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A Thermodynamically Consistent Relaxation Model for Turbulent, Binary Mixture Undergoing Phase Transition

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Abstract

Non-equilibrium phenomena within a turbulent, binary mixture undergoing a phase transition are modelled based on the one fluid, homogeneous approach. The set of governing evolution equations is given and the averaged basic balance laws are considered. The continuum under consideration consists of two constituents of which the first is undergoing a phase transition (vaporisation, cavitation, flashing, condensation) during the flow with turbulent transport of mass, heat and momentum. Starting from the Clausius-Duhem inequality for the recoverable specific entropy, several thermodynamical relationships for equilibrium and non-equilibrium fields are developed. The relaxation-retardation constitutive model for turbulent, phasic and diffusive fluxes are described. It is shown that the resulting model uncovers a few known two-phase models of turbulence and also the classical relaxation models as limiting cases.

1. Introduction

Recently, there have been a number of promising developments in the formulation of turbulent, multiphase, multi-component transport processes within flowing mixtures undergoing phase transitions [1–5]. The models developed are stemmig from governing equations that have the form of conservative equations and could be easily implemented with the existing computer codes [6–10]. In this paper we shall extend the approach developed since 1994 at IFFM PAS-ci Gdańsk in the Centre of Fluid Thermomechanics under Professor Zbigniew Bilicki's leadership.

The subject of our consideration is a category of two-phase flows, including turbulent flows undergoing phase transitions. As a special case of these flows one can consider bubbly flows, slurry flows, gas-particle and gas-droplet flows. The flow of solid dispersive particles is omitted, since such proceses, including fluidised bed reactors, particle generation and reaction processes, solid transport and separation phenomena

Table 1. Possible theoretical backgrounds for models.

	Source and origins of the basic approach	Examples of applications
1	Fundamental equation of kinetic gas theory with Maxwell's closure for the collision integral	Extended Irreversible Thermodynamics [36,35]
2	Fundamental equation of kinetic gas theory with probability density function	Statistical and PDF models of turbulence [63]
3	Fundamental equation of kinetic gas theory with Boltzmann's non-equilibrium PDF	Non-equilibrium turbulence [42] Non-local continua [51]
4	Fundamental equation of kinetic gas theory with constrains of the Tait, Reissner type	Thermodynamics of continua with the internal parameters [49] Continua with microstructure [53] Non-equilibrium phase transition [21,41]
5	Reynolds' splitting of mass, momentum and energy equations into sub-systems	Classical "RANS" averaged modes of turbulence [26] Two-fluid models of mixture [18]
6	Lagrangian-Hamilitonian variation approach	Variation statement of irreversible phenomena [38] Configurational forces [52] Equilibrium phase transition [59,31]

should be described via more complex models in which the turbulent interaction between the fluid and the particle plays a key role. Our considerations are connected with finding a consistent numerical model for turbulent fluid mixtures undergoing phase transition (mainly: *stress induced phase transition*).

There are a few candidates for such mathematical models accounting for the state of turbulence, phase, transition and diffusion of constituents. The most familiar models are shown in Table 1, and the Internal Variables Approach is preferred in this article. This approach stems from Joseph Kestin's line of reasoning [11,12] and assumes that the non-equilibrium turbulent sub-structure and the non-equilibrium phasic sub-structure can be described within the framework of the thermodynamics of internal parameters.

2. Basic Balances for the Homogeneous Non-Equilibrium Model

2.1. Basic variables

In contrast to the two-fluid (two-field) approach, let us suppose that a particle of a continuum is homogeneous enough to be treated as a medium which possesses properly phenomenological parameters such as: *density*, *velocity* and *temperature*. The phasic, turbulent and diffusive sub-structure of the particle will be called here phasic, turbulent and diffusive microstructure, respectively. As usual in thermomechanics, three fundamental balances are postulated in the following form:

Balance of mass:

$$\frac{\partial}{\partial t}(\rho) + \operatorname{div}(\rho \mathbf{v} + \mathbf{p}_\rho) = \operatorname{div}(\mathbf{J}^t_\rho + \mathbf{J}^{op}_\rho + \mathbf{J}^d_\rho) + \rho s_\rho. \tag{2.1}$$

Balance of momentum:

$$\frac{\partial}{\partial t}(\rho\mathbf{v} + \mathbf{p}_\rho - \mathbf{J}^t_\rho - \mathbf{J}^{op}_\rho - \mathbf{J}^d_\rho) + \operatorname{div}(\rho\mathbf{v}\otimes\mathbf{v} + \mathbf{v}\otimes\mathbf{p}_\rho + \mathbf{p}_\rho\otimes\mathbf{v} + \mathbf{p}_\rho)$$
$$= \operatorname{div}(\tau + \mathbf{J}^t_\rho + \mathbf{J}^{op}_\rho + \mathbf{J}^d_\rho) + \rho\mathbf{b}. \tag{2.2}$$

Balance of energy:

$$\frac{\partial}{\partial t}(\rho e) + \operatorname{div}(\rho e\mathbf{v} + \mathbf{p}_p\mathbf{v} + \mathbf{p}_e) = \operatorname{div}(T\mathbf{J}_s + \mathbf{J}^t_e + \mathbf{J}^{op}_e + \mathbf{J}^d_e + \tau^c\mathbf{v}) + \rho s_e. \tag{2.3}$$

Here, subscripts ρ, p, e, for instance, in $\mathbf{J}_\rho$, $\mathbf{J}_p$, $\mathbf{J}_e$ denote fluxes of mass, momentum and energy, respectively. Superscripts t, op, d denote turbulent, operational (phasic) and diffusive fluxes, respectively. In the above equations, three kinds of fluxes are postulated:

$$\begin{aligned}
&\text{convective :} && \rho\mathbf{v}, \rho\mathbf{v}\otimes\mathbf{v}, \rho e\mathbf{v},\\
&\text{recoverable :} && \mathbf{p}_\rho, \mathbf{p}_p, \mathbf{p}_e,\\
&\text{dissipative :} && \mathbf{J}^\alpha_\rho, \mathbf{J}^\alpha_p, \mathbf{J}^\alpha_e, \quad \alpha = t, op, d,
\end{aligned}$$

and the conventional fluxes: τ – the viscous flux of momentum, $\mathbf{J}_s$ – the flux of entropy.

2.2. *Two-fluid connections*

Let us consider a mixture of two constituents (water and air) and assume the motion of the first constituent to undergo the phase transition and let the mass fraction of a new phase be denoted by x. Let $\rho_\beta(\mathbf{x}, t)$, $\beta = w, a$ (water, air) be the density and $\mathbf{v}^\beta(\mathbf{x}, t)$ the velocity of constituent β at the point $\mathbf{x}$ at time t. Based on fundamental results [13–15], we introduce the following definitions for the mixture density ρ, the concentration c_β of constituent β, the barycentric (phenomenological) velocity $\mathbf{v}$, the slip velocity $\mathbf{u}$, and the mass fraction x of the new phase of the water constituents:

$$\rho = \rho_w + \rho_a, \quad c_\beta = \rho_\beta/\rho, \tag{2.4}$$

$$\mathbf{v} = c_w\mathbf{v}^w + c_a\mathbf{v}^a = c_\beta\mathbf{v}^\beta, \quad \beta = w, a, \tag{2.5}$$

$$\mathbf{u} = \mathbf{v}^w - \mathbf{v}^a, \quad \rho_w\left(1 + x\frac{\rho'_w}{\rho''_w} - x\right) = \rho'_w. \tag{2.6}$$

Here ρ'_w, ρ''_w are the density on the situration line dividing the water and vapour from the matastable state, respectively [16,17].

The basic unknowns, from the point of view of the two-fluid approach, are ρ_w, ρ_a, $\mathbf{v}^w$, $\mathbf{v}^a$. However, ρ, $c = c^a$, $\mathbf{v}$, $\mathbf{u}$ are taken here, as the basic unknowns. Since the mass concentration of air $c^a = c$, in technical applications is usually small, it is acceptable to use the volumetric air fraction φ instant of c.

2.3. Comments on balance of mass

The balance of mass (2.1) has been obtained from the averaging procedure adopted by Ishii [18] in which a fluid has a phasic, turbulent and diffusive microstructure. It is assumed that the vectors $\mathbf{p}_\rho$, $\mathbf{J}^t_\rho$, $\mathbf{J}^{op}_\rho$, J^d_ρ represent an internal mass transport within the continuum particle and that this transport is flux-free, which means practically that the fluxes under considerations fulfill the following condition:

$$\operatorname{div}(\mathbf{p}_\rho) = \operatorname{div}(\mathbf{J}^t_\rho + \mathbf{J}^{op}_\rho + \mathbf{J}^{\mathrm{d}}_\rho) + \rho s_\rho. \tag{2.7}$$

This equation requires some kind of self-agreed evolution of the phasic, turbulent and diffusive mass transport. It can be interpreted as a sort of pseudo-mass balance, postulated in analogy to the pseudo-momentum and pseudo-energy balances [19–21]. Taking Kestin's line of argument [11] as a pattern of approach, one finds that Eq. (2.7) describes ''mass derived forces'' in analogy to ''momentum derived forces'' [22]:

$$\operatorname{div}\mathbf{C} = \rho_a \mathbf{f}_a + \rho_w \mathbf{f}_w, \tag{2.8}$$

where $\mathbf{C} = C_{ij}\mathbf{e}_i \otimes \mathbf{e}_j$ is the pseudo-momentum flux (or the chemical potential tensor) and the forces $\mathbf{f}_a$, $\mathbf{f}_w$ are acting on the both sides of an inter-phase surface.

Having fulfilled Eq. (2.7), the balance of mass of binary turbulent mixture undergoing a phase transition is simply written as:

$$\frac{\partial}{\partial t}(\rho) + \operatorname{div}(\rho \mathbf{v}) = 0. \tag{2.9}$$

The sources of mass s_ρ in Eqs. (2.1) and (2.7) are defined as a simple sum of mass sources growing in local balances of constituents, and usually it is set to zero.

2.4. Recoverable fluxes

The additional recoverable flux of mass $\mathbf{p}_\rho$, that appears in Eq. (2.1), comes from the nature of mass transport in a turbulent, phasic and diffusive mixture that does not have purely dissipative character. The momentum transfer posseses the same recoverable-dissipative character. Usually, an inter-phase surface, which divides both the state of medium (laminar-turbulent, parent-new, nondifussional-difussional), possesses an operational, recoverable elasticity. Let us recall that a part of these elastic properties is commonly described as the surface tension σ (i.e., $\mathbf{C} = \sigma\delta_{\alpha\beta}\mathbf{e}_\alpha \otimes \mathbf{e}_\beta$, $\alpha, \beta = 1, 2$) or the surface moments $C_{(1)}$, $C_{(2)}$ [23,20]. Following these arguments, some recoverable fluxes $\mathbf{p}_\rho$, $\mathbf{p}_p$, $\mathbf{p}_e$ should be postulated as responsible for the transport of elastic properties of the microstructure[1]. The presence of $\mathbf{p}_\rho$, $\mathbf{p}_p$, $\mathbf{p}_e$ in the balance follows also from the variational formulation of a fluid undergoing a phase transition that takes into

account the space gradients of internal parameters describing the evolution of the phasic, turbulent and diffusive microstructure. In particular, one can support this line of reasoning with the kind of variational principles developed by Natanson [24], Eglit [25] and Grmela [26][2]. Generally, all these principles up from the Gibbs variational formulation [23], and can be easily extended to modern situations [22,27]. It should be pointed out that according to the variational approach, the recoverable energy flux $\mathbf{p}_e$ is obtained as a supplementation of the balance of energy.

