

Kolumban Hutter · Lukas Schneider

Important aspects in the formulation of solid–fluid debris-flow models. Part I. Thermodynamic implications

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Abstract This article points at some critical issues which are connected with the theoretical formulation of the thermodynamics of solid–fluid mixtures of frictional materials. It is our view that a complete thermodynamic exploitation of the second law of thermodynamics is necessary to obtain the proper parameterizations of the constitutive quantities in such theories. These issues are explained in detail in a recently published book by Schneider and Hutter (Solid–Fluid Mixtures of Frictional Materials in Geophysical and Geotechnical Context, 2009), which we wish to advertize with these notes. The model is a saturated mixture of an arbitrary number of solid and fluid constituents which may be compressible or density preserving, which exhibit visco-frictional (visco-hypoplastic) behavior, but are all subject to the same temperature. Mass exchange between the constituents may account for particle size separation and phase changes due to fragmentation and abrasion. Destabilization of a saturated soil mass from the pre- and the post-critical phases of a catastrophic motion from initiation to deposition is modeled by symmetric tensorial variables which are related to the rate independent parts of the constituent stress tensors.

Keywords Debris flow · Second law of thermodynamics · Mixture theory · Frictional material · Exterior calculus

1 Motivation

The literature on the dynamical interaction between a fluid and a solid or fluids and solids mixed to a heterogeneous body is immense and equally conflicting in several elements. The mechanical and thermal processes exhibited by such complex systems arise in many fields of the engineering and natural sciences. Examples are fluidized beds in chemical process engineering, particle laden flows in fluvial hydraulics and typhoon or hurricane and earthquake induced landslides in catastrophic avalanche flows, to name a few, for more details see Hutter [15]. One characterization of such flows is that they often arise as interacting species flows, in which the different species are more or less continuously intermixed. It is then only a small step of abstraction to postulate, that (thermo)-dynamical models for them can be deduced by postulating that the various species continuously fill the space and form what is called a mixture. However, it is already at this level of the

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K. Hutter (✉)
Bergstrasse 5, 8044, Zurich, Switzerland
E-mail: Hutter@vaw.baug.ethz.ch

L. Schneider
Heinrich-Fuhr-Str. 3, 64287 Darmstadt, Germany
E-mail: lks.schneider@gmail.com

construction of a mathematical model that scientists tend to disagree in their opinion what a basic formulation of a mathematical model might be. According to a second alternative, known as ‘multiphase systems’, understanding the species interaction is achieved by an averaging or homogenization operation of the effects exerted on one species element by all the other species elements that are present in the assemblage of the species.

The terms ‘mixture’ and ‘multi-phase system’ characterize slightly different approaches to physical processes in minglings and have led to controversial disagreements. However, there is no need for disagreement, because at last ‘mixtures’ and ‘multi-phase systems’ are structurally the same. Why? Well, in multi-phase systems, the essential steps, done to reach structurally the same governing equations as in mixture theories (balances of mass, momenta, energy and entropy) from which models are deduced, are the motivation and formulation of interaction laws between the species elements and subsequently, the performance of a so-called phase averaging operation, by which the discrete distribution of the species elements is smeared or smoothed over a representative volume element. The emerging equations are balance laws as in mixture formulations, often, and inappropriately, called conservation laws for quantities typical of those arising in classical physics. Expert presentations of the two approaches are by Truesdell [38] and Müller [30] on the mixture side, and Jackson [21], Anderson and Jackson [2] and Drew and Passman [10] on the multi-phase systems side. Of course, by postulating interaction laws between the species elements and performing the phase averaging process, detailed knowledge and information has gone into the phase averaged equations, which is useful, but these equations still contain unspecified variables, e.g. stresses for which constitutive relations must be written down to arrive at a complete so-called closed system of equations. An illustrative example is given by Pitman and Le [31].

The mixture and multi-phase systems approaches lead to systems of equations which have essentially the same balance structure for continuously differentiable fields, but both have, at this level, still unspecified fields which must be adequately parameterized to close the system of equations. Since these equations have the same structure, and their variables are obviously continuously occupying all points of the space of the body, it is not absolutely necessary to differentiate between ‘mixtures’ and ‘multi-phase systems’. We shall treat these denotations as synonymous. This does not, however, remove all controversies. These start anew with the choice or postulation of the unspecified terms mentioned above. In fact, the disagreement between scientists seems often to be caused by performing ad hoc closure statements at this level.

In order to explain the various issues, consider a binary mixture of a particle laden fluid. Let $\bar{\rho}_{f,s}$, $\bar{c}_{f,s}$, $\mathbf{v}_{f,s}$, $\bar{p}_{f,s}$, $\bar{\mathbf{T}}_{f,s}$, $\bar{\mathbf{m}}_{f,s}$ and $\bar{\rho}_{f,s}\mathbf{g}$ be the partial densities, the constituent mass production rate densities, the constituent pressures, the constituent stress tensors, the specific interaction forces and the external body forces of the fluid (f) and solid (s) constituents, respectively. Moreover, let $\nu_{f,s}$ be the volume fractions and $\rho_{f,s}$ the true densities¹ of the fluid and the solid constituents, respectively. Then, accept the fact (we shall explain this in detail later) that $\bar{\mathbf{T}}_{f,s}$ are symmetric tensors, the balances of mass and linear momentum can be written down for the solid and the fluid as follows:

$$\begin{aligned} \frac{\partial \bar{\rho}_f}{\partial t} + \nabla \cdot (\bar{\rho}_f \mathbf{v}_f) &= \bar{c}_f, \\ \frac{\partial \bar{\rho}_s}{\partial t} + \nabla \cdot (\bar{\rho}_s \mathbf{v}_s) &= \bar{c}_s, \\ \frac{\partial (\bar{\rho}_f \mathbf{v}_f)}{\partial t} + \nabla \cdot (\bar{\rho}_f \mathbf{v}_f \otimes \mathbf{v}_f) &= -\nabla \bar{p}_f + \nabla \cdot \bar{\mathbf{T}}_f + \bar{\mathbf{m}}_f + \bar{\rho}_f \mathbf{g}, \\ \frac{\partial (\bar{\rho}_s \mathbf{v}_s)}{\partial t} + \nabla \cdot (\bar{\rho}_s \mathbf{v}_s \otimes \mathbf{v}_s) &= -\nabla \bar{p}_s + \nabla \cdot \bar{\mathbf{T}}_s + \bar{\mathbf{m}}_s + \bar{\rho}_s \mathbf{g}, \end{aligned} \quad (1)$$

in which

$$\bar{c}_f = -\bar{c}_s, \quad \bar{\mathbf{m}}_f = -\bar{\mathbf{m}}_s, \quad (2)$$

since mass and momentum of the mixture body are conserved (see main text for justification). Moreover, irrespective of whether the solid and the fluid constituents are compressible or not, one has

$$\bar{\rho}_{f,s} = \nu_{f,s} \rho_{f,s}. \quad (3)$$

Assume now that we wish to derive a model for this binary mixture that is only based on the partial differential equations (1) (i.e. not involving the variables $\nu_{f,s}$ and $\rho_{f,s}$). Then, Eqs. (1) and (2) comprise eight equations for 26 unknowns, namely $\bar{\rho}_{f,s}$ (2), $\mathbf{v}_{f,s}$ (6), $\bar{c}_{f,s}$ (1), $\bar{p}_{f,s}$ (2), $\bar{\mathbf{m}}_{f,s}$ (3) [see (2)] and $\bar{\mathbf{T}}_{f,s}$ (12). Treating

¹ The ‘true’ density is the mass of a constituent per volume of that constituent.

