volmer's monograph (1939)).

[7]Let us recall that the central part of the theory called *extended thermodynamics* deals with the formulation of evolution equations for dissipative, irreversible fluxes. By analogy, the theory of hidden variables deals with the formulation of evolution equations for dissipative part of the order parameter.

[8]For instance, the Cahn-Hilliard equation is an example of this. It has been obtained for a microstructure which is responsible for diffusion-controlled phase transition.

[9]As an example one can find the Ginzburg-Landau equation, called now the time dependent Ginzburg-Landau equation (TDGL).

to identify the evolution equations for the nonconserved order parameter with the relaxational evolution equation [66].

1.2   Flashing of water – some additional physical motivations

The phenomenon of flashing in a flowing water at ordinary temperature ($\sim 59^o F$) and ordinary pressure (14.70 lbs/in^2) was observed for the first time by Osborne Reynolds in his experiments with a converging-diverging nozzle[10]. On the ground of Reynolds' idea it supports his successful observation that two different phenomena such as pool boiling and flashing flow can posses something in common. Reynolds' analysis of the sound generation in a kettle, a phenomenon related to sudden collapse of bubbles in boiling water, led him to the conclusion that the acoustic phenomena accompanying both the pool boiling and flashing flow have the same origin.[11]

Thus, Reynolds finally asserts that boiling can occur not only due to the external gradient of temperature but also due to the gradient of pressure. In hydrodynamics it is customary to consider physical properties of the fluid as consisting of incompressibility and perfect fluidity only, no account being taken of internal cohesion. Therefore, as Reynolds remarked, the ,,disruption" of fluid is possible under unusual circumstances when the pressure is everywhere positive.

Nowadays, experiments with cavitating water are frequently repeated, especially when nonequilibrium properties of hetero- and homogeneous nucleation must be novelized or corrected.[12]

1.3   Purposes and main results of this note

In this paper, as we already mentioned, a model of ideal fluid with a scalar microstructure is considered in details. Our primary goal is to construct a mathematical model of continuum which, posseses a simple microstructure. By the phrase ,,a simple microstructure" we mean a microscopic scalar field which, after some transition to macroscopic, continual level, shall become a single function of $\xi(\mathbf{x}, t)$. This field variable, called here *the order parameter,* behaves like a weekly

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[10]O.Reynolds (1894).

[11],,It is a matter of familiar observation that the flow of water through pipes under great pressure, as when, in the water supply of a town, the water is brought from below the surface of a reservoir on a continuous slope into houses or mains several hundred feet below the reservoir, and is generally attended with a hissing noise; and of this I believe no explanation has hitherto been given. Nor have I ever heard anyone suggest that there is any connection between the singing of the kettle and the hiss which almost invariably attends the opening of a tap in a pipe under considerable pressure as in a town's service. Yet when observed the hiss of the pipe closely resembles the harshest sound of the kettle" - O.Reynolds (1894),p. 44.

[12]see, for example, a reinterpretation of the *Moby Dick* experiments made by Bilicki, Kestin and Pratt (1990).

non-local function. It practically means, that it will appear in the theory together with its spatial $\nabla\xi$ and time gradients $\partial_t\xi$.[13]

We shall especially be interested in the description of the effects which follow from the microstructure, and are available at the macroscopic level in the form of any collective contributions.[14] Our attention is paid to a concise derivation of a unified model that incorporates every recoverable (convective), relaxational, diffusive, viscous and inertial influences of $\xi, \nabla\xi, \partial_t\xi$. The model is postulated in the form of balance equations, which usually are formulated for such empirical quantities as mass, momentum, energy and entropy. Speaking more directly, we wish to give satisfactory answers to two questions. The first is: *how the microstructure can change the classical model of the ideal fluid?*. The second sounds: *in which manner the evolution equation for ξ should be postulated?*

Before starting the analysis of fluids with a scalar microstructure, let us only recall that the model of ideal fluid, which is the simplest case of the Cauchy continuum, includes only purely recoverable (elastic) properties of the medium. For such fluids the Cauchy momentum flux $\mathbf{\Pi}^{\mathrm{re}}$ is reduced to conduction via thermodynamic pressure $p(\mathbf{x}, t)$ and to convection via velocity field $\mathbf{v}(\mathbf{x}, t)$

$$\mathbf{\Pi}^{\mathrm{re}}(\mathbf{x}, t) = p\mathbf{I} + \rho\mathbf{v} \otimes \mathbf{v}. \tag{1}$$

Similarly, the flux of energy $\mathcal{J}_{\mathbf{e}}^{\mathrm{re}}(\mathbf{x}, \mathbf{t})$ is a purely recoverable[15], independent object and does not contain any contribution from the heat flux $\mathbf{q}$. If $e = \rho\epsilon + 1/2\rho\mathbf{v}^2$ is the total energy density then $\mathcal{J}_e^{\mathrm{re}}$ is defined as a sum of convective and mechanical parts:

$$\mathcal{J}_e^{\mathrm{re}} = e\mathbf{v} + (\mathbf{\Pi}^{\mathrm{re}} - \rho\mathbf{v} \otimes \mathbf{v})\mathbf{v} = (e + p)\mathbf{v} = (\rho h + 1/2\rho\mathbf{v}^2)\mathbf{v}, \tag{2}$$

where, according to the notation used by $L\&L$ authors[16], $h = \epsilon + p/\rho$ is the specific enthalpy, ϵ is the internal energy and ρ is the mass density. Having equations (1), (2) the set of governing equations for the model of inviscid, nonconducting, ideal fluid is usually presented in the form of balance equations for mass, momentum, energy and entropy [26]:

$$\partial_t\rho = -\mathrm{div}(\rho\mathbf{v}) = -\mathrm{div}\mathcal{J}_\rho, \tag{3}$$

$$\partial_t(\rho\mathbf{v}) = -\mathrm{div}(p\mathbf{I} + \rho\mathbf{v} \otimes \mathbf{v}) = -\mathrm{div}\mathbf{\Pi}^{re}, \tag{4}$$

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[13]The model under consideration is mainly a mathematical one, what does not mean that numerous heuristic motivations have not been taken into account.

[14]e.i. phenomenological level.

[15]it was discovered by Peter Umov(1874) and Vito Volterra (1899).

[16]Landau & Lifshitz, this is an analogy to celebrated $T\&T$(Thomson&Tait, Truesdell&Toupin) another pairs of authors.

$$\partial_t(\rho\epsilon + \frac{1}{2}\rho\mathbf{v}^2) = -\text{div}(\rho h\mathbf{v} + 1/2\rho\mathbf{v}^2\mathbf{v}) = -\text{div}\mathcal{J}_e^{re}, \qquad (5)$$

$$\partial_t(\rho\eta) = -\text{div}(\rho\eta\mathbf{v}) = -\text{div}\mathcal{J}^{\eta}. \qquad (6)$$

The first three equations have a clear empirical meaning, which is traditionally applicable to continua balanced within the Eulerian description. The clearness is lost in the case of the balance of entropy. This equation is sometimes interpreted as an evolution equation which is postulated independently [52].

Answering our first question, it appears that the inclusion of the gradients $\partial_t\xi$ and $\nabla\xi$ leads to the introduction of some extra terms into the fluxes of momentum, energy and entropy. These extra terms contribute both to reversible and dissipative parts of the equations. For instance, we shall show in Chapter III, that the extra recoverable momentum flux comprises an additional pressure as well as additional recoverable shear stresses. A recoverable heat flux $\mathbf{q}_\xi$ also appears, which, in general, leads to nonisothermal flows of ideal fluids.

However, the additional contributions to the dissipative parts of the fluxes are of great novelty in the frame of ideal fluid description. These dissipative fluxes appear since, apart from the main contribution to dissipation following from the action of the rate of ξ on itself affinity, there is a possibility of the existence of cross and nonlinear effects in the Onsager kinetic equations. It thus appears that the extra dissipative fluxes $\mathbf{\Pi}^{ir}, \mathbf{q}^{ir}$ are indispensable to exactly satisfy the momentum and energy equations.

Passing on to the second question we wish to pay reader's attention to the fact that the majority of available evolution equations that are known in the literature, are *ad hoc* postulated. Though most of recent work in the theory of hidden variables has been dedicated to the deeper foundation of this theory[17], complex evolution equations are most aptly handled. Thus, in this paper, we try to solve this problem staying on the ground of verified mathematical tools. We shall apply the Poisson and dissipation bracket theory for derivation a diffusion-relaxation model.

2   Continua with a scalar microstructure – a short review of previous works

2.1   Models with relaxation of hidden variable

Let us review the history of the development of mathematical modelling of thermodynamic relaxation by means of a single hidden variable ξ. In this paragraph we restrict ourselves only to the models without gradients, removing models with $\nabla\xi$ to paragraph 2.2.

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[17] for instance - mezoscopic derivation on the basis of the Maxwell or Boltzmann kinetic theory.

So as to study the theory of hidden variables we should return to the methods and mathematical tools that have been known in analytical mechanics since the previous century. It seems that the notion of hidden variable is an analogue of the notion of cyclic variables. The concept of cyclic variables, that was introduced for the first time by Lagrange and Poisson, has later been developed by E. J. Routh on the grounds of analytical mechanics and hydrodynamics. It was W. J. M. Rankine[18] who first introduced the concept of a single hidden variable to modern thermodynamics. In his centrifugal model of elastic fluid particle the phenomenological temperature played a role of an additional hidden parameter. This line of reasoning was extended to Hamiltonian mechanics and presented in the form of variational principle by Szily[19], who called the systems with single cyclic (hidden) variable the mono-cyclic systems. Taking this mono-cyclic system as a starting point, J. J. Thomson[20] extended the concept to the poly-cyclic systems. These systems are capable of describing not only temperature but also recoverable electricity, magnetism, capillarity, hydrodynamics of viscous flows, etc.

The next important step was done by Wladyslaw Natanson[21]. Trying to extend the fundamentals of the concept of relaxation he introduced a hidden variable in the form of symmetric dyad

$$
\mathbf{e}^* = \epsilon^* \mathbf{i}_x \otimes \mathbf{i}_x + \phi^* \mathbf{i}_y \otimes \mathbf{i}_y + \psi^* \mathbf{i}_z \otimes \mathbf{i}_z +
$$
$$
+ \alpha^* (\mathbf{i}_y \otimes \mathbf{i}_z + \mathbf{i}_z \otimes \mathbf{i}_y)/2 + \beta^* (\mathbf{i}_x \otimes \mathbf{i}_z + \mathbf{i}_z \otimes \mathbf{i}_x)/2 + \gamma^* (\mathbf{i}_y \otimes \mathbf{i}_x + \mathbf{i}_x \otimes \mathbf{i}_y)/2, \tag{7}
$$

for which he postulated the following evolution (relaxation) equation:

$$
\frac{d}{dt}\mathbf{e}^* = \mathbf{d} - \frac{1}{\theta}\Big(\mathbf{e}^* - \frac{1}{3}(tr\mathbf{e}^*)\mathbf{I}\Big). \tag{8}
$$

The symmetric dyad $\mathbf{d}$ is the so-called rate of deformation

$$
\mathbf{d} = 1/2(grad\mathbf{v} + \mathrm{grad}^T\mathbf{v}) = (u_{,x})\mathbf{i}_x \otimes \mathbf{i}_x + (v_{,y})\mathbf{i}_y \otimes \mathbf{i}_y + (w_{,z})\mathbf{i}_z \otimes \mathbf{i}_z +
$$
$$
+(w_{,y}+v_{,z})(\mathbf{i}_z \otimes \mathbf{i}_y + \mathbf{i}_y \otimes \mathbf{i}_z)/2 + (u_{,z}+w_{,x})(\mathbf{i}_x \otimes \mathbf{i}_z + \mathbf{i}_z \otimes \mathbf{i}_x)/2 + \tag{9}
$$
$$
+(v_{,x}+u_{,y})(\mathbf{i}_y \otimes \mathbf{i}_x + \mathbf{i}_x \otimes \mathbf{i}_y)/2,
$$

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[18] Rankine (1851).
[19] Szily (1872).
[20] J.J. Thomson (1887).
[21] Natanson (1901).

and θ is the characteristic time of relaxation. The quantities $\mathbf{d}$ and $\frac{d}{dt}\mathbf{e}^*$ are generally different. It is since the former is related to an *apparent* deformation of the fluid whereas the latter is connected with the *real* state of material. Only for entirely elastic fluids the notion of the *real* rate of deformation becomes identical with that of *apparent*.