2.5. Dissipative momentum fluxes

The fluxes of momentum on the right side of Eq. (2.2), represent a dissipative manner of the momentum transport that, as follows from the principle of stress additivity [21,28], can be independently postulated in the form:

$$\begin{aligned}
&\boldsymbol{\tau} && - \text{ viscous stresses of mixture (Newton stress)},\\
&\mathbf{J}_p^{op} = O_{ij}\mathbf{e}_i \otimes \mathbf{e}_j && - \text{ operative (phasic) flux of momentum},\\
&\mathbf{J}_p^{t} = J^t{}_{ij}\mathbf{e}_i \otimes \mathbf{e}_j && - \text{ turbulent flux of momentum (Reynolds-like stress)},\\
&\mathbf{J}_p^{d} = D_{ij}\mathbf{e}_i \otimes \mathbf{e}_j && - \text{ diffusive flux of momentum (Fick stress)}.
\end{aligned}$$

The role of the dissipative fluxes τ_{ij}, $J^t{}_{ij}$, D_{ij} is generally well explained and usually accepted in the literature (see [17,29]). However, a word of explanation should be given as to why the operative flux O_{ij} is included. The motivation for considering it is based on the papers of Maldenstam and Leontovich [30]. They found that if the internal energy contains a contribution from the internal parameter then from the arguments of the Clausius-Duhem inequality it follows that an additional viscous pressure must be taken into account. An operative (phasic) second (bulk) viscosity defines the viscous operative pressure. Recently, different closures for operative bulk viscosity have been worked out [32,33] and included in the set of governing equations [5] as well as numerically verified [8,10,31,32,34,35].

2.6. Dissipative energy fluxes

We are considering a general case in which both constituents (water and air) and both phases of water have different temperatures. Especially important, from the point of view of the Homogeneous Non-Equilibrium Model [15,18,36], is the case of thermal non-equilibrium that arises in a flow containing a subcooled liquid undergoing a very fast (a few milliseconds) out flow into a low pressure medium. This thermal non-equilibrium model is especially important for determination of mass flow rates in critical flashing flows of vapour-liquid mixtures. Bilicki *et al.* [37–39] pointed out the importance of considering the thermal disequilibrium and slip between phases to predict critical mass flow rates. On the basis of analytical predictions and some

[1] The recoverable flux of momentum $\mathbf{p}_p$ has been postulated in literature as the recoverable Korteweg stress tensor [31].

[2] The full review and re-evaluation of the set of variational principles one can find in Sieniutycz's monograph [19].

available experimental data [40–43], they have shown that when the void fractions are small, the interface slip can be neglected. In such a case the fluid can be considered as a bubbly mixture, where the vapour bubbles are dragged along by the liquid and it is only the slip **u** between two constituents (water and air).

The thermal non-equilibrium between phases only becomes significant when the bubble nucleation is incipient [6]. In general, the mechanical and thermal non-equilibrium has an influence on the form of the energy balance equation. In Eq. (2.3) it has been postulated that the following energy fluxes exist:

$$\begin{aligned}
&\mathbf{J}_s = J_i^s \mathbf{e}_i && - \text{ vector of entropy flux,}\\
&\mathbf{J}_e^t = J_i^t \mathbf{e}_i && - \text{ vector of turbulent heat flux,}\\
&\mathbf{J}_e^{op} = J_i^{op} \mathbf{e}_i && - \text{ vector of operative heat flux,}\\
&\mathbf{J}_e^d = J_i^d \mathbf{e}_i && - \text{ vector of diffusive heat flux.}
\end{aligned}$$

The recoverable energy flux $\mathbf{p}_e$ has been postulated with regard to the gradient mixture model [18,36], the gradient turbulence model [44–46] and the gradient phase transition model [27,34,47]. Other fluxes are: the turbulent heat flux $\mathbf{J}_e^t$ and the diffusive heat flux $\mathbf{J}_e^d$, which appear frequently in the framework of models of homogeneous mixtures, but are formulated on the basis of sometimes contradictory assumptions (see, for instance, [18,48,49]). The operative energy flux $\mathbf{J}_e^{op}$ has been introduced and numerically verified by Kardás [7]. This flux is responsible for an additional dissipative transport of energy in the fluid undergoing stress induced phase transition like shock condensation and flashing.

Here, the flux of entropy also appears as $\mathbf{q} = T\mathbf{J}_s$. Now we adopt the heat flux as a special subcategory of microstructure – the heat microstructure [33,50]. This microstructure is mass-less but possesses the abilities of transient phenomena and heat super-conducting properties.

2.7. Total energy

The reason for adopting the energy balance in the above form follows from the experimentally documented fact that the internal specific energy, which is understood here as a recoverable energy, could also contain some part of the dissipation energy which is permanently locked in at a continuum particle. After removing motion, this energy is recovered as a relaxational flow. Therefore, in Eq. (2.3) the total energy e is: $\rho e = \rho u + \rho \mathbf{v}^2/2 + E^{op+t+d}$, where E^{op+t+d} denotes a recoverable part of energy associated with any purely dissipative flow. For flows undergoing a phase transition such an energy has been postulated by Maldenstam and Lenntonovich [30, see 1,11,15] and for turbulent flows by Elghobashi and Abu-Arab [13, see 52,53].

2.8. Governing evolution equations for the microstructure

In the literature, there are a few fundamental statements which allow to formulate equations for the inception, growth, evolution and decay of a microstructure [27,53,54]. Our line of reasoning is to develop the Internal Parameter approach for two important

cases: first, *flux-less evolutions*, where an evolution equation has a form of time evolution (Ginzburg-Landau type) and second, *flux-affinity evolutions*, where an evolution equation has a form of space-time evolution (Chan-Hillard type). In both cases similarities to Extended Irreversible Thermodynamics can be found [5,33,50].

Let us consider, for simplicity, an arbitrary internal parameter α (scalar, vector, tensor), that describes, in phenomenological manner, any property of the phasic, turbulent or diffusive microstructure. According to the basic statements of the Internal Variables Thermodynamics [12,55,56], an internal phenomenon on the macroscopic level can appear only via a function within two functionals: first – the recoverable internal energy $e = e(s, v, \alpha, \dot{\alpha}, \nabla\alpha)$ and second – the dissipative energy functional $D = D(\nabla T, \nabla \mathbf{v}, \dot{\alpha}, \nabla\dot{\alpha}, \ddot{\alpha})$. Connected to both functions, the recoverable and the dissipative energy, are the configurational forces, recoverable and dissipative, respectively. However, for the flux-less evolution and flux-affinity evolution the dissipative forces are differently defined.

The flux-less evolution approach

If the state of the macro-system is described by the specific entropy, certain mechanical variables and the internal parameter with first space and time derivatives, the system having a total energy $e = e(s, v, \alpha, \partial_t\alpha, \nabla\alpha)$ and a specific dissipation function $D = D(\nabla T, \nabla \mathbf{v}, \dot{\alpha}, \nabla\dot{\alpha}, \ddot{\alpha})$, it is defined, in the framework of continuum thermomechanics, according to the following reversible configurational forces [27]:

$$\boldsymbol{A}^{(r)} = \frac{\delta e}{\delta \alpha} = \frac{\partial e}{\partial \alpha} - \frac{\partial}{\partial x_i}\left(\frac{\partial e}{\partial(\partial_i \alpha)}\right) - \frac{d}{dt}\left(\frac{\partial e}{\partial \dot{\alpha}}\right), \tag{2.10}$$

and, the irreversible configurationl forces [53]:

$$\boldsymbol{A}^{(ir)} = \frac{\delta D}{\delta \dot{\alpha}} = \frac{\partial D}{\partial \dot{\alpha}} - \frac{\partial}{\partial x_i}\left(\frac{\partial D}{\partial(\partial_i \dot{\alpha})}\right) - \frac{d}{dt}\left(\frac{\partial D}{\partial \ddot{\alpha}}\right), \tag{2.11}$$

where the symbol $\delta/\delta\alpha$ denotes the Volterra type derivative that is to be defined correctly on the grounds of the variational approach [19,57]. In the case of a flux-less evolution approach, both forces, the reversible $\boldsymbol{A}^{(r)}$ and the irreversible $\boldsymbol{A}^{(ir)}$ (called sometimes – the affinity) do not contribute to the balance of energy. Therefore, the total cofigurational force is

$$\boldsymbol{A}^{(tot)} = \boldsymbol{A}^{(r)} + \boldsymbol{A}^{(ir)} = 0. \tag{2.12}$$

It follows from Eqs. (2.10) and (2.11) that the above condition leads to the equation

$$\frac{\partial e}{\partial \alpha} - \frac{\partial}{\partial x_i}\left(\frac{\partial e}{\partial(\partial_i \alpha)}\right) - \frac{d}{dt}\left(\frac{\partial e}{\partial \dot{\alpha}}\right) = -\left[\frac{\partial D}{\partial \dot{\alpha}} - \frac{\partial}{\partial x_i}\left(\frac{\partial D}{\partial(\partial_i \dot{\alpha})}\right) - \frac{d}{dt}\left(\frac{\partial D}{\partial \ddot{\alpha}}\right)\right], \tag{2.13}$$

which connects the internal parameter α with its rates $\dot{\alpha}, \ddot{\alpha}, \dddot{\alpha}$, and space gradients $\alpha_{,ij}, \dot{\alpha}_{,ij}$. Equation (2.13), in general, because of its complex form, describes an extended evolution [5,33] which is similar to the well-known Ginsburg-Landau equations for governing non-equilibrium phase transitions in solids [54]. Therefore, one can say that (2.13) governs the return of the system towards equilibrium.

In general, both sides of (2.13) are non-linear in $\dot{\alpha}, \ddot{\alpha}, \dddot{\alpha}, \alpha_{,ij}, \dot{\alpha}_{,ij}$. However, it has been noted [1,8,11,56] that in the vicinity of the equilibrium configuration α^{eq}, by linearization of (2.10) and (2.11) one obtains:

$$\frac{\partial e}{\partial \alpha} = \frac{1}{2} k(\alpha - \alpha^{eq}), \quad \frac{\partial D}{\partial \dot{\alpha}} = \frac{1}{2} \lambda \dot{\alpha}. \tag{2.14}$$

Hence, we obtain an evolution equation [1–7,12,16,30–32,37–41,44,58,59] of the relaxation type

$$\dot{\alpha} = \frac{1}{\tau}(\alpha - \alpha^{eq}), \tag{2.15}$$

in which $\tau = \lambda/k$ is the relaxation time. In the literature, Eq. (2.15) is sometimes treated as the Onsager-Casimir relation between the dissipative fluxes (J_α) and their conjugate general forces (X_α). Probably such an erroneous interpretation follows from an expression for the rate of entropy production $\sigma_s = \boldsymbol{A}^{(ir)}\dot{\alpha} = -\boldsymbol{A}^{(r)}\dot{\alpha} \geq 0$ [30,36,60,61], which, according to the basic statements of Irreversible Thermodynamics contains dissipative fluxes and conjugate forces.