$\bar{\rho}_f$, $\bar{\rho}_s$, \mathbf{v}_f and \mathbf{v}_s as the basic fields, closure relations are needed for all quantities arising on the right-hand side of (1). For the most simple case of vanishing constituent mass production $\bar{c}_f = \bar{c}_s = 0$, we then need closure statements for $\bar{p}_{f,s}$, $\bar{\mathbf{T}}_{f,s}$ and $\bar{\mathbf{m}}_f$. Taking a very naive view, we may set $\bar{\mathbf{T}}_f = \mathbf{0}$ on grounds that the fluid is ideal, and we may conjecture Newtonian viscous behaviour for the solid stress $\bar{\mathbf{T}}_s$. This still leaves us with closure relations for $\bar{p}_{f,s}$ and $\bar{\mathbf{m}}_f$. For the latter, we may write down a Darcy type relation: $\bar{\mathbf{m}}_s = \gamma(\mathbf{v}_f - \mathbf{v}_s)$, where γ is a permeability, but this ignores the fact that there may be a buoyancy contribution to $\bar{\mathbf{m}}_f$ of the fluid exercising a static force on the solid, see Jackson [21] or Pitman and Le [31]. Leaving this question aside for the moment, we are still left with equations of state for $\bar{p}_{f,s}$. For a single fluid, the thermal equation of state follows from thermodynamics via the second law, and there it is a relation involving the true density (which is the same as the partial density for a single constituent material). Here, however, since according to (3) partial mass densities may change by changes of the true mass densities or the volume fractions or both, we must conclude that (i) introduction of single constituent pressures \bar{p}_f and \bar{p}_s is insufficient and (ii) a model based on Eqs. (1) and (2) alone is equally defective. Furthermore, we suspect the existence of *thermodynamic pressures* $p_{f,s}^{\text{th}}$, which must be governed by changes of the true mass densities, and so-called *configuration pressures* $p_{f,s}^{\text{conf}}$, that are then governed by variations of the volume fractions. Obviously, this calls for a rigorous thermodynamic derivation which delivers explicit formulae for the pressures. This requires that the partial densities $\bar{\rho}_{f,s}$ are not basic field variables, but instead $\rho_{f,s}$ and $v_{f,s}$ are, and that the volume fractions are treated as internal variables for which also evolution equations are required, because $v_{f,s}$ obviously describe the configuration change of the mass distribution. We write these equations in the form

$$\frac{\partial v_f}{\partial t} + \nabla \cdot (v_f \mathbf{v}_f) = n_f, \quad \frac{\partial v_s}{\partial t} + \nabla \cdot (v_s \mathbf{v}_s) = n_s, \quad (4)$$

where $n_{f,s}$ are production rate densities.

There are further compelling demands for a thermodynamic foundation of the theory. To see this, assume that the fluid and solid are both density preserving. This means that the true mass densities $\rho_{f,s}$ are constant and that the mass balance Eq. (1)_{1,2} reduce to Eq. (4)_{1,2} with

$$n_f = \frac{c_f}{\rho_f}, \quad n_s = \frac{c_s}{\rho_s} \quad (5)$$

for consistency. If we then, for some reason, would assume that the constitutive relations do not depend on $v_{f,s}$ either, the pressure terms $p_{f,s}^{\text{th}}$, $p_{f,s}^{\text{conf}}$ would both vanish, a strange behaviour, in particular for equilibrium conditions. Therefore, dropping $v_{f,s}$ as independent constitutive variables will in this case most likely lead to singular behaviour.

There is still a further case which gives rise to concern. Suppose that we want to use Eq. (1) for the situation that the mixture is saturated. This means that

$$v_f + v_s = 1 \quad (\text{saturation}). \quad (6)$$

This equation expresses that the fluid constituent fills the entire pore space. Its requirement amounts to loosing an independent variable. Equation (6) may thus be interpreted as a constraint condition and as such gives therefore rise to a constraint pressure, just as the pressure in incompressible fluids. This pressure is called *saturation pressure* ζ , so that in this case

$$\bar{p}_{f,s} = \bar{p}_{f,s}^{\text{th}} + \bar{p}_{f,s}^{\text{conf}} + \bar{p}_{f,s}^{\text{sat}}, \quad (7)$$

with

$$\bar{p}_f^{\text{sat}} = \lambda \zeta, \quad \bar{p}_s^{\text{sat}} = (1 - \lambda) \zeta, \quad (8)$$

distributing this pressure via a parameter λ among the constituents. In the usual approaches, this distribution is postulated in an ad hoc manner, just as now, since the effect of a single variable of the nature of stress must somehow be distributed among the constituents in a reasonable manner. ‘Reasonable’ means that the sum over the constituent pressures ought to be equal to the total saturation pressure. However, is this correct and what is the functional form for λ ? It can take any finite value, but is, in the literature, unanimously postulated to have the form

$$\lambda = v_f, \quad (9)$$

see Iverson [17], Iverson and Denlinger [20], Denlinger and Iverson [9], Pitman and Le [31], Jackson [21] and many others. Assumption (9) or its generalization

$$\bar{p}_\alpha^{\text{sat}} = \nu_\alpha \zeta \quad (\alpha = 1, \dots, n), \quad \sum_{\alpha=1}^n \nu_\alpha = 1 \quad (10)$$

for saturated mixtures of n constituents is called the ‘assumption of pressure equilibrium’.² It is only correct for special cases. Its validity or replacement must and can be proved by thermodynamic arguments.

Nothing specific has yet been said about the interaction forces $\bar{\mathbf{m}}_{f,s}$ except that their sum must vanish, an obvious statement in view of Newton’s third law. However, experts in multi-phase systems emphasise that the interaction forces can take different forms, see Anderson and Jackson [2] and Jackson [21]. Conceptually, this is quite obvious if $\bar{\mathbf{m}}_f$ is thought to be additively decomposed as follows:

$$\bar{\mathbf{m}}_f = \bar{\mathbf{m}}_f^{(1)} + \nabla \cdot \bar{\mathbf{T}}_f^{(1)}. \quad (11)$$

For instance, from an a priori estimate,³ one might have a first guess of the contribution of $\bar{\mathbf{m}}_f$ and it often happens that it arises as a divergence term. Then, the right-hand sides of (1)_{3,4} could be written in the form

$$\begin{aligned} \text{RHS}(1)_3 &= -\nabla \bar{p}_f + \nabla \cdot ({}^{(1)}\bar{\mathbf{T}}_f^{\text{New}}) + \bar{\mathbf{m}}_f^{(1)} + \bar{\rho}_f \mathbf{g}, \\ \text{RHS}(1)_4 &= -\nabla \bar{p}_s + \nabla \cdot ({}^{(1)}\bar{\mathbf{T}}_s^{\text{New}}) - \bar{\mathbf{m}}_f^{(1)} + \bar{\rho}_s \mathbf{g}, \end{aligned} \quad (12a)$$

or even as

$$\begin{aligned} \text{RHS}(1)_3 &= -\nabla \bar{p}_f + \nabla \cdot ({}^{(2)}\bar{\mathbf{T}}_f^{\text{New}}) + \bar{\mathbf{m}}_f^{(1)} + \bar{\rho}_f \mathbf{g}, \\ \text{RHS}(1)_4 &= -\nabla \bar{p}_s + \nabla \cdot ({}^{(2)}\bar{\mathbf{T}}_f^{\text{New}} - {}^{(2)}\bar{\mathbf{T}}_f^{\text{New}}) - \bar{\mathbf{m}}_f^{(1)} + \bar{\rho}_s \mathbf{g}, \end{aligned} \quad (12b)$$

with

$${}^{(1)}\bar{\mathbf{T}}_f^{\text{New}} = \bar{\mathbf{T}}_f + \bar{\mathbf{T}}_f^{(1)}, \quad {}^{(1)}\bar{\mathbf{T}}_f^{\text{New}} = \bar{\mathbf{T}}_s - \bar{\mathbf{T}}_f^{(1)}, \quad (13a)$$

and

$${}^{(2)}\bar{\mathbf{T}}_f^{\text{New}} = \bar{\mathbf{T}}_f + \bar{\mathbf{T}}_f^{(1)}, \quad {}^{(2)}\bar{\mathbf{T}}_f^{\text{New}} = \bar{\mathbf{T}}_s + \bar{\mathbf{T}}_f, \quad (13b)$$

respectively. In these equations, $\bar{\mathbf{T}}_{f,s}^{\text{New}}$ and $\bar{\mathbf{m}}_f^{(1)}$ are still left arbitrary. Obviously, in a constitutive postulate these terms must be determined in thermodynamic formulations. Needless to say, that the representations (1)_{3,4} and (12), (13) are equivalent to one another if indeed a decomposition of the form (11) exists.

Looking at (13), one might be tempted to conclude that ${}^{(1)}\bar{\mathbf{T}}_f^{\text{New}}$ exhibits only fluid properties, whilst ${}^{(1)}\bar{\mathbf{T}}_f^{\text{New}}$ expresses both fluid and solid properties. However, such an interpretation is not compelling, for if one writes (11) as

$$\bar{\mathbf{m}}_s = \bar{\mathbf{m}}_s^{(1)} + \nabla \cdot \bar{\mathbf{T}}_s^{(1)}, \quad (14)$$

which expresses the same as (11), since $\bar{\mathbf{m}}_s + \bar{\mathbf{m}}_f = \mathbf{0}$, (12a) is still obtained, but (13a) now takes the form

$${}^{(1)}\bar{\mathbf{T}}_f^{\text{New}} = \bar{\mathbf{T}}_f - \bar{\mathbf{T}}_s^{(1)}, \quad {}^{(1)}\bar{\mathbf{T}}_f^{\text{New}} = \bar{\mathbf{T}}_s + \bar{\mathbf{T}}_s^{(1)}, \quad (15)$$

and the new interaction–force–sum relation, $\bar{\mathbf{m}}_s^{(1)} + \bar{\mathbf{m}}_f^{(1)} = \mathbf{0}$, is preserved. Now, the new solid stress seems to exhibit pure solid properties, whilst the fluid stress is ‘mixed’.