Another important thing which was noticed by Natanson is that the hidden variable $\mathbf{e}^*$ can be removed from considerations instead of some complications in the constitutive equations for the flux of momentum. It can be done with the help of the assumption that the Hooke law can be extended into fluids modeled within the Eulerian description. The difference is that the Hooke constitutive equation has to be applied not to the dyad of *apparent deformation* but to that of *real deformation*. Accepting this hypothesis, we obtain the following recoverable constitutive equation which provides relation between the traceless flux of momentum Π and the traceless dyad of $\mathbf{e}^*$

$$\mathbf{\Pi} - p\mathbf{I} = -\eta\mathbf{e}^* - \left(k - \frac{2}{3}\eta\right)tr\mathbf{e}^*\mathbf{I}, \qquad (10)$$

which comprises two elasticity-like coefficients: η - the modulus of rigidity and k - the modulus of compressibility. Combining (9) and (10) we finally obtain:

$$\frac{d}{dt}\mathbf{\Pi} + \frac{1}{\theta}\left(\mathbf{\Pi} - p\mathbf{I}\right) = -\eta\mathbf{d} - \left(k - \frac{3}{2}\eta\right)tr\mathbf{dI}. \qquad (11)$$

Assuming the following rule for the evolution of pressure

$$\frac{d}{dt}p = -k'\frac{d}{dt}\left(tr\mathbf{e}^*\right), \qquad (12)$$

and making use of Eq. (11) we arrive at

$$\frac{d}{dt}\left(\mathbf{\Pi} - p\mathbf{I}\right) + \frac{1}{\theta}\left(\mathbf{\Pi} - p\mathbf{I}\right) = -\eta\mathbf{d} - \left(k - k' - \frac{2}{3}\eta\right)(tr\mathbf{d})\mathbf{I}, \qquad (13)$$

where all the terms of higher order are neglected. Equation (13) is the evolution equation for the traceless flux $\mathbf{P} = \mathbf{\Pi} - p\mathbf{1}$ and is similar to the Maxwell relaxation equation. It is important to note that the above quations are exactly the same as those introduced within the framework of extended thermodynamics. It is also worth noticing that the relaxation time in the evolution equation (7) is equal to the relaxation time for the momentum flux in Eq. (13). It practically means that there is always a possibility to find an equivalent hidden variable which would change the constitutive equations for irreversible parts of the fluxes of mass, momentum and energy in a manner commonly used in extended thermodynamics. The simplest possible proof is the presence of the same relaxation times in both equations. Contemporary, Natanson's line of reasoning seems to be continued in

the works by F. Bampi&A. Morro. They are the authors of an analysis entitled *Extended Thermodynamics versus Hidden Variables.*[22] For this reason we propose here to distinguish both relaxation times usin θ and τ, respectively.

This distinction is not only formal but also has a physical foundation. The time θ usually comes from the kinetic theory of gases and represents the property of pure, one-component, single-phase media. The time τ represents only the collective contribution of nonequilibrium interactions of two phases. If the time θ is called the molecular relaxation time then the time τ should be called the substitute (or structural) relaxation time.

An interesting application of Natanson's hidden variable to the problem of scattering of light in liquid can be found in the paper by M. Leontonovich.[23] Quite similar method was applied to the problem of sound absorption[24]. This phenomenon is physically interpreted as a result of collisions between the sound quanta and the Debye heat quanta.

At the same time, the concept of single hidden variable appeared in numerous investigations on sound dispersion in gases and liquids. The effect of sound dispersion and absorption usually occurs when molecular vibrations become excited. This is possible when the translational and rotational energy of a system can be exchanged with the molecular vibrations. Thus, Landau and Teller, considering the passage of sound which transforms the medium from the nonexcited to the excited state proposed an evolution equation[25] which can be expressed in the following form:

$$\frac{d}{dt}n_1 = -n_1 div\mathbf{v} + k_0 n_0 - k_1 n_1, \tag{14}$$

where n_0 and n_1 denote the concentration of nonexcited and exited molecules, respectively, and k_0 and k_1 are probabilities of these transitions. If $n = n_0 + n_1$, then the relative concentration is $\xi = \frac{n_1}{n}$ together with its equilibrium value ξ_0. Substituting this into Eq. (14) and transforming the part containing div$\mathbf{v}$, we obtain

$$\frac{d}{dt}\xi = -\frac{1}{\tau}\Big[(\xi - \xi_0) + \psi_{\xi T}(T - T_0) + \psi_{\xi\rho}(\rho - \rho_0)\Big], \tag{15}$$

with the relaxation time defined as

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[22]F. Bampi&A. Morro (1984). Apart from this comprenhensive paper there are also the papers by Meixner (1949) and Biot (1955) where Natanson's reasoning is repeated. Natanson's approach has many points in common with the procedure of "diabatic elimination" which is commonly known in modern nonlinear physics as a method of *slow-fast mode dynamics* (see [58]).

[23]M. Leontovich (1941).

[24]L. Landau&G. Rumer (1937).

[25]Landau&Teller (1936).

$$\tau = \frac{1}{(k_0 + k_1)}.$$

(16)

It appears that the above form of evolution equation for the parameter ξ was introduced for the first time by Mandelstam and Leontovich[26]. The derivatives of the free energy: $\psi_{\xi T} = \frac{\partial \psi}{\partial \xi \partial T}, \psi_{\xi \rho} = \frac{\partial \psi}{\partial \xi \partial \rho}$ that appeared in Eq. (15) are due to a fruitful concept of extending the free energy function for nonequilibrium states, i.e. $\psi = \psi(T, \rho, \xi)$. It is assumed that the free energy ψ depends on the nonequilibrium parameter ξ in such a way that

$$\mathcal{A} = \frac{\partial}{\partial \xi} \psi \big(T, \rho, \xi \big),$$

(17)

the recoverable affinity $\mathcal{A}$ is described by the derivative of ψ[27]. In equilibrium the variable ξ attains a finite value (ξ_0) which depends on pressure and temperature. Its value can be obtained from the follownig condition of thermodynamic equilibrium[28]

$$\mathcal{A} = \psi_{,\xi} = 0.$$

(18)

The results of the analysis of the conditions of sound propagation led Mandelstam&Leontovich to the conclusion that in the medium with relaxing scalar microstructure there are two kinds of sound velocity: the first a_e is the ordinary Laplace value for very low frequences ω , whereas the second one a_f is the velocity at $\omega \to \infty$[29].

The second important feature of the relaxing scalar microstructure, also discovered in the cited paper of Maldenstam&Leontovich, is the operational second (bulk) viscosity. This property appears in the model mainly due to the presence in Eq. (15) of the coefficient $\psi_{\xi \rho}$. Finally, the coefficient of second (operational) viscosity is given in terms of the relaxation time and the difference between the frozen and equilibrium speed of sound[30]:

$$\eta'_{oper} = \tau'(a_f^2 - a_e^2)\rho,$$

(19)

in which $\tau' = \tau C/c$, where C and c are the heat capacities for any fixed ξ and for equilibrium ξ_0, respectively.

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[26]L.I. Mandelstam&M.A. Leontovich (1937).

[27]Yet another recoverable affinity is to be obtained in thermoplasticity where $\boldsymbol{\sigma}_p = \frac{\partial \psi}{\partial \mathbf{e}_p}$ and the internal variable $\mathbf{e}_p$ is the plastic deformation.

[28]ibidem, eq(1).

[29]these velocities are nowadays known as: the equilibrium and frozen speed of sound, respectively.

[30]there is a printer error in the original formulae here.

Further researches on the fluids with a scalar microstructure were carried out by numerous authors[31]. For instance, R.E. Nettleton proposed a consistent theory of a scalar microstructure which includes micro inertia effects as well as the wave theory of thermal relaxation. Generally, these researches proved a capability of the new thermodynamic tool consisting in the description of irreversible processes by means of the evolution of scalar microstructure.

2.2 Weakly non-local models with spatial gradient of the hidden variable

As we already mentioned, the essential postulate that the free energy function should be determined not only by the local state parameters but also by their spatial derivatives at the same point, comes from the studies of such pioneers as van der Waals, Fuchs, Gibbs, Rayleigh and others.[32]

In 1950 Landau and Ginzburg re-derived a similar result for a microstructure governed by a complex order parameter.[33] They assumed that the free energy of a medium undergoing phase transition from normal to superconducting state, in the presence of external magnetic field $\mathcal{H}$ in the vicinity of critical temperature T_c should be given as[34]

$$\psi_{s\mathcal{H}} = \psi_{s0} + \mathcal{H}^2/8\pi + 1/2m \mid -i\hbar \text{grad}\Psi - e/c\mathbf{A}\Psi \mid^2, \qquad (20)$$

$$\psi_{s0} = \psi_{n0} + \alpha \mid \Psi \mid^2 + \beta/2 \mid \Psi \mid^4 . \qquad (21)$$

It is seen that the complex hidden variable Ψ occurs in Eqs (20) and (21) mainly in the form of the scalar $\mid \Psi \mid^2$ which is called concentration. These expressions for the free energy density, successfully tested on normal-superconducting phase transitions, play nowadays a role of a pattern in many modern models.

During the last thirty years the Ginzburg-Landau approach was a basis for many works, not only on phase transitions, but also on thermodynamics of critical points, spinodal decomposition, wetting, etc. In particular, Cahn&Hilliard[35] analyzed in details the general form of the free energy and its relation to the three-dimensional theory of nucleation as well as to certain properties of the interfacial energy. Their expression for the total free energy:

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[31]Meixner (1949), Biot (1949), Broer (1958), Szaniawski (1958), Polyakova (1959), Nettleton (1961) and others.

[32]see for details van der Waals (1893).

[33]L.D. Landau&W.I. Ginzburg (1950).

[34]ibidem, Eq. (9).

[35]J.W. Cahn&J.E. Hillard (1958).

$$\mathcal{F} = \int \rho\psi dv = \int \rho[\psi_0(T, \rho, \xi) + \kappa(\nabla\xi)^2]dv \qquad (22)$$

was assumed as a sum of two contributions, the second of which is a function of the gradient of the order parameter. It appears that if we substitute Eq. (22) into the integral over an interface thicknes then the above free energy together with the chemical potentials μ_0, μ_1 both for n_0 and n_1 will result in the specific interfacial free energy σ defined as

$$\sigma = n \int [\psi_0(\xi) + \kappa(\nabla\xi)^2 - \xi\mu_1 - (1 - \xi)\mu_0]dz. \qquad (23)$$

It also appears that, according to Eq. (23), the more diffuse the interface is, the smaller will be the contribiution of the gradient term $\kappa(\xi_{,z})^2$ in σ. In equilibrium the variation of ξ will be such that the integral (23) attains a minimum. This is equivalent to the requirement that the chemical potential $\mu(\mathbf{x}, t)$ must be constant throughout the medium.