The flux-affinity evolution approach

Not always can each force be decomposed into the reversible and the irreversible parts (2.12). The reversible force $\boldsymbol{A}^{(r)}$ is a state variable since it is obtained, according to Eq. (2.9), by the variational differentiation of the internal energy. The irreversible force $\boldsymbol{A}^{(ir)}$, in the case when $\boldsymbol{A}^{(tot)} \neq 0$, cannot be further defined as the purely dissipative one (2.11). Hence an irreversible force is to be defined as follows:

$$\boldsymbol{A}^{(ir)} = \boldsymbol{A}^{(tot)} - \boldsymbol{A}^{(r)}. \tag{2.16}$$

This means that the connections of the irreversible forces with the dissipative function D are not completely determined. The dissipation function, in this case, depends on the time and space change of the recoverable forces, being a function of a change of state: $D = D(\nabla \boldsymbol{A}^{(r)}, \dot{\boldsymbol{A}}^{(r)})$. Then, the dissipative function lead to the determination of the flux $\mathbf{J}^\alpha$ and the source s^α:

$$\mathbf{J}^\alpha = \frac{\partial D}{\partial \nabla \boldsymbol{A}^{(r)}}, \quad s^\alpha = \frac{\partial D}{\partial \dot{\boldsymbol{A}}^{(r)}}. \tag{2.17}$$

These variables appear in the general flux-affinity evolution equation [32,44,57]:

$$\frac{\partial}{\partial t}(\rho\alpha) + \operatorname{div}(\rho\alpha\mathbf{v} + \mathbf{p}^{\alpha}) = \operatorname{div}(\mathbf{J}^{\alpha}) + \rho s^{\alpha}. \tag{2.18}$$

This equation has the form of the Chan-Hillard equation for describing the non-equilibrium phase transition. It often has been applied to describe stress-induced phase transitions in a solid continuum [11,20,21,33]. An additional recoverable flux $\mathbf{p}^{\alpha}$, that appears in Eq. (2.18), follows from the fact that a part of the dissipative phenomena is attached to a process and can be removed from the flow in a fully recoverable manner.

3. Evolution Equations for the Turbulent Microstructure

3.1. Turbulent transport modelling

The study of turbulence of multi-component, multiphase mixtures has a long history with numerous turning points in experimentation and mathematical modelling (see reviews [18,36]). It is a characteristic feature of mathematical modelling of turbulence, phase transition and mixture diffusion coupled together in the flow of a real fluid that they have always been treated separately. In the literature of phenomenological turbulence the main efforts of researchers are concentrated only on turbulent transport of momentum within viscous, incompressible isothermal simple fluids [62,63].

Only a few studies on the turbulent transport of thermal energy have been performed [13,29,36,48,52,60,61,64]. Nowadays, accepted for industrial calculations the two-parameter model of turbulence, called $\mathscr{k} - \varepsilon$ [62], deals with the transport of linear momentum and treats the turbulent transport of heat as a secondary quantity governed only by velocity fluctuations. Even the mostly accepted $\mathscr{k} - \varepsilon$ model of phenomenological turbulence does not possess a clear explanation as a thermodynamically consistent transport equation. It is shown in the literature [48] that the controversy revolves around the question which averaged form of entropy inequality is proper.

To be in good agreement with the original Reynolds' approach [65], it should be emphasized that only instantaneous balances of mass, linear momentum and energy can undergo a decomposition, nowadays frequently interpreted as averaging in space.

3.2. Reynolds' splitting procedure into mean and relative parts [65]

The original Reynolds' approach to turbulence phenomena, can be recognised as one which models two thermodynamic subsystems – a mean and a fluctuation subsystem. In other words, this approach asserts that the first subsystem corresponding to mean values is a fully recoverable macroscopic transport of mass, momentum and energy, whereas the second one corresponding to the fluctuation values is a non-equilibrium

Table 2. The two subsystem approach as a common framework for modelling turbulence and phase transition.

	Mean and Relative subsystems of turbulent flow	Mean and Relative subsystems of two phase flow
The basic unknowns (general models)	$\bar{\rho} = \varsigma''$ and ρ' $\bar{v} = v''$ and v' $\bar{e} = e''$ and e'	$\bar{\rho} = \rho_m$ and c $\bar{v} = v_m$ and u $\bar{e} = e_m$ and ΔT
The full non-equilibrium model	$\bar{u}, \bar{\rho}, \bar{e}$ k, k_θ, k_ρ $\varepsilon, \varepsilon_\theta, \varepsilon_\rho$ } turbulent microstructure	$\bar{u}, \bar{\rho}, \bar{e}$ x, u Δe } phasic microstructure
Two parameter homogeneous model	$\bar{u}, \bar{\rho}, \bar{e}$ k – turbulent kinetic energy ε – rate of dissipation of k	$\bar{u}, \bar{\rho}, \bar{e}$ x – dryness fraction θ – relaxation time of x

subsystem. Since our knowledge about the relative subsystem is still far from complete, we describe it approximately as a kind of turbulent microstructure. Finally, going strictly with Reynolds' line of reasoning, the locally homogenous (mean) model possesses the form of a single continuum endowed with a turbulent microstructure. The $k - \varepsilon$ model requires two evolution equations describing the most important features of turbulence shown in Table 2.

It should be once again emphasized that in [65] there is no averaging of the *linear momentum balance* but only splitting of the momentum balance for a sum of the mean and relative subsystems [Reynolds called them the referential (resultant) and relative subsystems of momentum balance, respectively [65, §3]]. The decomposition is quite similar to that used in two-phase systems or binary-mixture systems. Upon introduction it asserts within every particle of a continuum an internal interface which separates the subsystem $(\mathbf{v})''$ (mean) from the subsystem $(\mathbf{v})'$ (relative). A possible interaction between the subsystems, i.e., exchange of momentum, is enabled by introducing an extra flux $(\rho'\mathbf{v}' \otimes \mathbf{v}')''$, called by Reynolds "the conductive flux of momentum" and nowadays identified with the Reynolds turbulent stress "tensor" [62]. Reynolds [65] considers only additive splitting of the velocity field $\mathbf{v} = \mathbf{v}'' + \mathbf{v}'$ and density $\rho = \rho'' + \rho'$ with a simplification $\rho' \equiv 0$ as well as splitting of the Cauchy flux of momentum $\mathbf{t} = \mathbf{t}'' + \mathbf{t}'$ into the mean and relative parts. After that operation on the balance of linear momentum we obtain:

$$\frac{\partial}{\partial t}(\rho\mathbf{v}'' + \rho\mathbf{v}') = -\mathrm{div}\{\mathbf{t}'' + \mathbf{t}' + \rho[(\mathbf{v}'' \otimes \mathbf{v}'') + \mathbf{v}' \otimes \mathbf{v}'' + \mathbf{v}'' \otimes \mathbf{v}' + \mathbf{v}' \otimes \mathbf{v}']\} + \rho\mathbf{b}. \tag{3.1}$$

Adding and subtracting $\pm\rho(\mathbf{v}' \otimes \mathbf{v}')''$ in Eq. (3.1) we have

$$\frac{\partial}{\partial t}(\rho\mathbf{v}'' + \rho\mathbf{v}') = -\mathrm{div}\{\mathbf{t}'' + \mathbf{t}' + \rho[(\mathbf{v}''\otimes'') + (\mathbf{v}' \otimes \mathbf{v}')'']\} + \rho\mathbf{b} - \mathrm{div}\{\rho[\mathbf{v}' \otimes \mathbf{v}'' + \mathbf{v}'' \otimes \mathbf{v}' + \mathbf{v}' \otimes \mathbf{v}' - (\mathbf{v}' \otimes \mathbf{v})'']\}, \tag{3.2}$$

with the linear momentum balance for the sum of the mean $\mathbf{v}''$ and the relative $\mathbf{v}'$ subsystems. It is now easy to split (3.2) in two-subsystems (i.e., macro-micro-subsystems) as follows [65, Eq. (15), (16)] ([44], Eq. (A14), (A15)]:

$$\mathbf{v}'': \quad \frac{\partial}{\partial t}(\rho\mathbf{v}'') = -\mathrm{div}\{\mathbf{t}'' + \rho[(\mathbf{v}''\otimes\mathbf{v}'') + (\mathbf{v}'\otimes\mathbf{v}')'']\} + \rho\mathbf{b}, \tag{3.3}$$

$$\mathbf{v}': \quad \frac{\partial}{\partial t}(\rho\mathbf{v}') = -\mathrm{div}\{\mathbf{t}' + \rho[\mathbf{v}'\otimes\mathbf{v}'' + \mathbf{v}''\otimes\mathbf{v}' + \mathbf{v}'\otimes\mathbf{v}' - (\mathbf{v}''\otimes\mathbf{v})'']\}. \tag{3.4}$$

It is seen that a direct simple connection between both balances of momentum is realised via the additional internal flux of momentum:

$$\mathbf{R} = \rho(\mathbf{v}'\otimes\mathbf{v}')'' = R_{ij}\mathbf{e}_i\otimes\mathbf{e}_j \approx \mathbf{J}^t_p \equiv (\rho'\mathbf{v}'\otimes\mathbf{v}')''.$$

Within the classical framework of the two-subsystem approach, where all interactions occur only within the appropriate sources, it is a fact of great novelty. Physically, it means that a universal model of a two-subsystem continuum permits interactions between both subsystems via internal fluxes as well as via additional internal sources.

3.3. Extension of the decomposition

Dividing the fundamental Reynolds' assumption about the additive splitting of basic balance variables into a mean and a relative part, we postulate three additional internal turbulent fluxes, which must be added into the set of mean balances of mass, momentum and energy[3]. These are:

$$\textit{turbulent flux of mass}: \qquad \mathbf{J}^t_\rho = (\rho'\mathbf{v}')'' = (\rho' v'_i)''\mathbf{e}_i = j^t_i e_i, \quad i = x,y,z, \tag{3.5}$$

$$\textit{turbulent flux of momentum}: \quad \mathbf{J}^t_p = (\rho'\mathbf{v}'\otimes\mathbf{v}')'' = (\rho' v'_i v'_j)''\mathbf{e}_i\otimes\mathbf{e}_j = J^t_{ij}\mathbf{e}_i\otimes\mathbf{e}_j, \tag{3.6}$$

$$\textit{turbulent flux of energy}: \qquad \mathbf{J}^t_e = (\rho' e'\mathbf{v}')'' = (\rho' e' v'_i)''\mathbf{e}_i = q^t_i\mathbf{e}_i. \tag{3.7}$$

Here superscripts *(t)* and further indices *(op)*, *(d)*, throughout this work denote: **turbulent, phasic, diffusive**, respectively. It should be noted, from the very beginning, that the mean balances of mass, momentum and energy (interpreted as the average Navier-Stokes and Fourier equations [29]) with three additional turbulent fluxes cannot continue to be a simple fluid with the Navier-Stokes and the Fourier constitutive closures. It means that from a linear model of viscous and heat fluxes, we

[3] Traditionally, in literature [18,29,62] a bar on the top of a letter stands for the expected average value in time whereas a mean, in the sense of Reynolds, denoted by *bis* means the average in a small part of space.

must go into a model of non-linear, anisotropic, non-Newtonian, compressible, non-Fourierian, relaxing and retarding, weakly non-local fluid. Therefore, from the point of view of the theory of generalised media [19,26,49,50], turbulent flow can be treated as a motion of a complex fluid which contains not only non-linear constitutive closures but also new degrees of freedom, like the operative compressibility within a mixture. Those degrees of freedom are fields and have the form of internal variables, order parameters, non-localities, etc.