In order to present an even further alternative, one may incorporate the divergence term in (11) into the fluid stress, but refrain from doing the analogous step in the momentum equation for the solid. In this case, the interaction forces of the new formulation do no longer sum up to zero, a requirement, which is generally left unquestioned. However, in all cases demonstrated so far, the fluid and solid momentum equations remain unchanged. This example suggests as if the constituent interaction forces do not need to sum up to zero, a conjecture, once expressed to us at the Isaac Newton Institute at Cambridge University, UK. We take the position that Truesdell’s requirement ‘the motion of the mixture as a whole is governed by the same equations

² In the literature, ‘pressure equilibrium’ seems to be applied to the total pressures not just to the saturation pressure.

³ In multi-phase systems of Anderson and Jackson [2,21] such a priori estimates are explicitly made.

as is a single body’ should not be abandoned. The interaction–force–sum relation is simply a hidden statement in this case, not straightforward to be fulfilled.

Obviously, even other decompositions are thinkable, a popular one is due to the multi-phase systems defenders, see, e.g. Jackson [21]. This author demonstrates by scrutinizing the forces that are exerted by a fluid flow on suspended particles that

$$\bar{\mathbf{m}}_f = -\bar{\mathbf{m}}_s = -\nu_s \nabla \cdot \bar{\mathbf{T}}_f + \bar{\mathbf{m}}_f^{(2)}. \quad (16)$$

With this choice, we may write for the right-hand sides of (1)_{3,4}

$$\begin{aligned} \text{RHS}(1)_3 &= -\nabla \bar{\rho}_f + \nu_f \nabla \cdot \bar{\mathbf{T}}_f + \bar{\mathbf{m}}_f^{(2)} + \bar{\rho}_f \mathbf{g}, \\ \text{RHS}(1)_4 &= -\nabla \bar{\rho}_s + \nabla \cdot \bar{\mathbf{T}}_s + \nu_s \nabla \cdot \bar{\mathbf{T}}_f - \bar{\mathbf{m}}_f^{(2)} + \bar{\rho}_s \mathbf{g}. \end{aligned} \quad (17)$$

These equations have lost the divergence property for the stresses. They are yet a different version of the constituent momentum equations, but they are obviously analogous to (1)_{3,4} provided that the decomposition (16) holds.⁴

It is now understandable that it must be very difficult to bring such disparate formulations into coincidence, or at least to establish a certain degree of harmony. We claim that rational thermodynamics is the vehicle to achieve this. In so doing, one must select a formulation, either Eqs. (1)_{3,4}, (12) or (17) for the balance laws of constituent momenta, postulate constitutive relations for a desired material class and subsequently exploit the entropy principle to reduce the constitutive relations to the adequate ‘minimal’ form. In principle, this can be done for all three of the above presented systems of balance laws or any other one that is available. If for different formulations, final results can be brought into coincidence, then the formally different theories describe indeed the same material behaviour of the mixture in question, if not, the decompositions (11) or (16) are doubtful. This holds for a system that can be derived from (1). We regard Eq. (1) to be the most primitive ones, because they have the structure of balance laws, which possess clearly defined global, integrated forms with the usual mathematical properties.

In the above, two constituent mixtures were the basis for us to explain the crucial issues that are encountered with such continuous complex systems, but it is quite clear that nothing essential changes, if the mixture or the multi-phase system consists of $n > 2$ components. In Schneider and Hutter [35], the theory is developed for arbitrary n but we are aware that $n = 2$ and perhaps $n = 3$ or $n = 4$ are the most significant cases. The analysis, not easy to grasp, demonstrates that the above mentioned uncertainties or open holes in the derivation of the models will all be resolved. There is no reason for scientists to disagree and debate on different reasonable ad hoc assumptions on some parts of the stresses or interaction forces in different formulations; the different theories may well agree with one another, but agreement or disagreement of two formulations can only be judged after both have been subjected to a complete thermodynamic analysis.

2 Mixtures and debris-flow models

Our own interest in fluid–solid mixtures is guided by their application to catastrophic movement of snow, ice and debris avalanches, by mud flows in fluvial hydraulics, e.g. as a result of heavy rain fall when soil on mountain sides or dams break off or when large river discharge triggers sediment erosion and generates its transport and deposition further down in the river basin, often giving rise to devastating effects to life and property by erosion and sedimentation. Such catastrophic events occur nowadays worldwide and can almost daily be found in the news media. Many avalanche models have been developed for dry granular fluids (for a collection of references, see Harbitz [13], Hutter [14], Pudasaini and Hutter [32], Ancey [1] and others). Such models are adequate for dry dense snow avalanches, for dry debris flows and landslides that may be triggered by an earthquake. For flow of water-soaked soil or debris, a large number of models for catastrophic motion are based on single constituent models, in which the constitutive relation for the stress tensor is motivated by non-Newtonian rheology. These models employ a closure relation, for which the stress is proportional to the strain rate tensor with scalar factor—the effective viscosity—which itself depends on the second invariant of the stress tensor, sometimes in a rather complex way, see e.g. Luca et al. [25].

⁴ Readers with advanced knowledge in structured mixture theory will realize that momentum equations based on (17) cannot become equivalent to the equations with the original variables, if for the constitutive theory the principle of phase separation is employed.

There is an extensive literature on this subject in the rheological sciences, mostly dealing with polymeric and other complex fluids and using stress-stretching relations of the class of visco-plastic materials. Rheologists differentiate between fluids exhibiting a yield stress (Bingham, Herschel Bulkley, De Kee–Turcotte fluids) and fluids without a yield stress (Newtonian, power law fluids with shear thinning and shear thickening behaviour). Ancy [1] reviews the recent literature, emphasizing the viscous and plastic nature of such models. Because of the singularities that arise in some of these fluid models (e.g. infinite viscosity at zero stretching for shear thinning fluids, an essential singularity for all plastic models at yield), regularizations have been introduced which remove these singularities. Such a regularization, making the behaviour mathematically viscous has been suggested by Zhu et al. [39] for the De Kee–Turcotte fluid. Luca et al. [25] proposed such a regularization for shear thinning and shear thickening fluids with Newtonian behaviour, at small stretching, and power law behaviour, at large stretching. They derive thin layer approximations on arbitrary topography for these kinds of fluid models and show that at least two classes of avalanche models must be differentiated, the first class being applicable for fluids with zero or small yield stress and the second class for materials exhibiting large yield stress.

These models are likely adequate for flows of particle laden systems up to moderately high solids concentration with negligible active solid–fluid separation. They are, however, likely inappropriate when sedimentation occurs or for flow at high solids concentration when frictional contact between the grains is frequent. In the debris flow community, mixture concepts have so far only been incorporated in a broad fashion. Geotechnical engineers and engineering geologists (McDougall and Hungr [28,29], Iverson [17,18], Iverson and Denlinger [20]) have early recognized that the role of the fluid, or more precisely the pore pressure, is decisive for the run-out of a granular mass subjected to an interstitial fluid. In a first attempt to quantify the role played by the fluid, Iverson assumed the saturated binary mixture to consist of a fluid and a solid constituent, but imposed the simplifying assumption that both constituents move with the same velocity, $\mathbf{v}_f = \mathbf{v}_s$. This implied that the interaction force (the Darcy term) disappeared from the formulation,⁵ but the total pressure needed to be distributed between the solid and the fluid pressures according to

$$p_f = \lambda p, \quad p_s = (1 - \lambda)p. \quad (18)$$

To close the system, an ad hoc closure relation is needed for the pore fluid pressure p or for λ . A similar procedure was also taken up by Pudasaini et al. [33] in a slightly different avalanche formulation, but using the same physics. Computations have shown that the pore (fluid) pressure exercises a significant effect on granular mass run-out distances. The major disadvantage of this model is the ad hoc nature of the distribution of the pore pressure among the constituents according to (18). This equation has no theoretical basis other than to close the system of equations. Computations have also shown that results depend chiefly on the choice of the parameterization of λ , an equation for which there is no rational background. In an attempt to introduce some notion of rationalism in such a simplistic approach, a diffusion equation for the pore pressure was derived from an independent principle; see [19]. However, such an approach does still not remove the fact that the pore pressure equation is not rationally connected to the mixture equations.