In the subsequent paper Cahn[36], defining the affinity with the help of the variationl derivative of the extended free energy function:

$$\mathcal{A} \equiv \frac{\delta\psi}{\delta\xi} = \frac{\partial\psi}{\partial\xi} - \mathrm{div}\Big(\frac{\partial\psi}{\partial\nabla\xi}\Big) \qquad (24)$$

derived the following condition, more general then that of Mandelstam&Leontovich,

$$\frac{\delta\psi}{\delta\xi} \equiv 0 \qquad (25)$$

which is valid together with the symmetry relations analogous with those of Maxwell. Such defined affinity $\mathcal{A}$ plays now an important part in describing diffusion-controlled evolution of the microstructure[37]:

$$\partial_t\xi = -\mathrm{div}(\mathcal{J}_\xi) = -\mathrm{div}(-\mathsf{M}\mathrm{grad}\mathcal{A}), \qquad (26)$$

where the thermodynamic flux $\mathcal{J}_\xi$ is related to the affinity $\mathcal{A}$ through the kinetic (Onsager) relation

$$\mathcal{J}_\xi = -\mathsf{M}\mathrm{grad}\mathcal{A}. \qquad (27)$$

The presence of the gradient $\nabla\xi$ in Eq. (24) and the Laplace operator $\Delta = \mathrm{divgrad}(.)$, in Eq. (26) leads, even in a linear case, to differential equations of fourth order with respect to spatial derivatives. The positive quantity M should generally be interpreted as a kind of interfacial diffusion coefficient and therefore

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[36]J.W. Cahn (1959).
[37]J. W. Cahn (1961).

it can be expressed by the properties of the interface.

While the method used by Cahn and Hilliard is of phenomenological nature, the method used by E.W. Hart is the variational one. Hart has derived extended set of the Gibbs variational conditions for equilibrium phase transitions[38]. This kind of the description of the kinetics of phase transition is a continuation of the Gibbsian variational treatment. Strictly speaking, Hart extends the classical Gibbs variational principle [4] into the case of gradient microstructure. Additionally, by a new definition of variation $\delta\xi$ at the moving interface boundary, he was able to redefine the momentum flux. Choosing only the part of Hart's definition, which contains the first gradient $\nabla\xi$, we have

$$\mathbf{\Pi}^{\mathrm{re}} = [p - \mathrm{div}(\xi\psi_{\nabla\xi})]\mathbf{1} - \nabla\xi \otimes \psi_{\nabla\xi}. \tag{28}$$

This redefined flux contains, apart from thermodynamic pressure p, an extra shear stress and extra pressure. Such extra contributions to the momentum flux were the subject of numerous researches[39], in which not only variational methods were used.

It is seen from Eq. (28) that the extra momentum flux depends on the approximation of the free energy ψ in terms of ξ and $\nabla\xi$. For example, from the Bearman-Kirkwood theory it follows that their extra stress has the form[40]:

$$\mathbf{\Pi}^{\mathrm{re}} = p_0(\xi)\mathbf{1} - \square : [1/4\xi^2\nabla\nabla\epsilon_2 + \xi(\nabla\xi) \otimes (\nabla\epsilon_2)] \otimes [2\xi\nabla\nabla\xi - (\nabla\xi) \otimes (\nabla\xi)] \tag{29}$$

with

$$\square \equiv \mathbf{1} \otimes \mathbf{1} + (\mathbf{i}_j \otimes \mathbf{i}_k \otimes \mathbf{i}_k \otimes \mathbf{i}_j + \mathbf{i}_j \otimes \mathbf{i}_k \otimes \mathbf{i}_j \otimes \mathbf{i}_k), \tag{30}$$

where ϵ_2 is a correlation potential which is easy to predict on the basis of the 6-12 Leonnard-Jones model of the free energy density.

Rewriting now the Ginzburg-Landau evolution equation in terms of our scalar order parameter ξ as

$$\partial_t\xi = -\Gamma\mathcal{A} = -\Gamma\Big(\frac{\partial\psi}{\partial\xi} - \mathrm{div}\Big(\frac{\partial\psi}{\partial\nabla\xi}\Big)\Big), \tag{31}$$

it is easy to notice its relaxational character. Detailed solutions of this equation, performed by Chan[41] and Truskinovsky[42] exhibit nonlocal brinks oscillations in the structure of shock or interface layer. It should be pointed out that many

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[38]E.W. Hart (1959).

[39]for instance: Roshchin&Truskinowski (1989), Grmela (1993).

[40]H.T. Davis&L.E. Scriven (1981).

[41]S-K. Chan (1977).

[42]L. Truskinovsky (1982), (1985).

recently obtained results[43] could not have been obtained within the classical treatment of the Cauchy continuum. Generally speaking, models with a gradient microstructure allow us to obtain and predict a wide class of microscopic phenomena such as: pattern forming instabilities, self organization, turbulence and others with a characteristic internal-length scale.

3 A diffusion – relaxation model

3.1 Recoverable and dissipative brackets

There are methods which occupy an important position in the logical structure of analytical dynamics. Two of these are: the Poisson brackets that played a specific role in the early stages of the development of quantum mechanics, and the Lagrange brackets which express the constancy of the Lagrange differential invariant or Poincare integral invariant of analytical dynamics. A field-theory analogue of the Lagrange bracket is yet unknown but there is a hypothesis that it can be a starting point for obtaining a generalized Onsager-type symmetry condition[44]

$$\frac{\partial \mathcal{J}_\alpha}{\partial \mathcal{X}_\beta} = \frac{\partial \mathcal{J}_\beta}{\partial \mathcal{X}_\alpha} \tag{32}$$

between thermodynamic fluxes $\mathcal{J}_\alpha$ and thermodynamic forces $\mathcal{X}_\alpha$.

The field-theory, analogue of the Poisson brackets, was at first defined as a mathematical tool acting within the frame of the Lagrangean description, where it is called a canonical Poisson bracket. It has been applied for the first time to an ideal non-dissipative fluid[45]. The non-canonical Poisson bracket, however, is the Eulerian equivalent of the canonical one. It is to be derived either by conscious mapping from the Lagrange to Euler description or by *at hoc* postulating.

In this note we wish, standing on the ground of the Hamiltonian analytical mechanics, to discuss the possibility of the extension of the classical Poisson bracket formulation of the ideal fluid into a modified non-canonical bracket approach to ideal fluid with a scalar microstructure. It can be done in two different ways. The first one follows from the necessity of incorporating a new field variable ξ in the bracket theory. The second way consists in a derivation of dissipative brackets, which would be responsible for the description of irreversible phenomena, both in macroscopic balance equations and in an evolution equation for the

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[43] A. Onuki (1989), Umantsev&Roitburd (1988), L. Truskinovsky (1991) and others.

[44] M.A. Biot (1955).

[45] It was probably A. Clebsh (1859) who first has made an effort in expressing hydrodynamics within the Lagrange description and Hamiltonian approach.

microstructure[46]. Keeping in mind necessary clearness, we shall call, according to Grmela, the classical Poisson brackets *the convective brackets*. The two dissipation brackets we shall call *the diffusion* and *relaxation brackets*, respectively.

In this paragraph, the Hamiltonian structure of ideal fluid is recalled since we try to present at first the simplest case which, we suppose, shall be a starting point in seeking a more general Hamiltonian field-theory framework. Let us introduce few definitions usually applied in the process of derivation of the Hamiltonian structure. In classical hydrodynamics the ideal fluid is described by means of five fields: the mass density $\rho(\mathbf{x}, t)$, the total energy density $e(\mathbf{x}, t) = \rho\epsilon + 1/2\rho\mathbf{v}^2$ and the momentum density $\mathbf{p}(\mathbf{x}, t) = \rho\mathbf{v}$. Additionally, $s = \rho\eta$ is the entropy density and

$$\mathcal{S} = \int_v s\, dv, \mathcal{M} = \int_v \rho\, dv, \mathcal{E} = \int_v e\, dv, \mathcal{U} = \int_v \mathbf{p}\, dv, \tag{33}$$

are functionals called the entropy, mass, energy and momentum, respectively. They are defined for the appropriate (fixed) volume element dv.

However, it appears that the set of four equations (3)-(6) defined for ideal fluid can not be obtained from a single *Hamiltonian evolution equation*. It probably follows from deeper, not yet clear to us, properties of the Hamiltonian mechanics. The problem consists in mutual interactions between the conservation of energy and conservation of entropy. Every Hamiltonian theory starts either with the energy representation or entropy representation and therefore either the conservation of entropy or conservation of energy can finally be obtained[47].

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[46]The concept of dissipative bracket seems to emanate from Grmela (1986).

[47]The fundamentals of both formulations are given by the two Gibbs variational principles of reversible thermodynamics (see Gibbs (1875)):

I.(entropy representation) ,,For the equilibrium of any isolated system it is necessary and sufficient that in all possible variations of the state of the system which do not alter its energy, the variation of its entropy shall either vanish or be negative

$$(\delta\eta)_\epsilon \leq 0''.$$

II.(energy representation) ,,For the equilibrium of any isolated system it is necessary and sufficient that in all possible variations in the state of the system which do not alter its entropy, the variation of its energy shall either vanish or be positive

$$(\delta\epsilon)_\eta \geq 0''.$$

In other words, the first Gibbs variational principle (the entropy representation) asserts that a maximum in entropy implies the state of equilibrium when matter is disturbed in the volume in such a way that the total energy and mass remain constant. Inversely, the second Gibbs variational principle (energy representation) asserts that for a given amount of mass and constant total entropy, the total energy has a minimum when equilibrium is established. Van der Waals extended these principles into next two which would be a base for next two representations, i.e. the free energy representation and the free enthalpy representation (van der Waals (1893)). More details concerning the entropy and energy representations the reader may find in the article

Let us consider an arbitrary functional $\mathcal{F} = \int_v f(\rho, s, \mathbf{p}, \xi, \nabla\xi) dv$ within the entropy representation. Then the time derivative of $\mathcal{F}$ is

$$\partial_t \mathcal{F} = \partial_t \Big(\int_v f(\rho, s, \mathbf{p}, \xi, \nabla\xi) dv \Big) =$$

$$= \int_v \Big(\frac{\partial f}{\partial \rho} \frac{\partial \rho}{\partial t} + \frac{\partial f}{\partial s} \frac{\partial s}{\partial t} + \frac{\partial f}{\partial \mathbf{p}} \cdot \frac{\partial \mathbf{p}}{\partial t} + \frac{\partial f}{\partial \xi} \frac{\partial \xi}{\partial t} + \frac{\partial f}{\partial (\nabla\xi)} \cdot \frac{\partial \nabla\xi}{\partial t} \Big) dv = \qquad (34)$$

$$= \Big(\mathcal{F}_\rho \frac{\partial \rho}{\partial t} + \mathcal{F}_s \frac{\partial s}{\partial t} + \mathcal{F}_\mathbf{p} \cdot \frac{\partial \mathbf{p}}{\partial t} + \mathcal{F}_\xi \frac{\partial \xi}{\partial t} \Big).$$

In the above equation $\mathcal{F}_\rho, \mathcal{F}_s, \mathcal{F}_\mathbf{p}, \mathcal{F}_\xi$ denote the so-called Volterra variational derivatives. They can be obtained, for instance, by switching the order of differentiation in $\partial \nabla\xi / \partial t$ and integrating by parts the last term of Eq. (34). Then

$$\mathcal{F}_\xi \equiv \frac{\delta \mathcal{F}}{\delta \xi} = \frac{\partial \mathcal{F}}{\partial \xi} - \mathrm{div}\Big(\frac{\partial \mathcal{F}}{\partial \nabla\xi} \Big), \qquad (35)$$

denotes the Volterra variational derivative. The symbol $\delta\mathcal{F}/\delta\xi$ is taken from the variational calculus. It denotes the Euler-Lagrange equation resulting from the variation of $\mathcal{F}$ with respect to the variables ξ. Since the variable $\rho, s, \mathbf{p}$ in the simple ideal fluid enter into the functional $\mathcal{F}$ without spatial gradients, then in this case the Volterra variational derivative reduces to a simple derivative which shall be denoted by an additional coma

$$\mathcal{F}_\rho \equiv \mathcal{F}_{,\rho} = \frac{\partial \mathcal{F}}{\partial \rho}, \mathcal{F}_s \equiv \mathcal{F}_{,s} = \frac{\partial \mathcal{F}}{\partial s}, \mathcal{F}_\mathbf{p} \equiv \mathcal{F}_{,\mathbf{p}} = \frac{\partial \mathcal{F}}{\partial \mathbf{p}}. \qquad (36)$$

The balance equations for mass, momentum, and entropy, defined by Eqs. (3), (4) and (6), within the framework of entropy representation, are expressed in the Hamiltonian form:

$$\partial_t \mathcal{F} = \{\mathcal{F}, \mathcal{E}\}_\mathcal{C}, \qquad (37)$$

with the bracket operation $\{.,.\}_\mathcal{C}$ defined as follows[48] :

$$\{\mathcal{B}, \mathcal{C}\}_\mathcal{C} \equiv \int_v dv [\mathbf{p}.(\mathrm{grad}(\mathcal{B}_\mathbf{p})\mathcal{C}_\mathbf{p} - \mathrm{grad}(\mathcal{C}_\mathbf{p})\mathcal{B}_\mathbf{p}) +$$

$$+ \rho(\mathrm{grad}(\mathcal{B}_\rho).\mathcal{C}_\mathbf{p} - \mathrm{grad}(\mathcal{C}_\rho).\mathcal{B}_\mathbf{p}) + s(\mathrm{grad}(\mathcal{B}_s).\mathcal{C}_\mathbf{p} - \mathrm{grad}(\mathcal{C}_s).\mathcal{B}_\mathbf{p})]. \qquad (38)$$

The symbol grad(.) denotes spatial derivating, for example:

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by Sieniutycz&Berry (1989).