3.4. Turbulent microstructure

Going further with this line of reasoning, one can say that the mean kinetic energy of turbulence $k = 1/2(v_i' v_i')''$ and the mean rate of turbulence dissipation $\varepsilon = (v_{i,j}' v_{i,j}')''$ could play the role of some internal parameters. The mean heat energy $k_\theta = (\rho' e' e')''$ and the mean heat dissipation $\varepsilon_\theta = (\rho' e'_{,i} e'_{,i})''$ can play the role of the conservative parameters, which are mainly responsible for statement and evolution of the turbulent flux of energy $\mathbf{J}_e^t$. Then, formulating appropriate closure assumptions for $\mathbf{J}_\rho^t, \mathbf{J}_p^t, \mathbf{J}_e^t$ with k, ε, k_θ ε_θ as the main deriving force we can omit the traditional way of finding turbulent fluxes via higher-order moment balances, which contain unknowns of higher-order cross-moments. The algebraic, differential, integral or any other closures for $\mathbf{J}_\rho^t, \mathbf{J}_p^t, \mathbf{J}_e^t$ must be supplied independently to ensure that a set of governing equations does or does not contain the equations of type (3.4). For instance, the closures for $\mathbf{J}_\rho^t, \mathbf{J}_p^t, \mathbf{J}_e^t$, if developed within the framework of the Extended Thermodynamics can lead to a more thermodynamically consistent model which is more flexible for further improvements.

In this paper, the complexity of description is entirely introduced by the presence of turbulent fluxes $\mathbf{J}_\rho^t, \mathbf{J}_p^t, \mathbf{J}_e^t$ that we shall call a turbulence microstructure. Speaking in the language of the theory of a continuum with microstructure [25–27], we call the evolution model based on four conservative parameters $k, \varepsilon, k_\theta, \varepsilon_\theta$ a four-scalar microstructure. The influence of a four microstructure parameters on the macroscopic level can occur only in closures of the fluxes $\mathbf{J}_\rho^t, \mathbf{J}_p^t, \mathbf{J}_e^t$. However, the influence on the evolution of the turbulent microstructure can also show up in macroscopic fields like the density ρ and the velocity $\mathbf{v}$.

3.5. Turbulent mass microstructure

We have a more complex situation in the case of turbulent mass transport occurring in binary-mixture flows like jets of cold air in cross-flow of flue gases during the cooling of first stage blades in a gas turbine. In such a situation, one has three different time scales in a turbulent transport. It is a different time scale of response for very large eddies (mass), large eddies (momentum) and fine-scale eddies (heat). Therefore, a complete model of turbulent transport also needs an independent evolution of the turbulent mass transport. To be in agreement with the two-parameter $(k - \varepsilon)$ turbulent microstructure responsible for momentum and the two-parameter $(k_\theta - \varepsilon_\theta)$ turbulent microstructure responsible for heat transport, we propose an additional two-parameter $(k_\rho - \varepsilon_\rho)$ microstructure responsible for the turbulent mass transport

Table 3. A general view of the logical structure of turbulence microstructure parameters.

	Two scalar equations	Scalar symmetric tensor equations	Other models
Turbulent mass microstructure	$k_\rho = (\rho'\rho')''$ $\varepsilon_\rho = (\rho'_{,i}\rho'_{,i})''$	$k_\rho = (\rho'\rho')''$ $\varepsilon^\rho_{ij} = (\rho'_{,i}\rho'_{,j})''$	$\varepsilon^\rho_{ij} = (\rho'\rho'_{,i})''$
Turbulent momentum microstructure	$2k = (\rho' v'_i v'_i)''$ $\varepsilon = (\rho' v_{i,j} v_{i,j})''$	$k_{ij} = (\rho' v'_i v'_j)''$ $\varepsilon_{ij} = (\rho' v_{i,k} v_{i,k})''$	$k = (\rho' v'_i v'_i)''$ and 9 component $\lambda_{ij} = (\rho v'_{i,j})''$
Turbulent energy microstructure	$k_\theta = (\rho' T' T')''$ $\varepsilon_\theta = (\rho' T'_{,i} T'_{,i})''$	$k_\theta = (\rho' T' T')''$ $\varepsilon^\theta_{ij} = (\rho' T'_{,i} T'_{,j})''$	$\varepsilon^\theta_i = (\rho' T_{,j})''$

within, especially, stratificated and mixture flows (see Table 3). According to Reynolds' splitting procedure, the parameters

$$k_\rho = (\rho'\rho')'', \quad \varepsilon_\rho = (\rho'_{,i}\rho'_{,i})'' \tag{3.8}$$

play the primary role in constituting the turbulent flux of mass $\mathbf{J}^t_\rho$ and a secondary or not so important role in constituting the rest of fluxes $\mathbf{J}^t_p$ and $\mathbf{J}^t_e$.

3.6. Hierarchy of scales in turbulent microstructure

There is a hierarchy of the scales of turbulent transport which separates some interactions, such as the direct influence of fine-scale heat microstructure from the very large-scale mass microstructure. Therefore, the emphasis should be thus laid upon improving models that describe such complex phenomena like anisotropy, turbulent flow subjected to extra strains caused by streamline curvature, interaction of multiple numbers of shear layers, shock wave-boundary layer interaction, etc. [17,52,64]. It is obvious, that the commonly used two-equation ($k - \varepsilon$) model with an algebraic closure for $\mathbf{J}^t_p$, can only approximately describe the heat turbulent flux $\mathbf{J}^t_e = \mathbf{J}^t_e(\nabla T, k, \varepsilon, Pr^t)$ with a constant turbulent Prandtl number $Pr^t = const$, and the turbulent mass flux being equal to zero, $\mathbf{J}^t_\rho = 0$. Therefore, one common inability of the two-equation $k - \varepsilon$ turbulence model (even with anisotropic and rate modelling of $\mathbf{J}^t_p$) is that it cannot account for a full ''non-equilibrium turbulence'' in a multiphase fluid mixture. This is due to the use of a single time scale to simultaneously describe three basic modes of transport related to mass, linear momentum and energy. The capability of the three-scale model of turbulent microstructure to solve widely different complex flows is attributed to its capability to describe the non-equilibrium turbulence of binary-mixtures undergoing phase transition.

3.7. Second order turbulence modelling

In the literature of turbulence, besides the above six-scalars turbulent microstructure, we can find another model of turbulent transport based on the vector and/or tensors

microstructure. Table 3 shows different basic parameters used as conservative order parameters in modelling of the non-equilibrium microstructure.

Since $k = J^t{}_{ii}$ is the trace of the tensor of the turbulent flux of momentum and turbulent distortion $\varepsilon = \varepsilon_{ii}$, then the isotropic evolution for $k_{ij} = J^t_{ij}$ and ε_{ij}, can be split into the evolution of a trace and a trace-less tensor that is: k and $a_{ij} = J^t_{ij} - \frac{1}{3}k\delta_{ij}$, $a_{ii} = 0$. Similarly we have, ε and $e_{ij} = \varepsilon_{ij} - \frac{1}{3}\varepsilon\delta_{ij}$. The evolution of e_{ij} ($e_{ii} = 0$) is usually dropped from modelling [46]. Sometimes, during the modelling of the turbulent momentum anisotropy, not only the first invariant of J^t_{ij} is considered, but also the second and third one. In constructing more advanced turbulence models it is quite useful to refer to the general scheme of evolution equations constructed on the basis of a higher-order approximation. The scheme of evolution equations is identical for every pair, which describes the mass, momentum and energy microstructure evolution. These equations are postulated in a form of balance for a conservative parameter [11,12]. Taking into account these internal parameters, which are listed in Table 3, we write the following evolution equations:

$$\textit{turbulent mass transport} \begin{cases} \dfrac{\partial}{\partial t} j^t_i + \dfrac{\partial}{\partial x_m}(j^t_i v_m) = \dfrac{\partial}{\partial x_m}(J^j_{im}) + S^j_i - \varepsilon^\rho_i \\ \dfrac{\partial}{\partial t} \varepsilon^\rho_i + \dfrac{\partial}{\partial x_m}(\varepsilon^\rho_i v_m) = \dfrac{\partial}{\partial x_m}(J^\rho_{im}) + S^\rho_i \\ \dfrac{\partial}{\partial t} k_\rho + \dfrac{\partial}{\partial x_m}(k_\rho v_m) = \dfrac{\partial}{\partial x_m}(J^{\varepsilon\rho}_m) + S^{k\rho} - \varepsilon_\rho \\ \dfrac{\partial}{\partial t} \varepsilon_\rho + \dfrac{\partial}{\partial x_m}(\varepsilon_\rho v_m) = \dfrac{\partial}{\partial x_m}(J^{\varepsilon\rho}_m) + S^{\varepsilon\rho} \end{cases}, \tag{3.9}$$

$$\textit{turbulent momentum transport} \begin{cases} \dfrac{\partial}{\partial t} J^t_{ij} + \dfrac{\partial}{\partial x_m}(J^t_{ij} v_m) = \dfrac{\partial}{\partial x_m}(J^t_{ijm}) + S^t_{ij} - \varepsilon_{ij} \\ \dfrac{\partial}{\partial t} \varepsilon_{ij} + \dfrac{\partial}{\partial x_m}(\varepsilon_{ij} v_m) = \dfrac{\partial}{\partial x_m}(J^\varepsilon_{ijm}) + S^\varepsilon_{ij} \\ \dfrac{\partial}{\partial t} k + \dfrac{\partial}{\partial x_m}(k v_m) = \dfrac{\partial}{\partial x_m}(J^k_m) + S^k - \varepsilon \\ \dfrac{\partial}{\partial t} \varepsilon + \dfrac{\partial}{\partial x_m}(\varepsilon v_m) = \dfrac{\partial}{\partial x_m}(J^\varepsilon_m) + S^\varepsilon \end{cases}, \tag{3.10}$$

$$\textit{turbulent heat transport} \begin{cases} \dfrac{\partial}{\partial t} q^t_i + \dfrac{\partial}{\partial x_m}(q^t_i v_m) = \dfrac{\partial}{\partial x_m}(J^q_{im}) + S^q_i - \varepsilon^q_i \\ \dfrac{\partial}{\partial t} \varepsilon^\theta_i + \dfrac{\partial}{\partial x_m}(\varepsilon^\theta_i v_m) = \dfrac{\partial}{\partial x_m}(J^\theta_{im}) + S^\theta_i \\ \dfrac{\partial}{\partial t} k_\theta + \dfrac{\partial}{\partial x_m}(k_\theta v_m) = \dfrac{\partial}{\partial x_m}(J^{k\theta}_m) + S^{k\theta} - \varepsilon_\theta \\ \dfrac{\partial}{\partial t} \varepsilon_\theta + \dfrac{\partial}{\partial x_m}(\varepsilon_\theta v_m) = \dfrac{\partial}{\partial x_m}(J^{\varepsilon\theta}_m) + S^{\varepsilon\theta} \end{cases} \tag{3.11}$$