Nevertheless, a rational connection of a diffusion equation for the pore pressure to the more standard formulations is possible. The pore pressure equation may be thought of as a balance equation of the form

$$\frac{dp}{dt} = \nabla \cdot \mathcal{F}_p + \pi_p \quad (19)$$

with a flux term $\mathcal{F}_p = -\kappa_p \nabla p$ with diffusivity κ_p and a production term π_p . If (19) is used, p takes the role of an internal variable. A loose connection to the standard theories of solid–fluid mixtures emerges, if λ in (18) is identified with v_f as in (9). In this case, (19) is a substitute for one of the Eq. (4).⁶ So, Iverson’s procedure, which is free of volume fraction variables, may also be interpreted as a partial recognition of volume fraction balance laws. On the other hand, one may maintain λ in (18) as an independent variable and postulate (19) or

$$\frac{d\lambda}{dt} = \nabla \cdot \mathcal{F}_\lambda + \pi_\lambda \quad (20)$$

as its balance law. Both (19) and (20), however, require additional boundary conditions, which are difficult to motivate. These thoughts seem to be new; they establish a weak connection of the pore pressure approach to the more standard mixture formulations with volume fraction balance laws.

⁵ Actually, only the dynamic part of the interaction force which is a function of $\mathbf{v}_f - \mathbf{v}_s$, vanishes in this case, the static contribution is arbitrarily assumed to vanish.

⁶ In (4), flux terms are missing since additional boundary conditions would then be needed as is the case for (19).

A mixture model, deserving the qualification ‘mixture’ and serving the purpose of describing water saturated debris flows, was presented by Pitman and Le [31] using the mass balances (1)_{1,2} and the momentum balances that are based on Eqs. (16) and (1)_{3,4}. Density preserving and saturation assumptions were also used. The constitutive theory uses a plastic description which is essentially a Mohr–Coulomb behaviour due to Rankine [34]. In a reduced model, the fluid acceleration terms are dropped, so that the fluid equation reduces to a classical Darcy equation. Only preliminary computations for this reduced model have been conducted, and they demonstrate that the fluid component enhances the run-out distances. Interestingly, this theory is complementary to that of Iverson; it emphasizes the role of the dynamic interaction force, whilst Iverson ignores it, and it ignores the pore pressure, whilst Iverson accounts for it. Both, however, predict run-out distances that are increased by the presence of the fluid.

Other solid–fluid mixture models in which the above mentioned simplifications are not made but other ad hoc assumptions are implemented to simplify the complexity of the formulation are Fernández-Nieto et al. [12] and Luca et al. [26,27]. These authors treat solid–fluid mixtures divided into two layers, of which the lower layer is a binary mixture, whilst the upper layer is a pure fluid, and fluid exchange between the layers may or may not exist. The model of Luca et al. is based on a reduced formulation deduced from the equations presented by Schneider and Hutter [35].

The above mixture models are the only ones we know of, which have been proposed to be applied to debris flows, landslides, etc. in the mentioned geological applications. They are of ad hoc nature, i.e. closure relations have been suggested by physical reasoning and plausibility arguments, without any detailed thermodynamic analysis. It is our belief that for a constitutive class, which acceptably embraces possibly successful debris flow models, a thorough thermodynamic analysis ought to be performed to achieve a high degree of certainty of the model equations from which fluid–solid avalanche models in the geophysical context can be further deduced.

3 Mixtures with frictional components

Landslides and debris flows are often initiated from slopes that have been artificially consolidated and exhibit a high degree of ‘stability’. Such flows can also develop from artificial dams. Soil slumps arise in such cases often in inhabited areas (e.g. Hong Kong as a well known site!). In these circumstances, the geotechnical engineer or engineering geologist wishes to have a theoretical model for the behaviour of the soil prior to any catastrophic movement when the soil structure is still stable under quasi-static loads, which allows also (i) the prediction of failure by identifying shear bands and other possible instability features and (ii) the determination of the catastrophic avalanching motion from this initial post-critical state through all phases of the motion to the deposition. The model should predict the pre-critical state of stress, the onset of the localisation or alternative instability, the initiation of the ensuing motion, the speeds and the mass distribution in motion as well as in the final deposition. The models mentioned in the preceding section lack the potential to describe all these phases.⁷ A stress ‘component’ capable of predicting the localization to identify the breaking soil mass is missing. There are several options to incorporate this component into the theory. We have decided to do this in a form that generalizes the well-known constitutive models of hypo-plasticity, see [23,3–8].

We wish to mention that (i) even though the hypo-plasticity models are likely in conformity with the Second Law of Thermodynamics, this has not been demonstrated and (ii) that the hypo-plastic models have so far not been set into a clear mixture concept with a number of fluid and solid constituents. It is not obvious how this can be done. When interstitial water plays a role, the mixture context shows up in the classical hypo-plastic models only indirectly via the somewhat ‘cryptic’ statement, that effective stresses are looked at. A thermodynamic

⁷ One of the referees of an earlier version of this article criticized our statement that the model ought to be able to produce shear banding (localizations) and states that, usually, displacement fields at failure have a chaotic nature and is not structured by any patterning. We do agree with this statement, but challenge its mode of exclusiveness. We have just completed a paper on laboratory experiments of dry sand base and slope failures and systematically found that base failure has two modes, (i) shear band failure at dense initial packing and (ii) punching shear failure at loose initial packing. Slope failures have always generated shear band failures. With water our laboratory experiments are in the planning phase. However, this is not the point. We need a hypo-plastic constitutive component for the above case of the failure mode to model the initial conditions for the catastrophic motion in this case. However, a plastic stress contribution is also needed for the deposition where a consolidation mode from viscous to plastic behaviour almost certainly takes place. Moreover, at inception the fluid constituent with all its peculiarities provides the element for exactly the chaotic failure mentioned by the referee. So, we admit that mixture failing modes may be “chaotic” or “unstructured”. The destabilization of a slope at rest is certainly strongly governed by pore pressure variations. However, the theory is more subtle than what has been proposed, e.g. by Iverson. Our theory has been designed for exactly such situations.

setting of their derivation is, however, useful per se, since it will pave the route for extending hypo-plasticity to mixtures with several solid constituents.

In Schneider and Hutter [35], incorporation of the frictional effects into the theoretical formulation is done in much greater generality than just for hypo-plastic materials. However, this approach allows us to prove how and under what conditions hypo-plasticity fulfils the Second Law of Thermodynamics. We shall show this for the situation that every constituent of the mixture entails hypo-plastic material behaviour, but allows for the possibility that it can be dropped for particular constituents, e.g. fluid components. The demonstration of the thermodynamic consistency has, however, not been easy, at least not in the initial stages. The reason is, that unlike the customary hypo-plastic approach, where an evolution equation for the Cauchy stress tensor is postulated, we introduce the hypo-plastic behaviour indirectly by adding an evolution equation for an objective symmetric second rank tensor valued internal variable, to the physical balance laws, and postulating its production rate density in plausible form. This has first been demonstrated by Svendsen et al. [37] for single phase dry granular materials on the basis of an idea by Svendsen and is in [35] generalized in the context of mixture theory. This is a necessary step, because it is not at all clear how one should postulate hypo-plastic contributions to the interaction forces or to the partial stress tensors of the solid constituents, if there are many constituents. The method can describe frictional behaviour more generally than just by hypo-plasticity, but our interest is primarily in the latter. We claim that this work forms the basis for a general material theory of a mixture of solid and fluid constituents that should in principle be able to describe the thermo-dynamical response of fully saturated soils from their quasi-static behaviour through a phase of destabilization via the formation of localization features, to the post-critical behaviour in catastrophic avalanching motions, from their initiation and while the material is subjected to large deformations, down to the deposition.

4 Kinematics, balance laws, saturation, constituent density constraints, constitutive relations, entropy principle

4.1 Kinematics of multi-phase mixtures

In this section, our aim is to take a closer look at the kinematics of multi-phase mixtures. Thus, we start, as in every continuum theory, from configurations and motions of a three-dimensional non-empty continuum \mathcal{B} , the so-called material body.

As we are dealing with mixtures, we must consider configurations one for each constituent and motions of a collection of n non-empty continua \mathcal{B}_α (for each constituent one), that constitute the body \mathcal{B} .