   [48]Grmela (1993).

$$\mathrm{grad}(\mathcal{B}_\mathbf{p}) = (\delta\mathcal{B}/\delta\mathbf{p}) \otimes \nabla = \partial_k(\mathcal{B}_{p_j})\mathbf{i}_j \otimes \mathbf{i}_k, \tag{39}$$

and the dot is a symbol of full contraction. The bracket (38) is the Poisson bracket since it is antisymmetric, $\{\mathcal{B},\mathcal{D}\}_\mathcal{C} = -\{\mathcal{D},\mathcal{B}\}_\mathcal{C}$ and satisfies the Jacobi identity, $\{\{\mathcal{B},C\},\mathcal{D}\}_\mathcal{C} + \{\{\mathcal{C},\mathcal{D}\},\mathcal{B}\}_\mathcal{C} + \{\{\mathcal{D},\mathcal{B}\},\mathcal{C}\}_\mathcal{C} = 0$.

Taking the functional $\mathcal{F} = \mathcal{F}(\rho, s, \mathbf{p})$ and the part of the definition (34) which is related to ρ, s and $\mathbf{p}$ only, the left-hand side of the evolution equation (37) takes the following form

$$\int_v (\mathcal{F}_{,\mathbf{p}}\,.\partial_t\mathbf{p} + \mathcal{F}_{,\rho}\,\partial_t\rho + \mathcal{F}_{,s}\,\partial_t s)dv, \tag{40}$$

whereas the right-hand side is

$$\int_v (\mathcal{F}_{,\mathbf{p}}\,.[-\mathrm{div}(\mathbf{p}\otimes e_{,\mathbf{p}}) - \mathbf{p}\mathrm{div}(e_{,\mathbf{p}}) - \rho\mathrm{grad}(e_{,\rho}) - s\mathrm{grad}(e_{,s})]+$$
$$+\mathcal{F}_{,\rho}\,[-\mathrm{div}(\rho e_{,\mathbf{p}})] + \mathcal{F}_{,s}\,[-\mathrm{div}(s e_{,\mathbf{p}})])dv. \tag{41}$$

Boundary conditions arising from the integration by parts are taken to be equal to zero. Since the *evolution equation* (37) holds for all functionals $\mathcal{F}$ from Eqs (37), (40) and (41) we obtain the set of equations that govern the evolution of mass, momentum and entropy, respectively:

$$\partial_t\rho = -\mathrm{div}(\rho e_{,\mathbf{p}}), \tag{42}$$

$$\partial_t\mathbf{p} = -\mathrm{div}(\mathbf{p}\otimes e_{,\mathbf{p}}) - \rho\mathrm{grad}(e_{,\rho}) - s\mathrm{grad}(e_{,s}) - \mathbf{p}\mathrm{grad}(e_{,\mathbf{p}}), \tag{43}$$

$$\partial_t s = -\mathrm{div}(s e_{,\mathbf{p}}). \tag{44}$$

It is not difficult to obtain the energy equation from the above equations. If we define the following quantity[49]

$$p(\mathbf{x}, t) \equiv -e + \rho e_{,\rho} + s e_{,s} + \mathbf{p}.e_{,\mathbf{p}}, \tag{45}$$

and make use of the following differential identity

$$\partial_i e = e_{,\rho}\,\partial_i\rho + e_{,s}\,\partial_i s + e_{,\mathbf{p}}\,.\partial_i\mathbf{p}, i = 1, 2, 3, \tag{46}$$

we will obtain the sought expression

$$-\mathrm{grad}p = -\rho\mathrm{grad}(e_{,\rho}) - s\mathrm{grad}(e_{,s}) - \mathbf{p}.grad(e_{,\mathbf{p}}). \tag{47}$$

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[49]Grmela (1993).

Using Eq. (47) and interpreting p as a thermodynamic pressure we note that the balance of momentum takes the familar form

$$\partial_t \mathbf{p} = -\text{div}(\mathbf{p} \otimes e_{,\mathbf{p}}) - \text{grad} p, \tag{48}$$

which, for $e_{,\mathbf{p}} \equiv \mathbf{v}$ and $\mathbf{p} = \rho \mathbf{v}$, is identical with Eq. (4). Starting with the following identity:

$$\partial_t e = e_{,\rho}\, \partial_t \rho + e_{,s}\, \partial_t s + e_{,\mathbf{p}}\, . \partial_t \mathbf{p}, \tag{49}$$

after some transformations we obtain

$$\begin{aligned}
\partial_t e &= -e_{,\rho}\, \text{div}(\rho e_{,\mathbf{p}}) - e_{,s}\, \text{div}(s e_{,\mathbf{p}}) - \\[4pt]
&\quad -e_{,\mathbf{p}}\,.[\text{div}(\mathbf{p} \otimes e_{,\mathbf{p}}) + \text{grad}(-e + \rho e_{,\rho} + s e_{,s} + \mathbf{p}.e_{,\mathbf{p}})] = \\[4pt]
&= -\text{div}(\rho e_{,s}\, e_{,\mathbf{p}}) + \text{grad}(e_{,\rho})(\rho e_{,\mathbf{p}}) - \\[4pt]
&\quad -\text{div}(s e_{,s}\, e_{,\mathbf{p}}) + \text{grad}(e_{,s})(s e_{,\mathbf{p}}) - \\[4pt]
&\quad -\text{div}(\mathbf{p}.e_{,\mathbf{p}}\, e_{,\mathbf{p}}) + \text{grad}(e_{,\mathbf{p}})(\mathbf{p} \otimes e_{,\mathbf{p}}) - e_{,\mathbf{p}}\,.\text{grad} p = \\[4pt]
&= -\text{div}[(\rho e_{,\rho} + s e_{,s} + \mathbf{p}.e_{,\mathbf{p}})e_{,\mathbf{p}}] = -\text{div}[(p + e)e_{,\mathbf{p}}].
\end{aligned} \tag{50}$$

Since $p + e = p + \rho\epsilon + 1/2\rho \mathbf{v}^2 = \rho(p/\rho + \epsilon) + 1/2\rho \mathbf{v}^2$, and $e_{,\mathbf{p}} = \mathbf{v}$ thus Eq. (50) is identical with Eq. (5):

$$\partial_t e = -\text{div}\mathcal{J}_e^{\text{re}}, \quad \mathcal{J}_e^{\text{re}} = (p + e)\mathbf{v}. \tag{51}$$

Let us now consider thermaly conducting and viscous fluid as an example of the extension of the Hamiltonian formulation of non-dissipative ideal fluid into a model of recoverable-dissipative fluid. Our task is, therefore, to introduce the irreversible part of the *evolution equation* using dissipative brackets defined as follows[50]

$$\begin{aligned}
\{\mathcal{F}, \mathcal{G}\}_{Diss} &= -\int_v dv \Big(\text{grad}_s(\mathcal{F}_{\mathbf{p}}) \frac{\delta\Phi}{\delta(\text{grad}_s(-\mathcal{G}_{\mathbf{p}}\mathcal{G}_s))} \Big) + \\[6pt]
&\quad +\text{grad}(\mathcal{F}_s)\Big(-\mathcal{G}_{\mathbf{p}}\mathcal{G}_s \frac{\delta\Phi}{\delta(\text{grad}_s(-\mathcal{G}_{\mathbf{p}}\mathcal{G}_s))} \Big) + \text{div}(\mathcal{F}_{\mathbf{p}}) \frac{\delta\Phi}{\delta(\text{div}(-\mathcal{G}_{\mathbf{p}}\mathcal{G}_s))} + \\[6pt]
&\quad +\text{grad}(\mathcal{F}_s)\Big(-\mathcal{G}_{\mathbf{p}}\mathcal{G}_s \frac{\delta\Phi}{\delta(\text{div}(-\mathcal{G}_{\mathbf{p}}\mathcal{G}_s))} \Big) + \text{grad}(\mathcal{F}_s)\Big(\mathcal{G}_s \frac{\delta\Phi}{\delta(\text{grad}(\mathcal{G}_s))} \Big).
\end{aligned} \tag{52}$$

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[50]Grmela (1986).

In the above definition Φ is a dissipative potential (Rayleigh dissipation function) which is a function of three variables: $\mathrm{div}\mathbf{v} = \mathrm{div}(e,_{\mathbf{p}})$, $\mathrm{grad}_s\mathbf{v} = 1/2(\mathbf{v} \otimes \nabla + \nabla \otimes \mathbf{v}) = \mathrm{grad}_s(e,_{\mathbf{p}})$ and $\mathrm{grad}(e,_s)$. In particular case, when Φ is chosen to be a quadratic potential, the dissipative evolution equation becomes either the Navier-Stokes (viscous) or Fourier (heat conducting) hydrodynamic equation. The dissipative bracket (52) is linear only with respect to $\mathcal{F}_\rho, \mathcal{F}_s, \mathcal{F}_{\mathbf{p}}$ and nonlinear with respect to the generating functional $\mathcal{G}$. Keeping in mind the commonly known Navier-Stokes-Fourier type of approximation we postulate additive convective and dissipative brackets within a general evolution equation

$$\partial_t \mathcal{F} = \{\mathcal{F}, \mathcal{E}\}_{\mathcal{C}} + \{\mathcal{F}, \mathcal{E}\}_{\mathcal{D}iss}. \tag{53}$$

Repeating the calculations showed in (52) and (50) it is easy to find the extended set of balance equations for conducting and viscous fluid:

$$\partial_t \rho = -\mathrm{div}(\rho e,_{\mathbf{p}}), \tag{54}$$

$$\partial_t \mathbf{p} = -\mathrm{div}(p \otimes e,_{\mathbf{p}}) - \mathrm{grad}p + \mathrm{div}\Big(\frac{\delta\Phi}{\delta(\mathrm{grad}_s e,_{\mathbf{p}})}\Big) + \mathrm{grad}\Big(\frac{\delta\Phi}{\delta(\mathrm{div}e,_{\mathbf{p}})}\Big), \tag{55}$$

$$\partial_t e = -\mathrm{div}\Big[(p + e)e,_{\mathbf{p}}\Big] + \mathrm{div}\Big(\frac{\delta\Phi}{\delta(\mathrm{grad}_s e,_{\mathbf{p}})}e,_{\mathbf{p}}\Big) +$$

$$+\mathrm{div}\Big(\frac{\delta\Phi}{\delta(\mathrm{div}e,_{\mathbf{p}})}e,_{\mathbf{p}}\Big) + \mathrm{div}\Big(e,_s \frac{\delta\Phi}{\delta(\mathrm{grad}e,_s)}\Big), \tag{56}$$

$$\partial_t s = -\mathrm{div}(se,_{\mathbf{p}}) + \mathrm{div}\Big(e,_s^{-1} \frac{\delta\Phi}{\delta(\mathrm{grad}e,_s)}\Big) + \frac{1}{e,_s}\sigma_{(s)}. \tag{57}$$