Throughout this work the regular Cartesian coordinate notation with Latin subscripts $(i, j, m, n \ldots \equiv x, y, z)$ is employed. Also, dyadic notation is used for a more compact notation; for instance Eq. (3.10) may be written as:

$$\operatorname{div}(\mathbf{J}_p^t \otimes \mathbf{v}) = (\mathbf{J}_p^t \otimes \mathbf{v})_{,m} \cdot \mathbf{e}_m = \frac{\partial}{\partial x_m}(J_{ij}^t v_m)\mathbf{e}_i \otimes \mathbf{e}_j. \tag{3.12}$$

3.8. Closure hierarchy

In Eqs. (3.9)–(3.11) new cross-fluxes and sources have appeared, according to the hierarchy of the moments equation "S". Usually, we simplify the modelling by setting constitutive closures not for J but for $\operatorname{div}(J)$. For instance, in the case of the evolution equation for Reynolds-stress fluxes $(3.9)_1$ we have:

$$\frac{\partial}{\partial x_m}(J_{ijm}^t) \equiv T_{ij}. \tag{3.13}$$

Here T_{ij} is frequently called the turbulent diffusion. Using such a simplification we could change the problem of modelling the cross-fluxes J into finding an algebraic closure for the diffusion T. The evolution equation for the Reynolds-stress flux J_{ij}^t simplifies considerably in case of isotropic and homogeneous turbulence, since T_{ij} is equal to zero and the dissipation rate dyadic ε_{ij} nearly isotropic so that we can set $\varepsilon_{ij} = \frac{1}{3}\varepsilon\delta_{ij}$. The source part S usually contains different contributions which are: **production** P, **slow** and **fast pressure-strain correlation** (Π) and **dissipation** (ε). According to Rotta's pioneering observation, the simplification $T_{ij} = 0, J_{ijm}^t = 0$ leads to an anisotropic, homogeneous turbulence by the application of a constant mean velocity gradient to a relaxation into a state of isotropy when the mean velocity gradients are removed. From the mathematical point of view it is obvious that the conservative evolution under the assumption of vanishing cross-fluxes takes the form of a relaxation equation.

3.9. Simplifications of turbulent transport

Basic simplifications usually deal with reduction of the number of independent evolution equations in the set (3.9)–(3.11). For instance, putting a simple assumption about the isotropy of the turbulent dissipation in the following form:

$$\varepsilon^\rho = C^\rho \varepsilon \frac{k^\rho}{k}, \quad \varepsilon_{ij} = \frac{1}{3}\varepsilon\delta_{ij}, \quad \varepsilon^\theta = C^\theta \varepsilon \frac{k^\theta}{k}, \quad \varepsilon_i^\theta = \varepsilon_{ij}^\theta = 0, \quad \varepsilon_i^\rho = 0, \tag{3.14}$$

where C^ρ, C^θ – are constants, one can reduce the 30 Eqs. (3.9)-(3.11) to 14 equations $(3.9)_1$, $(3.10)_1$, $(3.10)_3$, $(3.10)_4$, $(3.11)_1$. There are many different simplifications of (3.4)–(3.6) and many of them have been patterned on the original Rotta's method of simplification of the differential equations on "J" into algebraic ones [62].

4. Special Examples of the Internal Parameters

4.1. Evolution of slip vector

Considering a mixture of two interpenetrating fluids within the Eulerian-Eulerian description, the governing equations as well as the basic unknowns are simply related to the balance of mass, momentum and energy. This means that within the framework of a two-fluid formulation, six equations of balance are employed to define six unknowns ρ_1, ρ_2, $\mathbf{v}^1$, $\mathbf{v}^2$, T_1, T_2. However, the one-fluid (homogeneous) approach besides the three basic unknowns fields ρ, $\mathbf{v}$, T also possesses the three internal fields, concentration of the second constituent c, slip velocity $\mathbf{u}$, and thermal non-equilibrium temperature difference ΔT. Since the fields c, $\mathbf{u}$ and ΔT have some similarity to the differences of $\rho_1 - \rho_2$, $\mathbf{v}^1 - \mathbf{v}^2$ and $T^1 - T^2$, respectively [18,36], one can expect that the evolution equations for c, $\mathbf{u}$, ΔT have a form of differences of balances of mass, momentum and energy between fluid (1) and (2).

The fields c, $\mathbf{u}$, ΔT, if they play the role of internal variables, can undergo an evolution equation governed by the Ginsburg-Landau-type Eq. (2.13) or the Chan-Hillard-type Eq. (2.18). Therefore, a simple explanation of the relations between those approaches does not have a short exhibition. In general, the evolution equations of type (2.13) or (2.17) should include interfacial exchange laws, which in the two-field balances take the form of algebraic closure laws. For example, the evolution equation for the slip vector $\mathbf{u}$ has the following form [4]:

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{v} + \mathbf{p}^u) = \operatorname{div}(\tau^u) + \rho \mathbf{b}^u, \tag{4.1}$$

where the recoverable $\mathbf{p}^u$, and the dissipative τ^u fluxes and source flow $\mathbf{b}^u$ can be interpreted in terms of two-fluid variables as [15,16,31]:

$$p^u_{ij} = c(1-c)u_i u_j + (c_{,i}u_j + c_{,j}u_i), \tag{4.2}$$

$$\tau^u_{ij} = c\tau^1_{ij} - (1-c)\tau^2_{ij} + (\tau^1_{im} + \tau^2_{im})(c_{,m}c_{,j}), \tag{4.3}$$

$$b^u_i = c(1-c)(b^1_i - b^2_i) + m^{1,2}_i. \tag{4.4}$$

Here τ^1_{ij}, τ^2_{ij} are the viscous stress tensors, b^1_i, b^2_i are the external body forces, and $m^{1,2}_i$ is the internal force density acting on constituent (1) and (2) due to the interchange of momentum between the constituents. It is important to note that $\mathbf{m}^{1,2}$ leading to in the source of the evolution Eq. (4.1). Therefore, it can be interpreted as an assumption algebraic closure of all equations.

According to the homogeneous equilibrium model, formulas like (4.2)–(4.4) cannot be more useful if the dissipative function D cannot be easily specified, than, for instance τ^u_{ij} could be postulated in the following form:

$$\tau^u_{ij} = \mu^u_1(c)d_{ij} + \mu^u_2(c)d^u_{ij} + \mu^u_3\Big[(d_{im} + d^u_{im})\omega^u_{mj} + \omega^u_{im}(d_{mj} + d^u_{mj})\Big], \tag{4.5}$$

which, according to the principle of objectivity represents a response of material that is frame dependent but objective [28,49] and μ_1^u, μ_2^u, μ_3^u are the slip viscosity coefficients. Such an objective set of variables is following:

$$d_{ij} = \frac{1}{2}(v_{i,j} + v_{j,i}), \quad d_{ij}^u = \frac{1}{2}(u_{i,j} + u_{j,i}), \quad \omega_{ij}^u = \frac{1}{2}(u_{i,j} - u_{j,i}), \tag{4.6}$$

4.2. Thermal dis-equilibrium

A more complex interpretation deals with the evolution equation for the non-equilibrium temperature ΔT. It is very difficult to find any similarity between differences in the energy balances (for T_1 and T_2, respectively) and the evolution equation for $\Delta T = T - T_{sat}(p, \rho)$. This problem has been discussed in [14,37,41,66]. It has been based on the assumption that during the nucleation of a new phase, the bubble growth is thermally controlled, i.e., the interfacial heat transfer is totally spent on the production of a new phase. This approach extends the experience of the theory of nucleation [9,14,54] and the literature of empirical and analytical correlation's [43,60]. Therefore, in this approach, the metastable state plays the main driving force in stress-induced phase transitions and the main source of thermal non-equilibrium.

5. Example 1 – Four Equation Model for Turbulence Flashing Flows

5.1. The $k - \varepsilon - x - \theta$ model of phasic, turbulent microstructure

Let us consider the simplest model of a continuum undergoing a phase transition. The crucial assumption of this model is that all non-equilibrium effects related to the turbulent and phasic phenomena are located at the interface. Thus, we will assume that both phases, separated by a surface of discontinuity, are perfect, non-conductive, non-viscous, full laminar fluids (liquid and its vapour). In particular, it means that the Reynolds fluxes of momentum, both in the liquid and gas, are equal to zero or at least negligibly small.

Keeping in mind the assumptions imposed above, we can consider the two-phase system as a fluid with a scalar, phasic-turbulent microstructure which determines the interfacial properties by four scalars $k - \varepsilon - x - \theta$. By the phasic-turbulent microstructure we will understand a microscopic region of the medium in which densities, volumetric or mass fractions, turbulence, compositions, etc., vary significantly over a distance whose order of magnitude is the range of molecular forces. To the limited extent to which the turbulence/phasic microstructure is defined, there is no difficulty in describing it by the four above mentioned scalar fields being four internal parameters.

Let us assume that the turbulence, which is induced within the interfacial zones, will be described only by the velocity fluctuation field $\mathbf{v}'$ and that another set of fluctuations ρ' and e' are left out as relatively small. Let the evolution of a phase be expressed in terms of a mass fraction x, called the dryness fraction [1,14,18]. Then two basic scalars k, x will describe the main sources of non-equilibrium within the

system. It follows from the above assumptions that both scalars have an identical point of incipiency.

To describe the evolution of the system towards thermodynamic equilibrium, we need two evolution equations for the scalars k and x, which are derived by sources that should also take into account higher spatial gradients. Therefore, both equations must depend on two additional parameters, denoted by ε and θ, which in turn are strongly dependent on the microstructure processes (see [1] for θ and [62] for ε). Moreover, to describe the evolution of the parameters ε and θ, we have to use further complex reasoning. It turns out to be simple in a special case when only the first spatial gradients are needed in the model.

5.2. Governing equations

Let us specify the balances of mass, momentum and energy (2.1–2.3). Note that the mechanisms of turbulent and phasic diffusion have some similarities and diffusiveness of turbulence is commonly compared to that of molecular diffusion wherein a molecule moves and collides with another. This process is particularly intensive within the interfacial zone. The sums of the turbulent operative (phasic) fluxes of mass are equal to zero, $\mathbf{J}^t_\rho + \mathbf{J}^{op}_\rho + \mathbf{J}^d_\rho = 0$ and so are the mass sources and the recoverable mass flux: $s_\rho = 0$, $\mathbf{p}_\rho = 0$. Then the mass, momentum and energy balances are postulated in the following form:

$$\frac{\partial}{\partial t}(\rho) + \operatorname{div}(\rho\mathbf{v}) = 0, \tag{5.1}$$

$$\frac{\partial}{\partial t}(\rho\mathbf{v}) + \operatorname{div}(\rho\mathbf{v}\otimes\mathbf{v} + p\mathbf{I}) = \operatorname{div}(\tau + \mathbf{J}^t_p + \mathbf{J}^{op}_p) + \rho\mathbf{b}, \tag{5.2}$$

$$\frac{\partial}{\partial t}(\rho e) + \operatorname{div}(\rho e\mathbf{v} + p\mathbf{v}) = \operatorname{div}(\mathbf{q} + \mathbf{J}^t_e + \mathbf{J}^{op}_e + (\tau + \mathbf{J}^t_p + \mathbf{J}^{op}_p)\mathbf{v}) + \rho\mathbf{b}\cdot\mathbf{v}, \tag{5.3}$$

where $\mathbf{q} = T\mathbf{J}^s$ is the molecular heat flux.