An element, X_α , of continuum \mathcal{B}_α can be understood as a name tag for one specific material particle of constituent K_α . An open set of these elements is called \mathcal{Q}_α and its surface $\partial\mathcal{Q}_\alpha$. Every \mathcal{B}_α has a set of configurations $\{\kappa_{\alpha\theta}\}_{\theta \in I}$ with $I \subset \mathbb{R}$ that are bijective mappings from \mathcal{B}_α into connected and compact regions, $\{\mathcal{R}_{\alpha\theta}\}_{\theta \in I}$, in the Euclidian space, \mathcal{E}^3 . In other words, one specific $\kappa_{\alpha\theta}$ assigns a vector $\mathbf{X}_{\alpha\theta}$ to the material particle X_α at a fixed time θ , i.e.

$$\begin{aligned} \kappa_{\alpha\theta} : \mathcal{B}_\alpha &\rightarrow \mathcal{E}^3, \\ \mathbf{X}_{\alpha\theta} &= \kappa_{\alpha\theta}(X_\alpha) \in \mathcal{R}_{\alpha\theta}, \end{aligned} \quad \text{for } \theta \text{ fixed,} \quad (21)$$

$\mathbf{X}_{\alpha\theta}$ is called the position vector of the corresponding material particle and $\mathcal{R}_{\alpha\theta}$ is the region occupied by constituent K_α .

Now, let us choose any element from the set of configurations and call it a reference configuration, $\kappa_{\alpha 0}$. $\mathcal{R}_{\alpha 0}$ and $\mathbf{X}_{\alpha 0}$ corresponding to $\kappa_{\alpha 0}$ are then $\mathcal{R}_{\alpha 0}$ and $\mathbf{X}_{\alpha 0}$, respectively. As already observed by Truesdell [38], $\kappa_{\alpha 0}$ can be different for every constituent. The present configuration can be obtained by sequentially applying the mappings $\kappa_{\alpha 0}^{-1}$ and $\kappa_{\alpha t}$ (see Fig. 1), where $\kappa_{\alpha t}$ is the mapping from the continuum \mathcal{B}_α to the present configuration. However, all constituents are located at the same present configuration \mathcal{R}_t , i.e. all $\mathcal{R}_{\alpha t}$ fall together to one \mathcal{R}_t and thus, in the present configuration we have only one *position vector* \mathbf{x} . In mathematical formulas \mathbf{x} can be expressed as

$$\mathbf{x} = \left(\kappa_{\alpha t} \circ \kappa_{\alpha 0}^{-1} \right) (\mathbf{X}_{\alpha 0}), \quad \text{or} \quad \mathbf{x} = \chi_\alpha (\mathbf{X}_{\alpha 0}, t), \quad (22)$$

where $\kappa_{\alpha t} \circ \kappa_{\alpha 0}^{-1}$ denotes a mapping that results from sequentially applying first $\kappa_{\alpha 0}^{-1}$ and then $\kappa_{\alpha t}$. The symbol χ_α denotes a vector-valued function of location $\mathbf{X}_{\alpha 0}$ and time t of which the value is \mathbf{x} . The function χ_α is called *the motion* of the constituent material body \mathcal{B}_α . With these definitions in mind we can now specify the

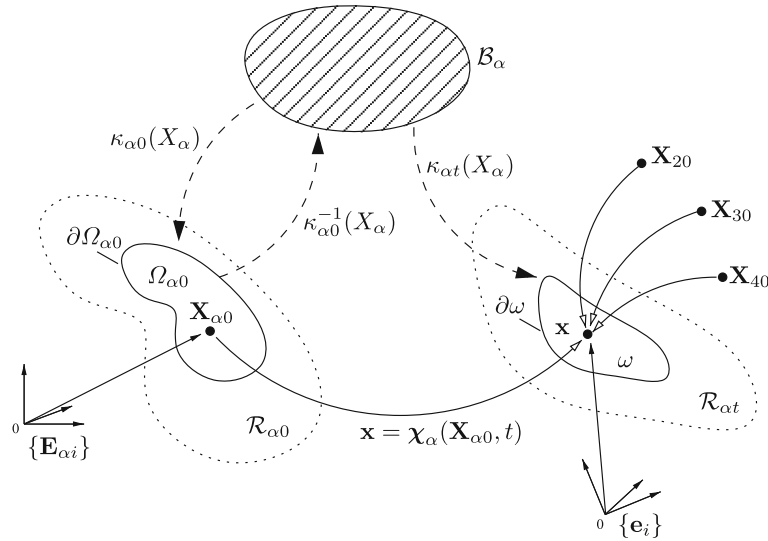


Fig. 1 Material body \mathcal{B}_α of constituent K_α . An open set $\mathcal{Q}_\alpha \subset \mathcal{B}_\alpha$ becomes in the reference configuration the material region $\Omega_{\alpha 0} \subset \mathcal{R}_{\alpha 0} \subset \mathcal{E}^3$ with boundary $\partial\Omega_{\alpha 0}$, and the material particle X_α is mapped onto $\mathbf{X}_{\alpha 0} \in \mathcal{R}_{\alpha 0}$. Similarly, in the present configuration, \mathcal{Q}_α is mapped into the open set $\Omega_{\alpha t} := \omega_\alpha \in \mathcal{R}_{\alpha t} \subset \mathcal{E}^3$ with boundary $\partial\Omega_{\alpha t} := \partial\omega_\alpha$, and the material particle X_α is mapped onto $\mathbf{x} \in \mathcal{R}_{\alpha t}$. $\{\mathbf{E}_{\alpha i}\}$ ($i = 1, 2, 3$) is a basis for K_α in the reference configuration, and $\{\mathbf{e}_i\}$ ($i = 1, 2, 3$) is a basis for K_α in the present configuration. Note that all different $\mathbf{X}_{\alpha 0}$ ($\alpha = 1, 2, \dots, n$) are mapped in the present configuration onto the same point \mathbf{x} . Therefore, ω_α and $\partial\omega_\alpha$ are the same region ω and boundary $\partial\omega$ for all α

constituent velocity \mathbf{v}_α , the material derivative $d^\alpha(\cdot)/dt$ following the motion of constituent K_α , the constituent acceleration \mathbf{a}_α , the constituent velocity gradient \mathbf{L}_α , its symmetric, \mathbf{D}_α , and skewsymmetric, \mathbf{W}_α , parts, the constituent deformation gradient \mathbf{F}_α and the constituent left Cauchy–Green deformation tensor \mathbf{B}_α . They are defined as

$$\begin{aligned} \hat{\mathbf{v}}_\alpha(\mathbf{X}_{\alpha 0}, t) &:= \frac{\partial \chi_\alpha(\mathbf{X}_{\alpha 0}, t)}{\partial t} = \left. \frac{d}{dt} \chi_\alpha(\mathbf{X}_{\alpha 0}, t) \right|_{\mathbf{X}_{\alpha 0}} \\ &= \frac{d^\alpha \chi_\alpha(\chi_\alpha^{-1}(\mathbf{x}, t), t)}{dt} =: \tilde{\mathbf{v}}_\alpha(\mathbf{x}, t) =: \dot{\mathbf{x}}_\alpha(\mathbf{x}, t), \end{aligned} \quad (23)$$

$$\begin{aligned} \hat{\mathbf{a}}_\alpha(\mathbf{X}_{\alpha 0}, t) &:= \frac{\partial^2 \chi_\alpha(\mathbf{X}_{\alpha 0}, t)}{\partial t^2} = \left. \frac{d^2}{dt^2} \chi_\alpha(\mathbf{X}_{\alpha 0}, t) \right|_{\mathbf{X}_{\alpha 0}} \\ &= \frac{d^{\alpha 2} \chi_\alpha(\chi_\alpha^{-1}(\mathbf{x}, t), t)}{d^2 t} =: \tilde{\mathbf{a}}_\alpha(\mathbf{x}, t), \end{aligned} \quad (24)$$

$$\mathbf{L}_\alpha := \nabla \mathbf{v}_\alpha = \mathbf{D}_\alpha + \mathbf{W}_\alpha, \quad (25)$$

$$\mathbf{D}_\alpha := \text{sym}(\nabla \mathbf{v}_\alpha), \quad \mathbf{W}_\alpha := \text{skw}(\nabla \mathbf{v}_\alpha).$$

$$\mathbf{F}_\alpha := \frac{\partial \chi_\alpha}{\partial \mathbf{X}_{\alpha 0}}(\mathbf{X}_{\alpha 0}, t), \quad (26)$$

$$\mathbf{B}_\alpha := \mathbf{F}_\alpha \mathbf{F}_\alpha^\top, \quad \mathbf{B}_\alpha = \mathbf{B}_\alpha^\top. \quad (27)$$

In these formulae, $(\dot{\cdot})_\alpha$ is an abbreviation for $d^\alpha(\cdot)/dt$, the material time derivative, following the motion of constituent K_α . Moreover, $|_{\mathbf{X}_{\alpha 0}}$ indicates that the indexed quantity is held fixed among the variables that are indexed; the functions $\hat{\mathbf{v}}_\alpha$ and $\tilde{\mathbf{v}}_\alpha$ take the same values for the same $\mathbf{X}_{\alpha 0}$, t and \mathbf{x} evaluated from (22)₂, but they are different functions, as they depend on different position vectors. The same is true for the accelerations.