Defining now the total fluxes of mass, momentum, energy and entropy as:

$$\mathcal{J}_\rho = \rho e,_{\mathbf{p}}, \tag{58}$$

$$\mathbf{\Pi} = \mathbf{\Pi}^{\mathrm{re}} + \mathbf{\Pi}^{ir} = (p\mathbf{I} + \mathbf{p}\otimes e,_{\mathbf{p}}) + \Big(-\frac{\delta\Phi}{\delta(\mathrm{grad}_s e,_{\mathbf{p}})} - \frac{\delta\Phi}{\delta(\mathrm{div}e,_{\mathbf{p}})}\mathbf{I}\Big), \tag{59}$$

$$\mathcal{J}_e \equiv \mathcal{J}_e^{\mathrm{re}} + \mathcal{J}_e^{ir} = ([e + p]e,_{\mathbf{p}}) + (\mathbf{\Pi}^{ir}e,_{\mathbf{p}} + \mathbf{q}^{ir}), \tag{60}$$

$$\mathcal{J}_\eta \equiv \mathcal{J}_\eta^{conv} + \mathcal{J}_\eta^{ir} = (se,_{\mathbf{p}}) + (\mathbf{q}^{ir}e_s^{-1}), \tag{61}$$

where the irreversible heat flux is given by

$$\mathbf{q}^{ir} = -e,_s \frac{\delta\Phi}{\delta(\mathrm{grad}e,_s)}, \tag{62}$$

we can rewrite the equations (54)-(57) in the standard form of conducting and viscous fluid

$$\partial_t \rho = -\text{div}\mathcal{J}_\rho, \tag{63}$$

$$\partial_t \mathbf{p} = -\text{div}\mathbf{\Pi}, \tag{64}$$

$$\partial_t e = -\text{div}\mathcal{J}_e, \tag{65}$$

$$\partial_t s = -\text{div}\mathcal{J}_\eta + e_s^{-1}\sigma_{(\eta)}. \tag{66}$$

From the properties of convexity of dissipative potential Φ it follows that the production of entropy $\sigma_{(\eta)}$ in Eq. (66) should satisfy

$$\sigma_{(\eta)} \geq 0. \tag{67}$$

3.2 Recoverable evolution equations for mass, momentum, energy, entropy and a hidden variable ξ

The evolution equation (53) is a prototype of the equation which combines in additive manner, both recoverable and dissipative properties of a material. This experimentally motivated way of splitting will be used in this paragraph. We shall try to extend the set of independent variables by our hidden scalar variable ξ.

The assumption on the additive decomposition of the recoverable-dissipative properties of the microstructure is physically strongly restrictive. There is no heuristic motivation for doing so. Therefore, it should be remembered that the restriction follows rather from the available mathematical tools. For example, it is a very well known property of the Hamiltonian approach that the entire system, e.g. the macroscopic ideal fluid and a scalar microstructure associated with it are governed by the same time-dependent evolution equation for all state variables.

These are $(\rho, s, \mathbf{p}, \xi)$ – in entropy representation, or $(\rho, e, \mathbf{p}, \xi)$ – in energy representation. We are especially interested in finding an evolution equation for the microstructure, which involves the extra contributions following from $\nabla\xi$.

We also assume, in analogy to Eq. (53), that the recoverable-dissipative time-dependent evolution equation, either for $(\rho, s, \mathbf{p}, \xi)$ or $(\rho, e, \mathbf{p}, \xi)$ posesses the following form

$$\partial_t \mathcal{F} = \{\mathcal{F}, \mathcal{E}\}_\mathcal{C} + \{\mathcal{F}, \mathcal{E}\}_\mathcal{R} + \{\mathcal{F}, \mathcal{E}\}_\mathcal{D}, \tag{68}$$

where the dissipative properties are carried either by the relaxational bracket $\{,\}_\mathcal{R}$ or the diffusional one $\{,\}_\mathcal{D}$. The total energy $\mathcal{E}$ is the generating functional.

Passing on to the analysis of the convective bracket $\{,\}_\mathcal{C}$, which is the main subject of this paragraph, it should be pointed out that the property of the Hamiltonian structure of the bracket $\{,\}_\mathcal{C}$ remains valid when the bracket is extended

into the scalar microstructure. Like in the case of ideal fluid, we assume that the total energy $\mathcal{E}$ is the generating functional, but it must be extended to include the recoverable contributions coming from ξ and $\nabla\xi$, e.i. $\mathcal{E} = \mathcal{E}(\rho, s, \mathbf{p}, \xi, \nabla\xi)$.

Following Grmela and others[51] we extend the recoverable bracket (38) as follows:

$$
\begin{aligned}
\{\mathcal{F}, \mathcal{G}\}_{\mathcal{C}} = & \int_v dv\rho[\mathrm{grad}(\mathcal{F}_\rho)\mathcal{G}_{\mathbf{p}} - \mathrm{grad}(\mathcal{G}_\rho)\mathcal{F}_{\mathbf{p}}] + \\
& + \int_v dv\mathbf{p}.[\mathrm{grad}(\mathcal{F}_{\mathbf{p}})\mathcal{G}_{\mathbf{p}} - \mathrm{grad}(\mathcal{G}_{\mathbf{p}})\mathcal{F}_{\mathbf{p}}] + \\
& + \int_v dvs[\mathrm{grad}(\mathcal{F}_s)\mathcal{G}_{\mathbf{p}} - \mathrm{grad}(\mathcal{G}_s)\mathcal{F}_{\mathbf{p}}] + \\
& + \int_v dv\xi[\mathrm{grad}(\mathcal{F}_\xi)\mathcal{G}_{\mathbf{p}} - \mathrm{grad}(\mathcal{G}_\xi)\mathcal{F}_{\mathbf{p}}].
\end{aligned}
\tag{69}
$$

It is easily noticed that the first integral in Eq. (69) coincides with that of Eq. (38), whereas the last integral in Eq. (69) is logically the simplest extension of Eq. (38) into a scalar microstructure. Unfortunately, there is only a single coupling, from four possible, of the microstructure with macroscopic fields $(\rho, s, \mathbf{p})$. We mean here the coupling via the momentum field $\mathbf{p}$. Undoubtedly, it is a serious disadvantage of the above definition. What is important, however, that the convective bracket (69) remains the Poisson bracket. It practicaly means that the definition (69) enables only recoverable, non-dissipative properties. To proof this statement let us notice that, similarly to (38), the bracket (69) depends linearly on $\mathcal{F}_\xi, \mathcal{G}_\xi$ and $\{\mathcal{F}, \mathcal{G}\}_{\mathcal{C}} = -\{\mathcal{G}, \mathcal{F}\}_{\mathcal{C}}$. By direct verification, the Jacobi identity can also be proved. Since no gradiends of $\rho, s, \mathbf{p}$ are accounted for in $\mathcal{F}_\rho, \mathcal{F}_s, \mathcal{F}_{\mathbf{p}}$, therefore these denotations mean practically $\mathcal{F}_{,\rho}, \mathcal{F}_{,s}, \mathcal{F}_{,\mathbf{p}}$, whereas $\mathcal{F}_\xi$ or $\mathcal{G}_\xi$ still denote the Volterra variational derivative defined by Eq. (35).

The non-dissipative time evolution of the fields $(\rho, s, \mathbf{p}, \xi)$ is given by the convective bracket (69) with $\mathcal{E}$ as a generating functional

$$
\partial_t \mathcal{F} = \{\mathcal{F}, \mathcal{E}\}_{\mathcal{C}},
\tag{70}
$$

which holds for an arbitrary functional $\mathcal{F}(\rho, s, \mathbf{p}, \xi, \nabla\xi)$. According to the definition (34) and (69) we obtain

$$
\partial_t \mathcal{F} = \int_v dv\{\mathcal{F}_{,\rho}\, \partial_t\rho + \mathcal{F}_{,s}\, \partial_t s + \mathcal{F}_{,\mathbf{p}}\, .\partial_t\mathbf{p} + \mathcal{F}_\xi\partial_t\xi\},
\tag{71}
$$

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[51] Gremla (1986), Edwards&Beris (1991).

$$\{\mathcal{F}, \mathcal{E}\}_{\mathcal{C}} = \int_v dv \{\mathcal{F}_{,\rho} \operatorname{div}(-\rho e_{,\mathbf{p}}) + \mathcal{F}_{,s} \operatorname{div}(-se_{,s}) + \mathcal{F}_{,\mathbf{p}} \operatorname{div}(-\mathbf{p} \otimes e_{,\mathbf{p}}) +$$

$$+ \mathcal{F}_\xi \operatorname{div}(-\xi e_\xi) + \operatorname{div}(\rho \mathcal{F}_{,\rho} e_{,\mathbf{p}}) + \operatorname{div}(s \mathcal{F}_{,s} e_{,\mathbf{p}}) + \operatorname{div}(\mathbf{p}.\mathcal{F}_{,\mathbf{p}} e_{,\mathbf{p}}) + \tag{72}$$

$$+ \operatorname{div}(\mathcal{F}_\xi \xi e_{\mathbf{p}}) + \mathcal{F}_{,\mathbf{p}}.[-\rho \operatorname{grad}(e_{,\rho}) - s \operatorname{grad}(e_{,s}) - \mathbf{p}.\operatorname{grad}(e_{,\mathbf{p}}) - \xi \operatorname{grad}(e_\xi)]\}.$$

Omitting at this stage the formulation of the model of the boundary conditions, which follow from the replacing the volume integral by the integral over its bounded surface, from (70), (71) and (72) we have

$$\mathcal{F}_{,\rho}: \qquad \partial_t \rho = -\operatorname{div}(\rho e_{,\mathbf{p}}), \tag{73}$$

$$\mathcal{F}_{,\mathbf{p}}: \partial_t \mathbf{p} = -\operatorname{div}(\mathbf{p} \otimes e_{,\mathbf{p}}) -$$
$$- [\rho \operatorname{grad}(e_{,\rho}) + s \operatorname{grad}(e_{,s}) + \mathbf{p}.grad(e_{,\mathbf{p}}) + \xi \operatorname{grad}(e_\xi)], \tag{74}$$

$$\mathcal{F}_{,s}: \partial_t s = -\operatorname{div}(se_{,\mathbf{p}}), \tag{75}$$

$$\mathcal{F}_\xi: \partial_t \xi = -\operatorname{div}(\xi e_{,\mathbf{p}}). \tag{76}$$

The momentum balance equation (74) can, similarly to Eqs. (45)-(48), be transformed to a more familiar form. If we define a ,,thermodynamic pressure" as

$$p = -e + \rho e_{,\rho} + s e_{,s} + \mathbf{p}.e_{,\mathbf{p}} + \xi e_{,\xi} + \nabla \xi.e_{,\nabla \xi}, \tag{77}$$

and remembering about the following identity ($k = 1, 2, 3$)

$$\operatorname{grad} e = [e_{,\rho} \partial_k \rho + e_{,s} \partial_k s + e_{,\mathbf{p}}.\partial_k \mathbf{p} + e_{,\xi} \partial_k \xi + e_{,\nabla \xi}.\partial_k(\nabla \xi)]\mathbf{i}_k, \tag{78}$$

we obtain the following simplified formula:

$$-\operatorname{grad} p = \rho \operatorname{grad}(e_{,\rho}) +$$
$$+ s \operatorname{grad}(e_{,s}) + \mathbf{p}.grad(e_{,\mathbf{p}}) + \xi \operatorname{grad}(e_{,\xi}) + \nabla \xi.\operatorname{grad}(e_{,\nabla \xi}). \tag{79}$$