5.3. Evolution equations for k and x

Generally the evolution equations for k and x contain two parts – diffusion and relaxation (source). Thus, having $(3.10)_3$ and (2.18) at hand we postulate the following evolution equations [33,45,62]:

$$\frac{\partial}{\partial t}(\rho k) + \operatorname{div}(\rho k\mathbf{v}) = \operatorname{div}(\mathbf{J}^k) + \rho s^k, \tag{5.4}$$

$$\frac{\partial}{\partial t}(\rho x) + \operatorname{div}(\rho x\mathbf{v} + \tau x(\mathbf{f} - \dot{\mathbf{v}})) = \operatorname{div}(\mathbf{J}^x) + \rho s^x. \tag{5.5}$$

Here an additional part in Eq. (5.5) (τ – is a time-like parameter) represents the recoverable microinertia contribution [4] and $\mathbf{f}$ is calculated as the Basset-like force

[16,62]. The diffusional fluxes $\mathbf{J}^k$, $\mathbf{J}^x$ represent a contribution coming from the interfacial surfaces. Therefore, the mutual interaction between k and x should be determined by means of simple algebraic closures, i.e.,

$$\mathbf{J}^x = C_{xx}\nabla x + C_{xk}\nabla k, \tag{5.6}$$

$$\mathbf{J}^k = C_{kx}\nabla x + C_{kk}\nabla k. \tag{5.7}$$

Similarly, an interaction between the turbulent and phasic sub-systems that follows from the relaxation part should have the following simple closures [38,63]:

$$\rho s^k = \rho\left[(\mathbf{J}_p^t + \mathbf{J}_p^{op})\cdot(\mathbf{v}\otimes\nabla) + (\mathbf{J}_e^t + \mathbf{J}_e^{op})\cdot\nabla T\right] - \rho\varepsilon, \tag{5.8}$$

$$\rho s^x = \rho\left[-\frac{1}{\theta}(x - x^{eq}) - \frac{1}{\tau}(k - k^{eq})\right]. \tag{5.9}$$

Here x^{eq}, k^{eq} are identified with some equilibrium values calculated from $\boldsymbol{A}^x = \boldsymbol{A}^k = 0$ [1,5,30,33]. However, the internal parameters ε and θ, which appear in Eqs. (5.8) and (5.9) can be evaluated according to the high order evolution equations:

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \operatorname{div}(\rho\varepsilon\mathbf{v}) = \operatorname{div}(\mathbf{J}^{\varepsilon}) + \rho s^{\varepsilon}, \tag{5.10}$$

$$\frac{\partial}{\partial t}(\rho\theta) + \operatorname{div}(\rho\theta\mathbf{v}) = \operatorname{div}(\mathbf{J}^{\theta}) + \rho s^{\theta}, \tag{5.11}$$

with the following closure equations [44,62]:

$$\mathbf{J}^{\varepsilon} = C_{\varepsilon 1}\nabla\varepsilon, \quad \mathbf{J}^{\theta} = 0, \tag{5.12}$$

$$\rho s^{\varepsilon} = \rho\frac{k}{\varepsilon}(C_{\varepsilon 2}\mathbf{J}_p^t\cdot(\mathbf{v}\otimes\nabla) + C_{\varepsilon 3}\varepsilon), \tag{5.13}$$

$$\rho s^{\theta} = \rho C_{\theta} p(\mathbf{v}\cdot\nabla), \tag{5.14}$$

where $C_{\varepsilon 1}, C_{\varepsilon 2}, C_{\varepsilon 3}, C_{\theta}$, are constants describing the property of the microstructure.

5.4. Momentum and energy fluxes

Having determined the evolution of the microstructure with the help of four parameters $k - \varepsilon - x - \theta$, it is possible to describe the closures for the operative and turbulent fluxes of momentum and energy. The most simple ones are algebraic equations for τ, $\mathbf{J}_p^t$, $\mathbf{J}_p^{op}$ and $\mathbf{q}$, $\mathbf{J}_e^t$, $\mathbf{J}_e^{op}$, usually postulated as functions of k, x and basic unknowns ρ, e, $\mathbf{v}$:

$$\tau + \mathbf{J}_p^t + \mathbf{J}_p^{op} = (\mu + \mu_t(k,\varepsilon) + \mu_{\mathrm{op}})(\mathbf{v}\otimes\nabla + \nabla\otimes\mathbf{v}) + (k + \lambda^{v}{}_{op})(\nabla\cdot\mathbf{v})\mathbf{1}, \tag{5.15}$$

$$\mathbf{q} + \mathbf{J}_e^t + \mathbf{J}_e^{op} = (\lambda + \lambda_t + \lambda_{op})\nabla T. \tag{5.16}$$

Reynolds-like closure procedures can be postulated by adding the spatial gradients of k, x. Then we get[4]

$$\mathbf{J}^t_{p\nabla} = \mathbf{J}^t_p + C^t_{pk}(\nabla\sqrt{k}) \otimes (\nabla\sqrt{k}), \tag{5.17}$$

$$\mathbf{J}^{op}_{p\nabla} = \mathbf{J}^{op}_p + C^{op}_{pk}\nabla x \otimes \nabla x, \tag{5.18}$$

$$\mathbf{J}^t_{e\nabla} = \mathbf{J}^t_e + C^t_e\left[k^{3/2}\nabla\rho + \rho\nabla(k^{3/2})\right], \tag{5.19}$$

$$\mathbf{J}^{op}_{e\nabla} = \mathbf{J}^{op}_e + C^{op}_e\left[x^{3/2}\nabla\rho + \rho\nabla(x^{3/2})\right]. \tag{5.20}$$

The algebraic closures describe only local properties of a turbulent phasic microstructure [29,62,63]. A real turbulent continuum behaves as some kind of continuum in time and space, which possesses its own history and memory as well as a flow induced anisotropy. However, it appears that for engineering purposes, it is sufficient to consider the closures only weakly non-local in time [26,51]. This kind of assumption leads to a differential model that requires only two new constants: the first one is the relaxation time of the operative and turbulent fluxes and the second is the retardation time for the thermodynamical forces.

Most commonly the weakly-non-local-in-time approach has been considered with respect to the turbulent transport of momentum. Let, as denoted by $\mathbf{d} = 0.5(\mathbf{v} \otimes \nabla + \nabla \otimes \mathbf{v})$, the rate of deformation and the Zaremba-Jaumann objective derivative equal [28,67]

$$\mathbf{d}^* = \frac{d^*}{dt}\mathbf{d} = \frac{\partial}{\partial t}\mathbf{d} + (\mathbf{d} \otimes \nabla)\mathbf{v} + \mathbf{w}^{\mathrm{T}}\mathbf{d} + \mathbf{d}\mathbf{w}, \tag{5.21}$$

where $\mathbf{v} \otimes \nabla = \mathbf{d} + \mathbf{w}$, $\mathbf{w}^{\mathrm{T}} = -\mathbf{w}$. Then, a weakly non-local closure for the turbulent flux of momentum can be written in the form of a retardation equation by setting

$$\mathbf{J}^t_p = \mu_t(k,\varepsilon)(\mathbf{d} + \tau^t_{ret}\mathbf{d}^*) + \lambda_t(k,\varepsilon)(tr\mathbf{d} + \tau^t_{ret}\mathbf{d}^*), \tag{5.22}$$

and, similarly, for the turbulent flux of energy

$$\mathbf{J}^t_p = \lambda_t(k,\varepsilon)(\nabla T + \tau^t_{ret}(\nabla T)^*), \tag{5.23}$$

where the retardation times for the deformation rate and the temperature gradients have different values.

The relaxation closure for the turbulent flux of momentum was defined by Reynolds as [45]:

$$\tau^{rel}(\mathbf{J}^t_p)^* + \mathbf{J}^t_p = \mu_t(\mathbf{v} \otimes \nabla + \nabla \otimes \mathbf{v}) + (k + \lambda^v_t)(\nabla \cdot \mathbf{v})\mathbf{1} + C^t_{pk}(\nabla\sqrt{k}) \otimes (\nabla\sqrt{k}), \tag{5.24}$$

[4] Further attempts along this line have never been successful. The 3/2 exponent in Eq. (5.20) was introduced by Reynolds in 1903 [45, originally Eq. (223)] and also derived by Kolgomorov in 1942.

where the relaxation time τ^{rel} an additional unknown to be determined. It is important not to confuse the so-called second-order closure for the Reynolds stress $\mathbf{J}_p^t$ [46,57,63] with the above relaxation Eq. (5.24). The second-order evolution equation for $\mathbf{J}_p^t$ needs an additional algebraic closure for a third-order flux, whereas our relaxation evolution equation needs only one additional constant (τ^{rel}) Therefore, the form of Eq. (5.24) is more similar to the evolution equations for the fluxes in Extended Irreversible Thermodynamics [24,49,51,55]. Note, that this closure leads to the hyperbolic conservation of mass, momentum and energy (the so-called telegraph equation). According to this the turbulent flux of momentum propagates with a finite velocity. In particular, a propagation speed of the turbulent fluctuation is given by [46]:

$$a_p^t = \sqrt{\frac{\mu_t}{\tau^{rel}}}. \tag{5.25}$$

It is in analogy to the speed of propagation of the viscous momentum. Formally, there is no reason to write the same closure equations for the operative fluxes of momentum and energy. In the absence of experimental data for the phase transition induced turbulence, the present homogeneous model with mutually interpenetrating phasic and turbulent microstructures seems to be an interesting and natural continuation of the Reynolds line of reasoning that splits the description into two subsystems.

6. Example 2 – Thermodynamics of Water-Air Turbulent Mixture

6.1. The set of internal parameters

The objective of this section is to describe the process of formulating different water-air structures arising under the condition of a strong turbulent momentum transport. In these circumstances, for an isothermal gas-liquid mixture without a phase transition ($x = \text{const}$), such internal variables as: φ [m^3/m^3] – the volume fraction of air, φ_{ij} [m^2/m^3] a tensor of fraction structure, k – the specific turbulent kinetic energy, J_{ij}^t – the Reynolds turbulent flux of momentum, ε – the specific turbulent dissipation rate, ε_{ij} – the turbulent distortion tensor, play the main role in the model. In order to alleviate a complicated notation related to the large number of internal parameters (21) (i.e., $\{\varphi, k, \varepsilon, \varphi_{ij}, J_{ij}^t, \varepsilon_{ij}\}$, $i, j = x, y, z$), let us introduce a common, short notation:

$$\alpha = \{\varphi, k, \varepsilon\}, \tag{6.1}$$

$$\alpha_{ij} = \{\varphi_{ij}, J_{ij}^t, \varepsilon_{ij}\}. \tag{6.2}$$

Additionally, three macroscopic unknowns, according to the balance of mass, momentum and energy are supplemented to the model: ρ, $\mathbf{v}$, T.