4.2 Balance equations

Let ψ_α be the true density of a physical quantity. It stands, in particular, for the mass density, momentum density, energy density and entropy density *per unit volume of constituent K_α* at every point within a region

Table 1 Densities for the constituent balance relations

Balance	ψ_α	π_α^ψ	ϕ_α^ψ	σ_α^ψ	γ_α^ψ
Mass	ρ_α	0	$\mathbf{0}$	0	$\rho_\alpha c_\alpha$
Momentum	$\rho_\alpha \mathbf{v}_\alpha$	$\mathbf{0}$	\mathbf{T}_α	\mathbf{b}_α	\mathbf{m}_α
Moment of momentum	$\mathbf{x} \times \rho_\alpha \mathbf{v}_\alpha$	$\mathbf{0}$	$\mathbf{x} \times \mathbf{T}_\alpha$	$\mathbf{x} \times \mathbf{b}_\alpha$	\mathbf{M}_α
Total energy	$\rho_\alpha (\varepsilon_\alpha + \frac{1}{2} \mathbf{v}_\alpha \cdot \mathbf{v}_\alpha)$	0	$\mathbf{T}_\alpha \mathbf{v}_\alpha - \mathbf{q}_\alpha$	$r_\alpha + \mathbf{b}_\alpha \cdot \mathbf{v}_\alpha$	e_α
Entropy	$\rho_\alpha \eta_\alpha$	$\pi_\alpha^{\rho\eta}$	$\phi_\alpha^{\rho\eta}$	$\sigma_\alpha^{\rho\eta}$	$\gamma_\alpha^{\rho\eta}$

ω_α . This density must be distinguished from $\bar{\psi}_\alpha$, which is defined as the physical quantity *per unit mixture volume*. In the sequel we shall denote densities carrying an overbar as *partial densities* and those without a bar as *true densities*. Whilst the former are related to the mixture volume, the latter are associated with the constituent volume. The two are related by

$$\bar{\psi}_\alpha = \nu_\alpha \psi_\alpha, \quad (28)$$

in which ν_α is the volume fraction density of constituent α . The physical quantity contained in ω_α is given by additivity over the volume as

$$\mathcal{G}_\alpha(t) = \int_{\omega_\alpha} \bar{\psi}_\alpha(\mathbf{x}, t) dv. \quad (29)$$

We now postulate the balance law

$$\frac{d\mathcal{G}_\alpha}{dt} = \mathcal{P}_\alpha + \mathcal{S}_\alpha + \mathcal{F}_\alpha, \quad (30)$$

where \mathcal{P}_α and \mathcal{S}_α , \mathcal{F}_α are the production, supply and flux densities of \mathcal{G}_α , which are given by

$$\mathcal{P}_\alpha(t) = \int_{\omega_\alpha} (\bar{\pi}_\alpha^\psi(\mathbf{x}, t) + \bar{\gamma}_\alpha^\psi(\mathbf{x}, t)) dv, \quad (31)$$

$$\mathcal{S}_\alpha(t) = \int_{\omega_\alpha} \bar{\sigma}_\alpha^\psi(\mathbf{x}, t) dv, \quad (32)$$

$$\mathcal{F}_\alpha(t) = \int_{\partial\omega_\alpha} {}^* \bar{\phi}_\alpha^\psi(\mathbf{x}, t, \mathbf{n}) da, \quad (33)$$

in which $\bar{\pi}_\alpha^\psi$, $\bar{\gamma}_\alpha^\psi$, $\bar{\sigma}_\alpha^\psi$ and ${}^* \bar{\phi}_\alpha^\psi$ are partial densities per unit mixture volume and unit mixture area, respectively. The partial production density has been divided into two contributions. We interpret henceforth $\bar{\pi}_\alpha^\psi$ as the (self) production rate of $\bar{\psi}_\alpha$ by constituent K_α , whilst $\bar{\gamma}_\alpha^\psi$ is the production rate of $\bar{\psi}_\alpha$ by all constituents other than K_α . This can be interpreted as production by interaction. For mass, linear and angular momentum, energy and entropy these quantities are defined in columns 3 and 6 of Table 1. Analogously, $\bar{\sigma}_\alpha^\psi$ is the partial density of the supply rate of $\bar{\psi}_\alpha$, a source of $\bar{\psi}_\alpha$ outside the body volume ω_α but affecting material points within ω_α .

The partial density of the flux of $\bar{\psi}_\alpha$ through the boundary of the body is defined per unit area on the surface $\partial\omega_\alpha$ and is denoted by ${}^* \bar{\phi}_\alpha^\psi$. Thus, the total flux through the boundary $\partial\omega_\alpha$ into the body volume ω_α is the surface integral (33). As opposed to $\bar{\psi}_\alpha$, $\bar{\pi}_\alpha^\psi$ and $\bar{\gamma}_\alpha^\psi$, which are only functions of \mathbf{x} and t , ${}^* \bar{\phi}_\alpha^\psi$ also depends on the unit exterior normal vector \mathbf{n} of $\partial\omega_\alpha$. In general, ${}^* \bar{\phi}_\alpha^\psi$ could also depend on other differential geometric properties of the surface, say the mean and Gaussian curvatures, but Cauchy restricted the dependence to merely one on \mathbf{n} (this is called the ‘Cauchy assumption’). The flux and supply terms for mass, linear and angular momentum, energy and entropy are listed in columns 4 and 5 of Table 1.

The bar in the representation ${}^* \bar{\phi}_\alpha^\psi(\mathbf{x}, t, \mathbf{n})$ indicates that the flux density in (33) is referred to a unit mixture area. To assume the relation

$${}^* \bar{\phi}_\alpha^\psi = \nu_\alpha {}^* \phi_\alpha^\psi, \quad (34)$$

we are postulating in fact that areal and volume fractions are the same. With this we have

$$\left\{ \bar{\boldsymbol{\psi}}_\alpha, \bar{\boldsymbol{\pi}}_\alpha^\psi, {}^* \bar{\boldsymbol{\phi}}_\alpha^\psi, \bar{\boldsymbol{\sigma}}_\alpha^\psi, \bar{\boldsymbol{\gamma}}_\alpha^\psi \right\} = \nu_\alpha \left\{ \boldsymbol{\psi}_\alpha, \boldsymbol{\pi}_\alpha^\psi, {}^* \boldsymbol{\phi}_\alpha^\psi, \boldsymbol{\sigma}_\alpha^\psi, \boldsymbol{\gamma}_\alpha^\psi \right\}. \quad (35)$$

If we then also employ Cauchy's lemma

$${}^* \boldsymbol{\phi}_\alpha^\psi(\mathbf{x}, t, \mathbf{n}) = \boldsymbol{\phi}_\alpha^\psi(\mathbf{x}, t) \mathbf{n}, \quad (36)$$

it can be shown that the local balance law for a physical quantity of constituent K_α takes the form

$$\partial \bar{\boldsymbol{\psi}}_\alpha - \nabla \cdot \left(\bar{\boldsymbol{\phi}}_\alpha^\psi - \bar{\boldsymbol{\psi}}_\alpha \otimes \mathbf{v}_\alpha \right) - \bar{\boldsymbol{\pi}}_\alpha^\psi - \bar{\boldsymbol{\sigma}}_\alpha^\psi - \bar{\boldsymbol{\gamma}}_\alpha^\psi = \mathbf{0}, \quad (37)$$

at all regular points of the present configuration.