Inserting now Eq. (79) into Eq. (74) and using the identity

$$\xi \operatorname{grad}(e_\xi) = \xi \operatorname{grad}(e_{,\xi}) - \operatorname{div}(\xi \operatorname{grad}(e_{,\nabla \xi})) + \nabla \xi \operatorname{grad}(e_{,\nabla \xi}), \tag{80}$$

we obtain a more familiar form of the balance of momentum

$$\partial_t \mathbf{p} = -\text{div}(\mathbf{p} \otimes e_{,\mathbf{p}}) - \text{grad}p - \text{div}\mathbf{\Pi}_\xi, \tag{81}$$

where the extra stress flux $\mathbf{\Pi}_\xi$ is defined as:

$$\mathbf{\Pi}_\xi = -\xi\text{grad}(e_{,\nabla\xi}) = [-\xi\partial_i(e_{,\partial_j\xi})]\mathbf{i}_j \otimes \mathbf{i}_i. \tag{82}$$

It is easy to notice that another definition of the extra pressure is obtained when the extra stress flux is equivalent to (77) and (82)

$$\partial_t \mathbf{p} = -\text{div}(\mathbf{p} \otimes e_{,\mathbf{p}}) - \text{grad}p' - \text{div}\mathbf{\Pi}'_\xi, \tag{83}$$

where[52]

$$p' = p - \text{div}(\xi e_{,\nabla\xi}), \tag{84}$$

$$\mathbf{\Pi}'_\xi = \nabla\xi \otimes e_{,\nabla\xi}. \tag{85}$$

Before passing on to the problem of energy balance, we note that there are two equivalent ways of obtaining the evolution equation for $\mathcal{E}$.

The first one is based on a type of calculations similar to (41)-(50), in which the Gibbs-like formula (49) plays an important role.

The second one, conceptually simpler, is based on changing the entropy representation by the energy representation, under the assumption that this transformation is the one-to-one mapping. Generally, this way is possible[53] if we replace the Volterra variational derivatives from the entropy to energy representations using the following mnemotechnic rules, respectively:

$$\frac{\delta}{\delta\rho} \longrightarrow \frac{\delta}{\delta\rho} + e_\rho\frac{\delta}{\delta e}, \qquad \frac{\delta}{\delta s} \longrightarrow e_s\frac{\delta}{\delta e},$$

$$\frac{\delta}{\delta\mathbf{p}} \longrightarrow \frac{\delta}{\delta\mathbf{p}} + e_\mathbf{p}\frac{\delta}{\delta e}, \qquad \frac{\delta}{\delta\xi} \longrightarrow \frac{\delta}{\delta\xi} + e_\xi\frac{\delta}{\delta e} - \text{div}(e_{\nabla\xi}\frac{\delta}{\delta e}), \tag{86}$$

where $e_{\nabla\xi} \equiv e_{,\nabla\xi}$ since $\partial e/\partial(\nabla \otimes \nabla\xi)$ is equal to zero from the definition. By inserting Eq. (86) into the original Poisson bracket (69) we obtain

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[52] The definition $\mathbf{\Pi}'_\xi$ is preferred by Truskinovski (1992) whereas the extra stress flux in the form of $\mathbf{\Pi}_\xi$ was used by Hart (1959).

[53] Grmela (1986).

$$\{\mathcal{F}, \mathcal{G}\}_{\mathcal{C}} = \int_v dv\{s[\mathrm{grad}(e_s\mathcal{F}_e).\mathcal{G}_\mathbf{p} - \mathrm{grad}(e_s\mathcal{G}_e).\mathcal{F}_\mathbf{p}] +$$

$$+\rho[\mathrm{grad}(\mathcal{F}_\rho + e_\rho\mathcal{F}_e).\mathcal{G}_\mathbf{p} - \mathrm{grad}(\mathcal{G}_\rho + e_\rho\mathcal{G}_e).\mathcal{F}_\mathbf{p}] +$$

$$+\mathbf{p}.[\mathrm{grad}(\mathcal{F}_\mathbf{p} + e_\mathbf{p}\mathcal{F}_e)\mathcal{G}_\mathbf{p} - \mathrm{grad}(\mathcal{G}_\mathbf{p} + e_\mathbf{p}\mathcal{G}_e)\mathcal{F}_\mathbf{p}] +$$

$$+\xi[\mathrm{grad}(\mathcal{F}_\xi + e_\xi\mathcal{F}_e)\mathcal{G}_\mathbf{p} - \mathrm{grad}(\mathcal{G}_\xi + e_\xi\mathcal{G}_e)\mathcal{F}_\mathbf{p}] -$$

$$-\xi[\mathrm{grad}(\mathrm{div}(e_\mathbf{p}\mathcal{F}_e))\mathcal{G}_\mathbf{p} - \mathrm{grad}(\mathrm{div}(e_\mathbf{p}\mathcal{G}_e))\mathcal{F}_\mathbf{p}] +$$

$$+\rho e_\mathbf{p}.[\mathrm{grad}(\mathcal{F}_\rho)\mathcal{G}_e - \mathrm{grad}(\mathcal{G}_\rho)\mathcal{F}_e] +$$

$$+\mathbf{p}\otimes e_\mathbf{p}.[\mathrm{grad}(\mathcal{F}_\mathbf{p})\mathcal{G}_e - \mathrm{grad}(\mathcal{G}_\mathbf{p})\mathcal{F}_e] -$$

$$-\xi e_\mathbf{p} \otimes e_{\nabla\xi}.[\mathrm{grad}(\mathrm{grad}(\mathcal{F}_e))\mathcal{G}_e - \mathrm{grad}(\mathrm{grad}(\mathcal{G}_e))\mathcal{F}_e] -$$

$$-\xi e_\mathbf{p}\mathrm{grad}^T(e_{\nabla\xi}).[\mathrm{grad}(\mathcal{F}_e)\mathcal{G}_e - \mathrm{grad}(\mathcal{G}_e)\mathcal{F}_e] +$$

$$+e_\mathbf{p}(\rho e + \mathbf{p}.e_\mathbf{p} + se + \xi e - \xi\mathrm{div}(e_{\nabla\xi})[\mathrm{grad}(\mathcal{F}_e)\mathcal{G}_e - \mathrm{grad}(\mathcal{G}_e)\mathcal{F}_e]\}.$$

$$(87)$$

This is the Poisson bracket for $(\rho, e, \mathbf{p}, \xi)$ variables in energy representation. Starting with the Gibbs-like formula (49) and using the right-hand sides of equations (73)-(76) we arrive at

$$\partial_t e = e_{,\rho}\left[-\mathrm{div}(\rho e_{,\mathbf{p}})\right] + e_{,s}\left[-\mathrm{div}(se_{,\mathbf{p}})\right] +$$
$$+e_{,\mathbf{p}}\left[-\mathrm{grad}p - \mathrm{div}(\mathbf{p}\otimes e_{,\mathbf{p}}) - \mathrm{div}\mathbf{\Pi}_\xi\right] + e_\xi[-\mathrm{div}(\xi e_{,\mathbf{p}})], \qquad (88)$$

which transforms to

$$\partial_t e = -\mathrm{div}(e_{,\rho}\,\rho e_{,\mathbf{p}} + e_{,\mathbf{p}}\,(\mathbf{p}\otimes e_{,\mathbf{p}}) + e_{,s}\,se_{,\mathbf{p}} + e_\xi\xi e_{,\mathbf{p}}) +$$

$$+\mathrm{grad}(e_{,\rho})\rho e_{,\mathbf{p}} + \mathrm{grad}(e_{,\mathbf{p}})(\mathbf{p}\otimes e_{,\mathbf{p}}) + \mathrm{grad}(e_{,s})se_{,\mathbf{p}} + \qquad (89)$$

$$+\mathrm{grad}(e_\xi)(\xi e_\xi) - e_{,\mathbf{p}}.(\mathrm{grad}p + \mathrm{div}\Pi_\xi).$$

Using the identities

$$-\mathrm{div}(e_\xi\xi e_{,\mathbf{p}}) = -\mathrm{div}([e_{,\xi} - \mathrm{div}(e_{,\nabla\xi})]\xi e_\mathbf{p}) =$$
$$= -\mathrm{div}(e_{,\xi}\,\xi e_{,\mathbf{p}} + e_{,\nabla\xi}.\nabla\xi e_{,\mathbf{p}}) + \mathrm{div}(\mathrm{div}(\xi e_{,\nabla\xi})e_{,\mathbf{p}}), \qquad (90)$$

$$\mathrm{grad}[e_{,\xi} - \mathrm{div}(e_{,\nabla\xi})](\xi e_{,\mathbf{p}}) =$$
$$= \mathrm{grad}(e_{,\xi})\xi e_{,\mathbf{p}} - \mathrm{div}(\mathrm{grad}^T(e_{,\nabla\xi})\xi)e_{,\mathbf{p}} + \nabla\xi.\mathrm{grad}(e_{,\nabla\xi})e_{,\mathbf{p}}, \qquad (91)$$

which lead to the exclusion of the expression $-e_{,\mathbf{p}}.\mathrm{grad}p$, one can obtain

$$\partial_t e = -\mathrm{div}[(\rho e_{,\rho} +\mathbf{p}.e_{,\mathbf{p}} +se_{,s} +\xi e_{,\xi} +\nabla\xi.e_{,\nabla\xi})e_{,\mathbf{p}}]-$$

$$-\mathrm{div}(\mathbf{\Pi}_\xi e_{,\mathbf{p}}) + \mathbf{\Pi}_\xi.\mathrm{grad}(e_{,\mathbf{p}}) - \mathrm{div}(\mathrm{grad}^T(e_{,\nabla\xi})\xi).e_{,\mathbf{p}} = \qquad (92)$$

$$= -\mathrm{div}[(p + e)e_{,\mathbf{p}}] - \mathrm{div}\mathbf{q}_\xi - \mathrm{div}(\mathbf{\Pi}_\xi e_{,\mathbf{p}}),$$

where the extra momentum flux $\mathbf{\Pi}_\xi$ is defined by Eq. (82) and the extra energy flux $\mathbf{q}_\xi$ is given by

$$\mathbf{q}_\xi = -\mathrm{div}(\xi e_{,\nabla\xi})e_{,\mathbf{p}} +\xi\mathrm{grad}(e_{,\nabla\xi})e_{,\mathbf{p}} . \qquad (93)$$

This is the equation which govern the non-dissipative time evolution of the total energy for simple ideal fluids with a scalar microstructure. This equation follows from the Gibbs-like formula (49) and the local equilibrium relation (77). It can also be proved by virtue of the calculation of the convective bracket (87) in energy representation. Note that the bracket (87) is again the Poisson bracket. Moreover, there exist a distinguished functional $\mathcal{C}$ ($\mathcal{C}$ - Casimir) for the bracket (87) which satisfies $\{\mathcal{F},\mathcal{C}\}_{\mathcal{F}}$. This distinguished functional is the total entropy

$$\mathcal{S} = \int_v sdv = \int_v \rho\eta dv, \qquad (94)$$

e.g. $\partial_t\mathcal{F} = \{\mathcal{F},\mathcal{S}\}_{\mathcal{C}} = 0$ which implies the non-dissipation condition. The vector $\mathbf{q}_\xi$ should rather be treated as a recoverable energy flux[54] even if this vector is responsible for the introduction of the gradient of temperature.

3.3   Dissipative contributions in the evolution equations

Having a set of four dynamical variables $\rho, s, \mathbf{p}, \xi$ we must select appropriate dissipative affinities. In the simplest case we shall assume the following set of the spatial gradients of affinities: $\mathrm{grad}(\frac{\delta e}{\delta\rho}), \mathrm{grad}(\frac{\delta e}{\delta s}), \mathrm{grad}(\frac{\delta e}{\delta\mathbf{p}}), \mathrm{grad}(\frac{\delta e}{\delta\xi})$ as a possible source of dissipation.