6.2. Internal energy

The specific internal energy is postulated be a function of the specific volume, specific entropy and of the internal variables: $u = u(v, s, \alpha, \alpha_{ij})$. Then, the First Law of

Thermodynamics for reversible processes has the form of an extended Gibbs equation [1,27]:

$$\begin{aligned} du &= \left.\frac{\partial u}{\partial \rho}\right|_{s,\alpha,\alpha_{ij}} d\rho + \left.\frac{\partial u}{\partial \rho}\right|_{s,\alpha,\alpha_{ij}} ds + \left.\frac{\partial u}{\partial \rho}\right|_{s,\alpha,\alpha_{ij}} d\alpha + \left.\frac{\partial u}{\partial \rho}\right|_{s,\alpha,\alpha_{ij}} d\alpha_{ij} \\ &= \mu d\rho + Tds + \boldsymbol{A}^{(r)} d\alpha + \boldsymbol{A}^{(r)} d\alpha_{ij}, \end{aligned} \tag{6.3}$$

where μ is the chemical potential, T the thermodynamic temperature, $\boldsymbol{A}^{(r)} \equiv \boldsymbol{A}$ and $\boldsymbol{A}^{(r)}_{ij} \equiv \boldsymbol{A}_{ij}$ are the scalar and tensor recoverable affinity. It is not a simple task to find an appropriate form of u with respect to α_{ij}, but, if this parameter in reference is a spherical tensor like: $\alpha^0_{ij} = k_0 \sigma_0 r_0^2 \delta_{ij}$ [32] (r_0 – radius of bubble), then:

$$u = u_\alpha(\rho, s, \alpha) + \alpha \left[k_0 \frac{\sigma}{\sigma_0} r_0^3 \left(\frac{3\alpha_{ij}}{k_0 r_0^2} - \delta_{ij} \right)^2 \right], \tag{6.4}$$

where $\sigma_0(r_0)$ is the surface tension. From definition (2.16) and (6.4) it follows that:

$$\boldsymbol{A}_{ij} = \boldsymbol{A}_{ji} = \alpha K \left(\frac{3\alpha_{ij}}{k_0 r_0^2} - \delta_{ij} \right). \tag{6.5}$$

6.3. Total energy

Note that the additional requirements for internal energy postulated in the balance of energy here are in (6.4). The total energy consists of the sum of the internal and the kinetic energy as follows:

$$e = u + \tfrac{1}{2} \mathbf{v} \cdot \mathbf{v}. \tag{6.6}$$

This equation is not a trivial one since, according to the classical modelling of internal variables [5], the dynamical contributions from $\dot{\alpha}$ and $\dot{\alpha}_{ij}$ are neglected. The vector of unknown conservative variables consists now of the following 26 fields:

$$\boldsymbol{U} = \{\rho, \mathbf{v}, e, \rho\alpha, \rho\alpha_{ij}\}. \tag{6.7}$$

6.4. Evolution equations

The variables ρ, $\mathbf{v}$, e are governed by the basic phenomenological balances of mass, linear momentum and energy, described by Eqs. (2.1)–(2.3). The internal variables α, α_{ij} undergo the evolution equation of the type (2.18). From the point of view of numerical discretization (Finite Volume Method or Finite Element Method), the formal mathematical structure should be the same for every evolution equation and should have the so-called ''conservative form'' [7,9,62,64]:

$$\partial_t \boldsymbol{U} + \operatorname{div}(\boldsymbol{F}^c + \boldsymbol{F}^e) = \operatorname{div}(\boldsymbol{F}^v) + \boldsymbol{S}. \tag{6.8}$$

Besides the conservative variable $\boldsymbol{U}$ (6.7), fluxes of three different types appear: the convective $\boldsymbol{F}^c$, recoverable $\boldsymbol{F}^e$ and dissipative $\boldsymbol{F}^v$ flux as well as the source $\boldsymbol{S}$.

In our case the equations of balance take the following local form:

Balance of mass

$$\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x_i}(\rho v_i) = 0, \tag{6.9}$$

Balance of momentum

$$\frac{\partial}{\partial t}(\rho v_i) + \frac{\partial}{\partial x_j}(\rho v_i v_j + p_{ij}) = \frac{\partial}{\partial x_j}(\tau^c_{ij}) + \rho b_i, \tag{6.10}$$

Balance of energy

$$\begin{aligned}\frac{\partial}{\partial t}(\rho e) + \frac{\partial}{\partial x_j}(\rho e v_j + p_{jk}v_k + p^\alpha_i \boldsymbol{A} + p^\alpha_{jik}\boldsymbol{A}_{ik}) \\ = \frac{\partial}{\partial x_j}(q^c_j + \tau^c{}_{ij}v_i + J^\alpha_j \boldsymbol{A} + J^\alpha_{jik}\boldsymbol{A}_{ik}) + \rho b_i v_i + \rho(\boldsymbol{A}^{(tot)}s^\alpha + \boldsymbol{A}^{(tot)}_{ij}s^\alpha_{ij}),\end{aligned} \tag{6.11}$$

Evolution of the scalar microstructure $\alpha = \{\varphi, k, \varepsilon\}$

$$\frac{\partial}{\partial t}(\rho\alpha) + \frac{\partial}{\partial x_j}(\rho\alpha v_j + p^\alpha_j) = \frac{\partial}{\partial x_j}(J^\alpha_j) + \rho s^\alpha, \tag{6.12}$$

Evolution of the tensor microstructure $\alpha_{ij} = \{\varphi_{ij}, J^t_{ij}, \varepsilon_{ij}\}$

$$\frac{\partial}{\partial t}(\rho\alpha_{ij}) + \frac{\partial}{\partial x_k}(\rho\alpha_{ij}v_k + p^\alpha_{ijk}) = \frac{\partial}{\partial x_k}(J^\alpha_{ijk}) + \rho s_{ij}{}^\alpha. \tag{6.13}$$

Here, according to Eqs. (2.2) and (2.3), the total dissipative momentum flux $\tau^c{}_{ij}$ is the sum of the molecular, operative, turbulent and diffusive fluxes:

$$\tau^c{}_{ij} = \tau_{ij} + J^{op}_{ij} + J^t_{ij} + J^d_{ij}, \tag{6.14}$$

and the total dissipative energy flux is:

$$q^c_j = TJ^s_i + J^{op}_i + J^t_i + J^d_i. \tag{6.15}$$

In the energy equation also appears the total affinity $\boldsymbol{A}^{(tot)}$, $\boldsymbol{A}^{(tot)}_{ij}$ that, according to Eq. (2.16) can be split into the recoverable and the irreversible part, respectively. Additionally, a diffusive flux of entropy $\mathbf{J}^s$ appears in (6.11). This flux multiplied by the temperature, according to the Clausius hypothesis about the "compensated heat transformation" [11], defines here the heat flux. Consequently, the heat micro-sub-structure governed by the evolution of the specific entropy scalar gives a contribution only the energy balance. The evolution equations for the entropy micro-sub-structure

are postulated to be:

$$\rho \frac{d}{dt} s \equiv \rho \dot{s} = \frac{\partial}{\partial t}(\rho s) + \frac{\partial}{\partial x_j}(\rho s v_j) = \frac{\partial}{\partial x_j}(J_j^s) + \rho \sigma_s, \tag{6.16}$$

where, according to the Second Law of Thermodynamics: $\sigma_s \geq 0$.

6.5. Irreversible properties of continua

The evolution equations give the recoverable as well as the irreversible contributions to the balance of energy (6.11). On the other hand, the balance of internal energy in the form of the Gibbs Eq. (6.3) contains only the recoverable contribution of energy. Therefore, taking the difference between (6.11) and (6.3) and making use of the balance of entropy (6.16) we are able to obtain the final expression for σ_s.

In this algorithm, first, the expression for $\dot{e}$ must be calculated as follows:

$$\rho \dot{e} = \rho \dot{u} + \rho v_i \dot{v}_i = \rho(\mu \dot{\rho} + T\dot{s} + \boldsymbol{A}\dot{\alpha} + \boldsymbol{A}_{ij}\dot{\alpha}_{ij} + v_i \dot{v}_i). \tag{6.17}$$

Several contributions for the above equation, i.e., $\mu\dot{\rho}, T\dot{s}, \boldsymbol{A}\dot{\alpha}, \boldsymbol{A}_{ij}\alpha_{ij}, v_i\dot{v}$ can be directly obtained by multiplication of:

the balance of mass by $\mu\dot{\rho}$

$$\mu\rho\left(\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x_i}(\rho v_i)\right) = \mu\rho\left(\dot{\rho} + \rho\frac{\partial}{\partial x_i}(v_i)\right) = 0, \tag{6.18}$$

the balance of momentum by v_i

$$\rho v_i(\dot{v}_i) + v_i \frac{\partial}{\partial x_j}(p_{ij}) = v_i \frac{\partial}{\partial x_j}(\tau^c{}_{ij}) + \rho v_i b_i, \tag{6.19}$$

the balance of scalar microstructure by $\boldsymbol{A}$

$$\rho\boldsymbol{A}(\dot{\alpha}) + \boldsymbol{A}\frac{\partial}{\partial x_j}(p_j^\alpha) = \boldsymbol{A}\frac{\partial}{\partial x_j}(J_j^\alpha) + \rho\boldsymbol{A}s^\alpha, \tag{6.20}$$

the balance of tensor microstructure by $\boldsymbol{A}_{ij}$

$$\rho\boldsymbol{A}_{ij}(\dot{\alpha}_{ij}) + \boldsymbol{A}_{ij}\frac{\partial}{\partial x_k}(p_{ijk}^\alpha) = \boldsymbol{A}_{ij}\frac{\partial}{\partial x_k}(J_{ijk}^\alpha) + \rho\boldsymbol{A}_{ij}s_{ij}^\alpha, \tag{6.21}$$

the balance of the specific entropy by T

$$\rho T\dot{s} = T\frac{\partial}{\partial x_j}(J_j^s) + \rho T\sigma_s. \tag{6.22}$$

According to Eq. (7.17), adding Eqs. (6.18)–(6.22) together, we find the expression for $\rho\dot{e}$. But, on the other hand, note that $\rho\dot{e}$ can also be expressed from the balance of energy (6.11) as

$$\rho\dot{e} + \frac{\partial}{\partial x_j}(p_{jk}v_k + p_i^{\alpha}\boldsymbol{A} + p_{jik}^{\alpha}\boldsymbol{A}_{ik}) = \frac{\partial}{\partial x_j}(TJ_j^s + \tau^c{}_{ij}v_i + J_j^{\alpha}\boldsymbol{A} + J_{jik}^{\alpha}\boldsymbol{A}_{ik}) + \rho b_i v_i + \rho(\boldsymbol{A}^{(tot)}s^{\alpha} + \boldsymbol{A}_{ij}{}^{(tot)}s_{ij}^{\alpha}). \quad (6.23)$$

Now, taking the difference between (6.17) and (6.22) and substituting additionally a few identities of the following type:

$$\frac{\partial}{\partial x_i}(\tau_{ij}^c v_j) = v_j\frac{\partial}{\partial x_i}(\tau_{ji}^c) + \tau_{ij}^c\frac{\partial}{\partial x_i}v_j, \quad (6.24)$$

we obtain as a result the following relation for the entropy production:

$$\rho T\sigma_s = \tau_{ij}^c(v_{i,j}) + J_j^s T_{,j} + J_j^a\boldsymbol{A}_{,j} + J_{jik}^{\alpha}\boldsymbol{A}_{ik,j} + \rho(\boldsymbol{A}^{(tot)} - \boldsymbol{A})s^{\alpha} + \rho(\boldsymbol{A}_{ij}^{(tot)} - \boldsymbol{A}_{ij})s_{ij}^{\alpha}. \quad (6.25)$$

Additionally, the recoverable momentum flux was assumed to be arbitrary and not only a spherical tensor $p_{ij} = p\delta_{ij}$. The associated dissipation functional $D = T\sigma_s$ is defined in [56].