The requirement that the mixture as a whole obeys local balance laws as if it were a single material implies the local balance law

$$\partial \boldsymbol{\psi} = \boldsymbol{\pi}^\psi + \nabla \cdot \left(\boldsymbol{\phi}^\psi - \boldsymbol{\psi} \otimes \mathbf{v} \right) + \boldsymbol{\sigma}^\psi, \quad (38)$$

for the mixture variables which are related to the constituent quantities via

$$\begin{aligned} \boldsymbol{\psi} &:= \sum \bar{\boldsymbol{\psi}}_\alpha, \\ \boldsymbol{\phi}^\psi - \boldsymbol{\psi} \otimes \mathbf{v} &:= \sum \left[\bar{\boldsymbol{\phi}}_\alpha^\psi - \bar{\boldsymbol{\psi}}_\alpha \otimes \mathbf{v}_\alpha \right], \\ \boldsymbol{\pi}^\psi &:= \sum \bar{\boldsymbol{\pi}}_\alpha^\psi, \\ \boldsymbol{\sigma}^\psi &:= \sum \bar{\boldsymbol{\sigma}}_\alpha^\psi, \end{aligned} \quad (39)$$

where

$$\rho := \sum \bar{\rho}_\alpha, \quad \rho \mathbf{v} := \sum \bar{\rho}_\alpha \mathbf{v}_\alpha. \quad (40)$$

We employ the balance laws for the physical quantities collected in Table 1. These can be written as follows:

- mass:

$$\mathcal{R}_\alpha := \partial \bar{\rho}_\alpha + \nabla \cdot (\bar{\rho}_\alpha \mathbf{v}_\alpha) - \bar{\rho}_\alpha c_\alpha = 0, \quad (41)$$

- linear momentum:

$$\mathcal{M}_\alpha := \partial (\bar{\rho}_\alpha \mathbf{v}_\alpha) - \nabla \cdot \left(\bar{\mathbf{T}}_\alpha - \bar{\rho}_\alpha \mathbf{v}_\alpha \otimes \mathbf{v}_\alpha \right) - \bar{\mathbf{m}}_\alpha - \bar{\mathbf{b}}_\alpha = \mathbf{0}, \quad (42)$$

- energy:

$$\mathcal{E} := \partial (\rho \varepsilon) + \nabla \cdot (\mathbf{q} + \rho \varepsilon \mathbf{v}) - \mathbf{T} \cdot \nabla \mathbf{v} - \rho r = 0, \quad (43)$$

- entropy:

$$\mathcal{H} := \partial (\rho \eta) + \nabla \cdot (\boldsymbol{\phi}^{\rho \eta} + \rho \eta \mathbf{v}) - \sigma^{\rho \eta} = \pi^{\rho \eta} \quad (44)$$

in which we require $\mathbf{T}_\alpha = \mathbf{T}_\alpha^T$, which holds true if exchange of angular momentum of constituent α is only due to exchange of linear momentum of the same constituent. In the above

$$\begin{aligned} \mathbf{u}_\alpha &:= \mathbf{v}_\alpha - \mathbf{v}, \quad \sum \mathbf{u}_\alpha = \mathbf{0}, \\ \sum_\alpha \bar{\rho}_\alpha c_\alpha &= 0, \quad \sum_\alpha \bar{\mathbf{m}}_\alpha = \mathbf{0} \end{aligned} \quad (45)$$

as well as

$$\mathbf{T} := \sum \bar{\mathbf{T}}_\alpha - \sum \bar{\rho}_\alpha \mathbf{u}_\alpha \otimes \mathbf{u}_\alpha = \mathbf{T}_I + \mathbf{T}_D, \quad (46)$$

$$\mathbf{T}_I := \sum \bar{\mathbf{T}}_\alpha, \quad \mathbf{T}_D := - \sum \bar{\rho}_\alpha \mathbf{u}_\alpha \otimes \mathbf{u}_\alpha \quad (47)$$

$$\mathbf{q} := \sum \bar{\mathbf{q}}_\alpha - \sum \bar{\mathbf{T}}_\alpha \mathbf{u}_\alpha + \sum \bar{\rho}_\alpha \left\{ \varepsilon_\alpha + \frac{1}{2} \{ \mathbf{u}_\alpha \cdot \mathbf{u}_\alpha \} \right\} \mathbf{u}_\alpha = \mathbf{q}_I + \mathbf{q}_D, \quad (48)$$

$$\mathbf{q}_I := \sum \bar{\mathbf{q}}_\alpha, \quad \mathbf{q}_D := - \sum \bar{\mathbf{T}}_\alpha \mathbf{u}_\alpha + \sum \bar{\rho}_\alpha \left\{ \varepsilon_\alpha + \frac{1}{2} \{ \mathbf{u}_\alpha \cdot \mathbf{u}_\alpha \} \right\} \mathbf{u}_\alpha. \quad (49)$$

Moreover, we also employ the following flux free *balance laws for the volume fractions*, v_α :

$$\mathcal{N}_\alpha := \partial v_\alpha + \nabla \cdot (v_\alpha \mathbf{v}_\alpha) - \bar{n}_\alpha = 0, \quad (50)$$

and for the *frictional stress like variables*, \mathbf{Z}_α ,

$$\mathcal{Z}_\alpha := \overset{\circ}{\bar{\mathbf{Z}}}_\alpha - \bar{\Phi}_\alpha = \mathbf{0}. \quad (51)$$

Here, \mathbf{Z}_α is a symmetric second rank tensor and $\overset{\circ}{\bar{\mathbf{Z}}}_\alpha$ is the objective time derivative

$$\overset{\circ}{\bar{\mathbf{Z}}}_\alpha = \partial \bar{\mathbf{Z}}_\alpha + (\nabla \bar{\mathbf{Z}}_\alpha) \mathbf{v}_\alpha - (\boldsymbol{\Omega}_\alpha \bar{\mathbf{Z}}_\alpha - \bar{\mathbf{Z}}_\alpha \boldsymbol{\Omega}_\alpha), \quad (52)$$

where $\boldsymbol{\Omega}_\alpha$ is a spin tensor, e.g. \mathbf{W} or \mathbf{W}_α . The quantities \bar{n}_α and $\bar{\Phi}_\alpha = \bar{\Phi}_\alpha^T$ are production rate densities, which eventually must be given by closure statements.

4.3 Saturation condition

The theory in Schneider and Hutter [35] is developed for a mixture satisfying the saturation condition

$$\sum_\alpha v_\alpha = 1. \quad (53)$$

It states that there is no material free void space within the mixture. Thus, if we write $v_n = - \sum_{\alpha=1}^{n-1} v_\alpha$, the volume fraction balance law for $\alpha = n$ is given by

$$\mathcal{N}_n := -\partial \left(\sum_{\beta=1}^{n-1} v_\beta \right) + \nabla \cdot \mathbf{v}_n - \nabla \cdot \left(\sum_{\beta=1}^{n-1} v_\beta \mathbf{v}_n \right) - \bar{n}_n = 0. \quad (54)$$

Obviously, only v_α , $\alpha = 1, \dots, n-1$ are independent fields.

4.4 Constituent density constraints

Schneider and Hutter [35] present their solid–fluid mixture model for the case that some or all of the constituent true mass densities are constant, i.e.

$$\rho_\alpha = \text{const.}, \quad \alpha = m+1, \dots, n \quad (0 \leq m \leq n) \quad (55)$$

If the constituent densities ρ_α are independent constitutive variables, the constraint conditions (55) reduce the number of independent constitutive variables by $(n-m)$. In particular, comparison of the constituent mass balance laws with the volume fraction balance laws implies

$$\bar{c}_\alpha = \bar{n}_\alpha, \quad \text{or} \quad c_\alpha = n_\alpha, \quad (\alpha = m+1, \dots, n) \quad (56)$$

for all density preserving constituents.

4.5 Constitutive relations

Schneider and Hutter [35] choose the constitutive equations to be of the form

$$\begin{aligned} \mathbf{C} &= \hat{\mathbf{C}}(\mathbb{S}), \\ \mathbb{S} &= \left\{ \theta, \dot{\theta}, \nabla\theta, \bar{\rho}, \bar{\nabla}\rho, \bar{v}, \bar{\nabla}v, \bar{\mathbf{v}}, \bar{\mathbf{B}}, \bar{\mathbf{D}}, \bar{\mathbf{W}}, \bar{\mathbf{Z}} \right\}, \\ \bar{\rho} &:= \rho_1, \dots, \rho_m, \quad \bar{v} := v_1, \dots, v_{n-1}, \\ \bar{\mathbf{v}} &:= \mathbf{v}_1, \dots, \mathbf{v}_n, \quad \bar{\mathbf{B}} := \mathbf{B}_1, \dots, \mathbf{B}_n, \\ \bar{\mathbf{D}} &:= \mathbf{D}_1, \dots, \mathbf{D}_n, \quad \bar{\mathbf{W}} := \mathbf{W}_1, \dots, \mathbf{W}_n, \\ \bar{\mathbf{Z}} &:= \bar{\mathbf{Z}}_1, \dots, \bar{\mathbf{Z}}_n. \end{aligned} \tag{57}$$

\mathbf{C} denotes any dependent constitutive variable and $\hat{\mathbf{C}}(\mathbb{S})$ is the functional describing⁸ it. That the independent set \mathbb{S} is assumed to be the same for all dependent constitutive variables is the expression of the rule of equivalence, which states that all constitutive quantities initially share the same dependences. Possible variable reductions ought to be deduced by proof. In (57), we already used the assumption that each constituent behaves as an isotropic material, i.e. an arbitrary rotation or a mirror reflection does not alter the material behaviour of a constituent (cf. Hutter and Jöhnk [16]). Thus, the shape of the constitutive law, (57), shall not be affected by these rotations or reflections.