In order to satisfy the mass balance in a simple fluid we put $\mathrm{grad}(e_\rho) = 0$ and obtain the following set of thermodynamic forces

$$\mathcal{X}_\alpha = \{\nabla e_s, \nabla e_\mathbf{p}, e_\xi, \nabla e_\xi\}, \qquad \alpha = 1, 2, 3, 4, \qquad (95)$$

which, in respect to the previous definitions $T = \frac{\delta e}{\delta s}, \mathcal{A} = \frac{\delta e}{\delta\xi}, \mathbf{v} = \frac{\delta e}{\delta\mathbf{p}}$, have the familiar form[55]

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[54]Grmela (1993).

[55]we are interested only in the symmetrical part of the velocity gradient, denoted earlier by $\mathbf{d}$.

$$\mathcal{X}_\alpha = \{\nabla T, \nabla \otimes \mathbf{v}, \mathcal{A}, \nabla \mathcal{A}\}. \tag{96}$$

A corresponding set of thermodynamic fluxes should now be defined as

$$\mathcal{J}_\alpha = \{\mathbf{q}^{ir}, \mathbf{\Pi}^{ir}, \sigma_\xi, \mathcal{J}_\xi\}, \tag{97}$$

where the first two arguments $\mathbf{q}^{ir}, \mathbf{\Pi}^{ir}$ are similar to those in the viscous and heat conducting Navier-Stokes-Fourier fluid. These are the vectors of irreversible heat and irreversible viscous momentum flux, respectively. Sometimes it is comfortable to split $\mathbf{\Pi}^{ir}$ into spherical $p^{ir}\mathbf{I}$ and traceless dyadic $\mathbf{\Pi}^{ir(d)}$. We wish here to extend the Mandelstam&Leontovich [14] concept according to which the irreversible pressure p^{ir} can exist in the phase transforming ideal fluid. It is because the transforming fluid possesses an artificial (operational) second viscosity $\eta'(\xi)$ which vanishes for $\xi = 0$ or $\xi = 1$:

$$p^{ir} = \eta' \mathrm{div}\mathbf{v}. \qquad . \tag{98}$$

We shall assume that the transforming ideal fluid also posesses an artificial thermal conductivity $k(\xi)$[56] and artificial shear viscosity $\eta(\xi)$. Although the kinetic relationships between $\mathcal{X}_\alpha$ and $\mathcal{J}_\alpha$ looks quite standard, the cross and nonlinear contributions should play an essential role. Denoting by $\mathcal{L}_{\alpha\beta}$ the kinetic coefficients, we can write down the relation

$$\mathcal{J}_\alpha = \mathcal{L}_{\alpha\beta} \mathcal{X}_\beta$$

between the generalized fluxes $\mathcal{J}_\alpha$ and corresponding generalized forces $\mathcal{X}_\beta$ in the following expanded form:

$$\mathbf{q}^{ir} = [\mathcal{L}_{11} + \mathcal{L}_{11\xi}e_\xi\mathbf{I} + \mathcal{L}_{11p}\nabla \otimes e_\mathbf{p} + \mathcal{L}_{11\mathbf{p}}^{''}(\nabla \otimes e_\mathbf{p})^2]\nabla(e_s) +$$
$$+[\mathcal{L}_{14} + \mathcal{L}_{14\xi}e_\xi\mathbf{I} + \mathcal{L}_{14\mathbf{p}}\nabla \otimes e_\mathbf{p} + \mathcal{L}_{14\mathbf{p}}^{''}(\nabla \otimes e_\mathbf{p})^2]\nabla(e_\xi) + \ldots, \tag{99}$$

$$\mathbf{\Pi}^{ir} = \mathcal{L}_{22}\nabla \otimes e_\mathbf{p} + \mathcal{L}_{22}^{''}(\nabla \otimes e_\mathbf{p})^2 + \mathcal{L}_{23}e_\xi\mathbf{I} + \mathcal{L}_{24}\nabla(e_\xi) \otimes \nabla(e_\xi) +$$
$$+\mathcal{L}_{24}\nabla(e_\xi) \otimes \nabla(e_\xi) + \mathcal{L}_{24}^{''}(\nabla(e_\xi) \otimes \nabla(e_\xi))^2 + \mathcal{L}_{21}^{''}(\nabla(e_s) \otimes \nabla(e_s))^2 + \ldots, \tag{100}$$

$$\sigma_\xi = \mathcal{L}_{33}e_\xi + \mathcal{L}_{32}\mathrm{div}(e_\mathbf{p}) + \mathcal{L}_{34}\nabla(e_\xi).\nabla(e_\xi) + \mathcal{L}_{31}\nabla(e_s).\nabla(e_s) + \ldots, \tag{101}$$

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[56]this quantity was introduced by D.Kardas for quite different reasons.

$$\mathcal{J}_\xi = (\mathcal{L}_{44} + \mathcal{L}_{44\xi} e_\xi \mathbf{I} + \mathcal{L}_{44\mathbf{p}} \nabla \otimes e_\mathbf{p} + \mathcal{L}''_{44\mathbf{p}} (\nabla \otimes e_\mathbf{p})^2) \nabla(e_s) +$$

$$+ (\mathcal{L}_{41} + \mathcal{L}_{41\xi} e_\xi \mathbf{I} + \mathcal{L}_{41\mathbf{p}} \nabla \otimes e_\mathbf{p} + \mathcal{L}''_{41\mathbf{p}} (\nabla \otimes e_\mathbf{p})^2) \nabla(e_\xi). \qquad (102)$$

These are hypothetical kinetic equations for the entirely coupled irreversible interactions of the scalar microstructure and macroscopic fields. In the above algebraic relations we prefer the notation according to the definition (95) instead of the classical one (96). It is since in Eq. (95) all the thermodynamic forces have the same logical status. They are the variational derivatives of the recoverable total energy.

The kinetic equations (99)-(102) provides us with the information on defining the dissipation potential Φ (similarly to Eq.(52)) as well as the analysis of the dissipation bracket. The form of the dissipation bracket depends upon the kind of representation employed for the system as well as upon dynamical variables. Extending the methodology used in the previous paragraphs, we choose entropy representation and a set dynamical variables given by Eq. (95). Since our generating functional represents the total energy $\mathcal{E}$, which according to the first law of thermodynamics remains constant, then, consequently $\partial_t \mathcal{E} = \{\mathcal{E}, \mathcal{E}\}_\mathcal{C} + \{\mathcal{E}, \mathcal{E}\}_{\mathcal{D}iss} = 0$ and $\{\mathcal{E}, \mathcal{E}\}_{\mathcal{D}iss} = 0$. Since, according to the second law of thermodynamics, the entropy production $\sigma_{(\eta)}$ must be positive thus we can write $\partial_t \mathcal{S} = \{\mathcal{S}, \mathcal{E}\}_{\mathcal{D}iss} \geq 0$.

Having the prototype of the dissipation bracket (52) we can define the required dissipation bracket[57]. Denoting by $f = (\rho, s, \mathbf{p}, \xi)$ and $g = (\rho, \mathbf{p}, \xi)$ two sets of dynamical variables and by $\frac{\delta \mathcal{E}}{\delta f} = (\frac{\delta e}{\delta \rho}, \frac{\delta e}{\delta s}, \frac{\delta e}{\delta \mathbf{p}}, \frac{\delta e}{\delta \xi})$ the variational derivatives of f, we obtain, for a generating functional $\mathcal{G}$, the dissipation bracket in the form:

$$\{\mathcal{F}, \mathcal{G}\}_{\mathcal{D}iss} =$$
$$\mathcal{I}\Big[\Big(\frac{\delta \mathcal{F}}{\delta g}, \nabla\Big(\frac{\delta \mathcal{F}}{\delta f}\Big)\Big)_{linear}, \frac{\delta \mathcal{G}}{\delta f}, \nabla\Big(\frac{\delta \mathcal{G}}{\delta f}\Big)\Big] + \frac{\delta \mathcal{F}}{\delta s} \Phi\Big(\frac{\delta \mathcal{G}}{\delta f}, \nabla\Big(\frac{\delta \mathcal{G}}{\delta f}\Big)\Big). \qquad (103)$$

In the above equation the integral $\mathcal{I}$ is linear with respect to $\frac{\delta \mathcal{F}}{\delta g}$ and $\nabla(\frac{\delta \mathcal{F}}{\delta f})$. Additionally, we pulled out the linear dependence on $\frac{\delta \mathcal{F}}{\delta s}$ and wrote it separately togheter with the dissipation potential Φ.

Generally, the quantities $\frac{\delta \mathcal{E}}{\delta f}$ and $\mathrm{grad}(\frac{\delta \mathcal{E}}{\delta f})$ represent the possible affinites. The former is associated with the relaxational phenomena and the latter with diffusional ones. Therefore, in practice, the dissipation bracket can be decomposed in the following way

$$\{\mathcal{F}, \mathcal{G}\}_{\mathcal{D}iss} = \{\mathcal{F}, \mathcal{G}\}_\mathcal{R} + \{\mathcal{F}, \mathcal{G}\}_\mathcal{D}, \qquad (104)$$

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[57]J. Edwards&A.N. Beris (1991)

into the relaxational and diffusional bracket, respectively. However, it must be pointed out that only the microstructural affinity $\frac{\delta e}{\delta \xi} = \mathcal{A}$ is included in the thermodynamic force $\mathcal{X}_\alpha$. Similarly, the gradient of $\frac{\delta e}{\delta \rho}$ is omitted in defining the diffusion bracket. The dissipation bracket for the system which is close to equilibrium will be linear also with respect to $\mathcal{G}$. In this case only few couplings from (99)-(102) will be possible:

$$\{\mathcal{F}, \mathcal{G}\}_{\mathcal{D}iss} = \int_v \mathcal{L}_{22}\mathrm{grad}(\mathcal{F}_\mathbf{p})\mathrm{grad}(\mathcal{G}_\mathbf{p})dv - \int_v \mathcal{L}_{11}\mathrm{grad}(\mathcal{F}_s)\mathrm{grad}(\mathcal{G}_s)dv -$$

$$- \int_v \mathcal{L}_{44}\mathrm{grad}(\mathcal{F}_\xi)\mathrm{grad}(\mathcal{G}_\xi)dv - \int_v \mathcal{L}_{33}(\mathcal{F}_\xi \mathcal{G}_\xi)dv - \int_v \mathcal{L}_{23}\mathrm{grad}(\mathcal{F}_\mathbf{p})\mathcal{G}_\xi dv -$$

$$- \int_v \mathcal{L}_{32}\mathrm{div}(\mathcal{G}_\mathbf{p})\mathcal{F}_\xi dv + \int_v \mathcal{L}_{22}\mathcal{F}_s(\mathrm{grad}(\mathcal{G}_\mathbf{p}) \otimes \mathrm{grad}(\mathcal{G}_\mathbf{p}))dv + \int_v \mathcal{L}_{33}\mathcal{F}_s(\mathcal{G}_\xi \mathcal{G}_\xi)dv + \tag{105}$$

$$+ \int_v \mathcal{L}_{11}\mathcal{F}_s(\mathrm{grad}(\mathcal{G}_s) \otimes \mathrm{grad}(\mathcal{G}_s))dv + \int_v \mathcal{L}_{44}\mathcal{F}_s(\mathrm{grad}(\mathcal{G}_\xi) \otimes \mathrm{grad}(\mathcal{G}_\xi)).$$