6.6. Onsager-Casimir relations

The theory of non-equilibrium thermodynamics always requires that the dissipation function must be non-negative and have a form of: $\boldsymbol{J}\circ\boldsymbol{X}$, where $\boldsymbol{J}$ are thermodynamic fluxes and $\boldsymbol{X}$ are the thermodynamic forces. According to (6.24) these are, respectively:

$$\boldsymbol{J} = \{\tau_{ij}^c, J_i^c, J_i^{\alpha}, J_{ijk}^{\alpha}, \rho s^a, \rho s_{ij}^{\alpha}\}, \quad (6.26)$$

$$\boldsymbol{X} = \{v_{i,j}, T_{,i}, \boldsymbol{A}_{,i}, \boldsymbol{A}_{ij,k}, \boldsymbol{A}^{(tot)} - \boldsymbol{A}, \boldsymbol{A}_{ij}{}^{(tot)} - \boldsymbol{A}_{ij}\}. \quad (6.27)$$

Since the fluxes $\boldsymbol{J}$ are given also by (2.17), in the linear case: $\boldsymbol{J_a} = \boldsymbol{L_{ab}}\boldsymbol{X_b}$, it is possible to check a simple closure relation consistent with the practices of non-equilibrium thermodynamics [3,19,54,56]. Thus, if $\boldsymbol{L_{ab}}$ is any matrix of constitutive coefficients, then the fluxes are given by:

the total dissipative momentum flux

$$\tau_{ij}^c = \boldsymbol{L}_{11}(\varphi, k, \varepsilon)d_{ij} + \boldsymbol{L}_{16}(\boldsymbol{A}_{ij}{}^{(tot)} - \boldsymbol{A}_{ij}) + [\boldsymbol{L}_{17}v_{i,i} + \boldsymbol{L}_{15}(\boldsymbol{A}^{(tot)} - \boldsymbol{A})]\delta_{ij}, \quad (6.28)$$

the entropy flux

$$J_i^c = Tq_i^c = \boldsymbol{L}_{22}T_{,i} + \boldsymbol{L}_{23}\boldsymbol{A}_{,i}, \tag{6.29}$$

the flux of scalar microstructure $\alpha = \{\varphi, k, \varepsilon\}$

$$J_i^\alpha = \boldsymbol{L}_{32}T_{,i} + \boldsymbol{L}_{33}\boldsymbol{A}_{,i}, \tag{6.30}$$

the flux of tensorial microstructure $\alpha_{ij} = \{\varphi_{ij}, J_{ij}^t, \varepsilon_{ij}\}$

$$J_{ijk}^\alpha = \boldsymbol{L}_{14}d_{ij,k} + \boldsymbol{L}_{44}\boldsymbol{A}_{ij,k}, \tag{6.31}$$

the scalar source $\alpha = \{\varphi, k, \varepsilon\}$

$$\rho s^\alpha = \boldsymbol{L}_{15}(\varphi, k, \varepsilon)d_{ii} + \boldsymbol{L}_{45}(\boldsymbol{A}_{ii}^{(tot)} - \boldsymbol{A}_{ii}) + \boldsymbol{L}_{35}(\boldsymbol{A}^{(tot)} - \boldsymbol{A}), \tag{6.32}$$

the tensorial source $\alpha_{ij} = \{\varphi_{ij}, J_{ij}^t, \varepsilon_{ij}\}$

$$\rho s_{ij}{}^\alpha = \boldsymbol{L}_{16}(\varphi, k, \varepsilon)d_{ij} + \boldsymbol{L}_{66}(\boldsymbol{A}_{ij}{}^{(tot)} - \boldsymbol{A}_{ij}) + \boldsymbol{L}_{63}(\boldsymbol{A}^{(tot)} - \boldsymbol{A})\delta_{ij}. \tag{6.33}$$

Note that the above equations consist of the cross-effects between the phasic $\alpha = \{\varphi\}$, $\alpha_{ij} = \{\varphi_{ij}\}$ and the turbulent $\alpha = \{k, \varepsilon\}$, $\alpha_{ij} = \{J_{ij}^t, \varepsilon_{ij}\}$ microstructure. For instance, if the Reynolds turbulent flux J_{ij}^t in (6.14) is determined via the evolution Eq. (6.13) supplemented by the closures (6.30) and (6.32), then Eq. (6.27) describes only viscous, phasic and diffusive parts of the flux of momentum. However, if we have to do with the classical $k - \varepsilon$ (two-equation) model of turbulence, and Eqs. $(3.10)_1$ and (6.13) do not appear in the considerations, then Eq. (6.27) should determine, by an algebraic closure, also J_{ij}^t. The same considerations apply to the turbulent flux of heat, which can be defined algebraically by (6.28) or by the evolution equation $(3.11)_1$.

6.7. Turbulent evolution of the water-air structure

In the case of the two component mixture flow, when the turbulent flow is responsible for the change of its structure, for instance, from bubble flow into slug flow, the turbulence microstructure can play a passive role. Then the internal variables can be reduced to $\alpha = \{\varphi, k, \varepsilon\}$ and $\alpha_{ij} = \{\varphi_{ij}, 0, 0\}$. In this case the sources $s^\varphi \equiv 0$ vanish since no phase change is observed, and $J_{ijk}^\varphi \equiv 0$ since a flux-less evolution of shape of the bubble flow into slug flow is usually observed [4,64]. In such a simplified case, one has the evolution equation $(3.10)_3$ and $(3.10)_4$ for k and ε and the following evolution equation for φ and φ_{ij}:

$$\rho\dot{\varphi} = \frac{\partial}{\partial x_i}(J_i^\varphi), \tag{6.34}$$

$$\rho\dot{\varphi}_{ij} = \rho s_{ij}^\varphi. \tag{6.35}$$

According to the definition (2.10) three scalar affinities $\boldsymbol{A}^{\varphi}$, $\boldsymbol{A}^{k}$, $\boldsymbol{A}^{\varepsilon}$ and one tensor $\boldsymbol{A}^{\varphi}_{ij}$ should be defined. Then, according to (6.27–6.32), the required closures are:

$$\begin{aligned}
\tau^{c}_{ij} &= 2(\mu+\mu_t+\mu_{op})d_{ij}+\lambda^{op}v_{i,i}\delta_{ij}+\mu_1(\boldsymbol{A}_{ij}{}^{tot}-\boldsymbol{A}^{\varphi}_{ij})\\
&\quad+[\mu_2(\boldsymbol{A}^{tot}_{k}-\boldsymbol{A}^{k})+\mu_2(\boldsymbol{A}^{tot}_{\varphi}-\boldsymbol{A}^{\varphi})]\delta_{ij},\\
J^{c}_{i} &= Tq^{c}_{i}=(\lambda+\lambda^{t})T_{,i}+\lambda_1\boldsymbol{A}^{\varphi}_{,i}+\lambda_2\boldsymbol{A}^{k}_{,i}+\lambda_3A^{\varepsilon}_{,i},\\
J^{\varphi}_{i} &= (\kappa+\kappa^{t})T_{,i}+\kappa_1\boldsymbol{A}^{\varphi}_{,i}+\kappa_2\boldsymbol{A}^{k}_{,i}+\kappa_3\boldsymbol{A}^{\varepsilon}_{,i},\\
\rho s^{\varphi}_{ij} &= \beta_1(\boldsymbol{A}_{ij}{}^{tot}-\boldsymbol{A}^{\varphi}_{ij})+\beta_2 d_{ij}+[\beta_3(\boldsymbol{A}^{tot}_{k}-\boldsymbol{A}^{k})+\beta_4(\boldsymbol{A}^{tot}_{\varphi}-\boldsymbol{A}^{\varphi})]\delta_{ij}.
\end{aligned}\tag{6.36}$$

The numerous coefficients: μ, μ^{t}, μ^{op}, μ_1, μ_2, μ_3, λ, λ^{op}, λ^{t}, κ, κ^{t},..., β_4, in general are functions of $\{\varphi, k, \varepsilon, \varphi_{ij}\}$. The weakest point of the derived equations is their linearity. Nevertheless, they possess the requited structure of a full coupling between phasic and turbulent microstructure.

7. Concluding Remarks

The existing models of multiphase turbulent flow can not be called thermodynamically consistent. The multiphase flows with various predictive strategies are based on the Eulerian-Eulerian description (one-field, homogenous or two-fluid approach) or Eulerian-Lagrangean description. For the flow of a fluid that undergoes a stress or temperature induced phase transition, the Eulerian description is commonly adopted for the prediction of kinetics of non-equilibrium phase transition [54] based on the experience of the metastable state description [53]. Turbulence accompanying this phenomenon can not be correctly described by the Reynolds averaging techniques since the turbulent fluxes arising from Reynolds averaging deal separately with the averaging procedure in one phase and a separate averaging procedure in the second phase [13,29,48]. These studies do not seem to have advanced any theoretical reasons for the Reynolds averaging technique, but have deduced it entirely from their experiments. In reducing these results to a single model, however, many things have to be taken into account and many misleading assumptions have been made. There is one assumption which upon the face of it seems to be contrary to general experience, this is, that the concurrent phase transition does not change the level of turbulence.

In this paper we approach the problem in another manner. Starting with the interpretation of the turbulent flux of momentum as an internal forces interchanging momentum between laminar and turbulent fluid within a continuum particle [44], we have endeavoured to deduce from analytical considerations the model for the thermodynamically consistent laws of transport mass, momentum and energy between the phasic, turbulent and diffusive microstructures. In the literature [13,29,48,62,63] there is one main direction of reasoning – to extend the achievements of the theory of turbulence from one phase to multiphase flows. Such a line of reasoning omits a specificity of phase transition phenomena. On the basis of our work on non-equilibrium phase transitions, [1–7,16,32,37–41,44,58,59], an opposite direction of approach has been presented here – from thermodynamically substantiated models of a laminar flow undergoing a

phase transition to a turbulent, phasic and diffusive flow. But as yet the advance in this direction has not been essential – because the discrepancy in the results of the various experiments is such that one cannot avoid the conclusion that not all important variables of the problem have been taken into account yet.

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