From the above equation a purely dissipative evolution equation for $\mathbf{p}, s, \xi$ follows:

$$\partial_t \mathbf{p} = -\mathrm{div}[\mathcal{L}_{22}\mathrm{grad}(e_\mathbf{p})] - \mathrm{grad}(\mathcal{L}_{23}e_\xi), \tag{106}$$

$$\partial_t s = -\mathrm{div}(e_s \mathcal{L}_{11}grad e_s) + \mathcal{L}_{22}.(\nabla e_\mathbf{p}) \otimes (\nabla e_\mathbf{p}) +$$

$$+ \mathcal{L}_{11}.\mathrm{grad}(e_s) \otimes \mathrm{grad}(e_s) + \mathcal{L}_{33}e_\xi e_\xi + \mathcal{L}_{44}.(\nabla e_\xi) \otimes (\nabla e_\xi), \tag{107}$$

$$\partial_t \xi = -\mathrm{div}(\mathcal{L}_{44}\nabla e_\xi) + \mathcal{L}_{33}e_\xi + \mathcal{L}_{32}\mathrm{div}(e_\mathbf{p}). \tag{108}$$

Taking the definition (101) and (102) into account, equation (108) can be rewritten as an evolution equation for the conservative order parameter ξ:

$$\partial_t \xi = -\mathrm{div}(\mathcal{J}_\xi) + \sigma_\xi. \tag{109}$$

This general form of the evolution of microstructure allows both for diffusional and relaxational contributions. One of the simplest case is a model with isotropic microstructure, i.e.

$$\sigma_\xi = -\Gamma \mathcal{A}, \tag{110}$$

$$\mathcal{J}_\xi = -\mathsf{M}\mathrm{grad}\mathcal{A}, \tag{111}$$

for which $\mathbf{\Pi}^{ir} = \mathbf{q}^{ir} = 0, \Gamma > 0, \mathsf{M} > 0, \mathcal{L}_{33} = -\Gamma, \mathcal{L}_{44} = -\mathsf{M}\mathbf{I}$. For an incompressible fluid $\mathrm{div}(e_\mathbf{p}) = 0$ and we arrive at

$$\partial_t \xi = -\mathrm{div}(-\mathsf{M}\mathrm{grad}\mathcal{A}) - \Gamma \mathcal{A}. \tag{112}$$

This is a relaxational-diffusive evolution equation for a microstructure. For $\mathsf{M} = 0$ the equation becomes a purely relaxational, whereas for $\Gamma = 0$ it is a purely diffusional one. The former form is called the Ginzburg-Landau equation and the latter is known as the Cahn-Hilliard equation. In the former case it is easy to find relaxational and diffusional brackets which satisfy Eq. (104). Assuming that only $\mathcal{L}_{33} = -\Gamma$ and $\mathcal{L}_{44} = -\mathsf{M}\mathbf{I}$ are different form zero, the dissipative bracket (105) reduces to:

$$\{\mathcal{F}, \mathcal{G}\}_{\mathcal{R}} = \int_v \frac{\delta\mathcal{F}}{\delta\xi}(-\Gamma)\frac{\delta\mathcal{G}}{\delta\xi}dv, \tag{113}$$

$$\{\mathcal{F}, \mathcal{G}\}_{\mathcal{D}} = \int_v \mathrm{grad}(\frac{\delta\mathcal{F}}{\delta\xi})(-\mathsf{M}\mathbf{I})\mathrm{grad}(\frac{\delta\mathcal{G}}{\delta\xi})dv. \tag{114}$$

These brackets have independently been postulated by Grmela [46].

Turning now to the energy equation, we notice that it can be obtained from

$$\partial_t e = -\mathrm{div}(\mathbf{q}^{ir}_\xi + \mathbf{\Pi}^{ir}e_{\mathbf{p}}), \tag{115}$$

where

$$\mathbf{q}^{ir}_\xi = \mathbf{q}^{ir} + e_\xi\mathcal{L}_{23}e_{\mathbf{p}} + e_\xi\mathcal{L}_{44}\mathrm{grad}(e_\xi), \tag{116}$$

and $\mathbf{q}^{ir}$ and $\mathbf{\Pi}^{ir}$ are defined by Eqs (90) and (100), respectively.

3.4 The final set of equations

The phenomenological (operational) coefficients $\mathcal{L}_{\alpha\beta}$ ($\alpha, \beta = 1, 2, 3, 4$) in the kinetic equations (99)-(102) have deliberately been unspecified so as to preserve the evolution equations as general as possible. These equations allow defining the final set of governing equations for ideal fluid with a scalar microstructure. They comprise the recoverable contributions (73), 81), (75), (92), (76) as well as dissipative ones expressed by Eqs. (106), (107), (108),(116), respectively. Finally, we obtain the evolution equations for mass, momentum, energy, entropy and microstructure:

$$\partial_t \rho = -\mathrm{div}(\mathcal{J}_\rho), \tag{117}$$

$$\partial_t \mathbf{p} = -\mathrm{div}(\mathbf{p}{\otimes}e_{\mathbf{p}}) - \mathrm{grad}p - \mathrm{div}(\mathbf{\Pi}_\xi + \mathbf{\Pi}^{ir}), \tag{118}$$

$$\partial_t e = -\mathrm{div}[(p + e)e_{\mathbf{p}}] - \mathrm{div}[\mathbf{q}_\xi + \mathbf{q}^{ir}_\xi + (\mathbf{\Pi}_\xi + \mathbf{\Pi}^{ir})e_{\mathbf{p}}], \tag{119}$$

$$\partial_t s = -\mathrm{div}[se_{\mathbf{p}} + e_s^{-1}\mathbf{q}^{ir}] + \sigma_{(\eta)}, \tag{120}$$

$$\partial_t \xi = -\mathrm{div}(\xi e_\mathbf{p} + \mathcal{J}_\xi) + \sigma_\xi, \tag{121}$$

where $\mathcal{J}_\rho, p, \boldsymbol{\Pi}_\xi, \Pi^{ir}, \mathbf{q}_\xi, \mathbf{q}_\xi^{ir}, \mathbf{q}^{ir}, \mathcal{J}_\xi, \sigma_\xi$ are given by Eqs. (58), (77), (82), (100), (93), (117), (99), (102) and (101), respectively, whereas $\sigma_{(\eta)}$, as it follows from Eq. (108), is

$$\sigma_{(\eta)} = \mathcal{L}_{22} \cdot (\nabla e_\mathbf{p}) \otimes (\nabla e_\mathbf{p}) + \mathcal{L}_{11} \cdot \mathrm{grad}(e_s) \otimes \mathrm{grad}(e_s) +$$
$$+ \mathcal{L}_{33} e_\xi e_\xi + \mathcal{L}_{44} \cdot \mathrm{grad}(e_\xi) \otimes \mathrm{grad}(e_\xi). \tag{122}$$

Equations (117)-(121) are the governing equations for classical ideal fluid with a scalar microstructure. This set of equations must be supplemented by boundary and initial conditions as well as by a condition for incipient point, e.g. the point where the evolution equation for ξ must start working.

3.5 A simple model of flashing flow

In flashing water flow the order parameter ξ is interpreted as a dryness fraction x, e.g. the mass fraction of vapour phase in two-phase medium [61]. The specific internal energy of the mixture is not only a function of specific energies of the constituent phases but depends also on the interfacial energy [62]. The internal energies of particular phases are determined by a specific entropy s and a specific volume v, whereas the internal energy of the interfaces is expressed by the dryness fraction x and its spatial gradient ∇x. This statement can be written as [63]:

$$\epsilon = x\epsilon_v(v, s) + (1 - x)\epsilon_l(v, s) + \epsilon_i(x, \nabla x) \tag{123}$$

The same definition is valid for the remaining potentials, e.g. enthalpy, free energy and free enthalpy.

One-dimensional balance equations are given as follows [64]:

- mass conservation for the mixture

$$\partial_t \rho + w\partial_z \rho + \rho \partial_z w = -\frac{A'}{A}\rho w \tag{124}$$

- momentum conservation for the mixture

$$\partial_t w + w\partial_z w + \rho^{-1}\partial_z p = -\frac{C\tau}{A\rho} - g \tag{125}$$

- energy conservation for the mixture

$$\partial_t h + w\partial_z h - \rho^{-1}\partial_t p - w\rho^{-1}\partial_z p = \frac{C\tau w}{A\rho} \tag{126}$$

• vapour production

$$\partial_t x + w\partial_z x = -\frac{x - \bar{x}}{\beta} - \frac{(x - \bar{x})^3}{\gamma} + \kappa\partial_z^2(x - \bar{x}) \tag{127}$$

The above set of equations can be written in a compact form [65]:

$$A\partial_t \sigma + B\partial_z \sigma = C + D\partial_z^2 \sigma \tag{128}$$

where A and B are the matrices of coefficients, C is the vector of algebraic sources and D stands for the matrix of differential source terms. Performing the analysis of small perturbations we obtain the following dispersion relation for the model with a relaxational-gradient microstructure [65]:

$$det[-i\omega A + ikB + k^2 D - \partial_\sigma C + E] = 0 \tag{129}$$

which under some assumptions reduces to [65]:

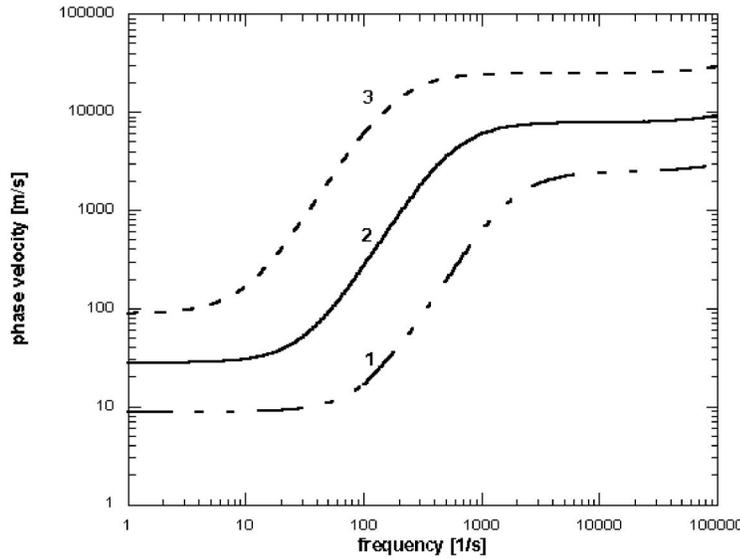$$[if_1]k^4 + [\omega f_2 + i(f_3 + \omega^2 f_4)]k^2 + [\omega^3 f_5 + i\omega^2 f_6] = 0 \tag{130}$$

Figure 1: Phase velocity c_{ph} versus frequency ω for different values of the capillarity coefficient: 1 - $\kappa = 0.08$, 2 - $\kappa = 0.8$, 3 - $\kappa = 8.0$.

This is a biquadratic equation with respect to the wave number k. It posesses four complex solutions which compose two pairs. The real parts of the solutions within one pair have the same magnitude and differ only in sign. It means that the model posesses two velocities of propagation of small perturbations which can propagate with these velocities in both directions. The most important is the higher of them since this velocity determines the conditions of choking. An example of the performed calculations is shown in Fig.1. This figure presents the dependence of the higher phase velocity $c_{ph}(\omega)$ on frequency ω and exhibits dispersive properties of the model. Futher results concerning of flashing flows are presented in [66].

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Model pynu doskonaego ze skalarn mikrostruktur.
Zastosowanie do opisu odparowania rozprnego wody.

Streszczenie

Opis pynu doskonaego, w ktrym zachodzi nierwnowagowa przemiana fazowa opisywana jedym parametrem skalarnym ξ (parametr porzdku typu stopie suchoci) uzupeniono o trzy elementy. Dwa pierwsze to dodatkowe strumienie pdu i energii wynikajce z obecnoci gradientw ∇_ξ zarwno w energii wewntrznej jak i w funkcji dysypacyjnej Rayleigha. Element trzeci to uoglnione rwnanie ewolucyjne na skalar ξ opisujce zarwno relaksacyjne jak i dyfuzyjne mody przemiany fazowej.