By combining the material isotropy with the requirement that every constitutive law must be objective, it is observed that all constitutive quantities must be *isotropic functions* of their dependent variables, i.e.

$$\begin{aligned} \mathbf{Q}_* \hat{\mathbf{C}} &= \hat{\mathbf{C}} \left(\theta, \dot{\theta}, \mathbf{Q}(\nabla\theta), \bar{\rho}, \mathbf{Q}(\bar{\nabla}\rho), \bar{v}, \mathbf{Q}(\bar{\nabla}v), \mathbf{Q}(\bar{\mathbf{v}}), \right. \\ &\quad \left. \mathbf{Q}\bar{\mathbf{B}}\mathbf{Q}^T, \mathbf{Q}\bar{\mathbf{D}}\mathbf{Q}^T, \mathbf{Q}\bar{\mathbf{W}}\mathbf{Q}^T, \mathbf{Q}\bar{\mathbf{Z}}\mathbf{Q}^T \right), \end{aligned} \tag{58}$$

for all orthogonal time-dependent tensors $\mathbf{Q}(t)$, where \mathbf{Q}_* denotes the action

$$\left(\mathbf{Q}_* \hat{\mathbf{C}} \right)_{i_1 i_2 \dots i_n} = Q_{i_1 j_1} Q_{i_2 j_2} \dots Q_{i_n j_n} \left(\hat{\mathbf{C}} \right)_{j_1 j_2 \dots j_n} \tag{59}$$

on the tensor valued quantity $\hat{\mathbf{C}}$.

4.6 Entropy principle

The union of the balance laws of mass, linear momentum, volume fraction and stress-like second order tensor variables, and constitutive relations for

$$\mathbf{C} = \left\{ \varepsilon, \eta, c_\alpha, \bar{n}_\alpha, \bar{\mathbf{m}}_\alpha, \mathbf{q}, \phi^{\rho\eta}, \mathbf{T}_\alpha, \bar{\Phi}_\alpha \right\} \tag{60}$$

form a set of non-linear partial differential equations for the variables

$$\left\{ \theta, \underbrace{\rho_1, \dots, \rho_m}_{\text{compressible}}, \underbrace{v_1, \dots, v_{n-1}}_{\text{saturation}}, \mathbf{v}_1, \dots, \mathbf{v}_n, \bar{\mathbf{Z}}_1, \dots, \bar{\mathbf{Z}}_n \right\}. \tag{61}$$

These equations are called *field equations*, and it is tacitly assumed that they are well posed in the sense that mathematical solutions to meaningful initial and boundary conditions do exist. Any such solution is called a *thermodynamic process*.

The balance law for the mixture entropy, $\mathcal{H} = \pi^{\rho\eta}$, was stated in Eq. (44). In terms of it, the second law of thermodynamics demands that the imbalance

$$\pi^{\rho\eta} = \partial(\rho\eta) - \nabla \cdot (\phi^{\rho\eta} - \rho\eta\mathbf{v}) - \sigma^{\rho\eta} \geq 0. \tag{62}$$

⁸ $\hat{\mathbf{C}}$ involves the variable $\bar{\mathbf{Z}}$, for which an evolution equation is formulated. So, as an expression, $\hat{\mathbf{C}}$ is a function, but since $\bar{\mathbf{Z}}$ is given by a functional relation involving the time derivative of $\bar{\mathbf{Z}}$, we may think of $\hat{\mathbf{C}}$ to have functional structure.

must be satisfied for all thermodynamic processes, i.e. all solutions of the field equations. According to Liu's assertion, [24], (which is based on Farkas's variational inequality theorem [11]), this statement is equivalent to the following extended inequality

$$*\boldsymbol{\pi}^{\rho\eta} := \pi^{\rho\eta} - \sum \lambda_{\alpha}^{\rho} \mathcal{R}_{\alpha} - \sum \lambda_{\alpha}^{\nu} \cdot \mathcal{M}_{\alpha} - \lambda^{\varepsilon} \mathcal{E} - \sum_{\alpha=1}^{n-1} \lambda_{\alpha}^{\nu} \mathcal{N}_{\alpha} - \lambda_n^{\nu} \mathcal{N}_n - \sum \lambda_{\alpha}^Z \cdot \mathcal{Z}_{\alpha} \geq 0 \quad (63)$$

or

$$\begin{aligned} *\boldsymbol{\pi}^{\rho\eta} &= \partial(\rho\eta) - \nabla \cdot (\boldsymbol{\phi}^{\rho\eta} - \rho\eta\mathbf{v}) \\ &\quad - \sum_{\alpha=1}^m \lambda_{\alpha}^{\rho} \{ \partial\bar{\rho}_{\alpha} + \nabla \cdot (\bar{\rho}_{\alpha}\mathbf{v}_{\alpha}) - \bar{\rho}_{\alpha}c_{\alpha} \} \\ &\quad - \sum \lambda_{\alpha}^{\nu} \cdot \{ \partial(\bar{\rho}_{\alpha}\mathbf{v}_{\alpha}) - \nabla \cdot (\bar{\mathbf{T}}_{\alpha} - \bar{\rho}_{\alpha}\mathbf{v}_{\alpha} \otimes \mathbf{v}_{\alpha}) - \bar{\mathbf{m}}_{\alpha} \} \\ &\quad - \lambda^{\varepsilon} \{ \partial(\rho\varepsilon) + \nabla \cdot (\mathbf{q} + \rho\varepsilon\mathbf{v}) - \mathbf{T} \cdot (\nabla\mathbf{v}) \} \\ &\quad - \sum_{\alpha=1}^{n-1} \lambda_{\alpha}^{\nu} \{ \partial\nu_{\alpha} + \nabla \cdot (\nu_{\alpha}\mathbf{v}_{\alpha}) - \bar{n}_{\alpha} \} \\ &\quad - \lambda_n^{\nu} \left\{ -\partial \left(\sum_{\beta=1}^{n-1} \nu_{\beta} \right) + \nabla \cdot \mathbf{v}_n - \nabla \cdot \left(\sum_{\beta=1}^{n-1} \nu_{\beta}\mathbf{v}_n \right) - \bar{n}_n \right\} \\ &\quad - \sum \lambda_{\alpha}^Z \cdot \left\{ \dot{\bar{\mathbf{Z}}}_{\alpha} - [\boldsymbol{\Omega}_{\alpha}, \bar{\mathbf{Z}}_{\alpha}] - \bar{\boldsymbol{\Phi}}_{\alpha} \right\} \\ &\geq 0, \end{aligned} \quad (64)$$

in which it was assumed that the supply terms sum up to zero, implying that

$$\sigma^{\rho\eta} = \sum \lambda_{\alpha}^{\nu} \cdot \bar{\mathbf{b}}_{\alpha} + \lambda^{\varepsilon} r. \quad (65)$$

Moreover, the various λ s are Lagrange multipliers to be determined together with restrictions of constitutive quantities as a result of the exploitation of (64). These steps of analysis are very long and are explicitly demonstrated in Schneider and Hutter [35]. Below we report on the most significant findings.

5 General results

For the mathematical exploitation of inequality (64), it is convenient to introduce the one-forms

$$\mathcal{P} = \sum_{I=1}^K \mathcal{P}_{x_I} dx_I := d(\rho\eta) - \lambda^{\varepsilon} d(\rho\varepsilon), \quad (66)$$

$$\mathcal{F} = \sum_{I=1}^K \mathcal{F}_{x_I} dx_I := d\boldsymbol{\phi}^{\rho\eta} + \lambda^{\varepsilon} (d\mathbf{q}) - \sum (d\bar{\mathbf{T}}_{\alpha}) \lambda_{\alpha}^{\nu}, \quad (67)$$

in which $x_I (I = 1, \dots, K)$ are the independent constitutive variables. Of help are also the following auxiliary variables:

$$l_{\alpha}^{\rho} := \lambda_{\alpha}^{\rho} + \lambda_{\alpha}^{\nu} \cdot \mathbf{v}_{\alpha}, \quad (68)$$

$$l_{\alpha}^{\nu} := \rho_{\alpha} l_{\alpha}^{\rho} + \lambda_{\alpha}^{\nu}, \quad (69)$$

$$\boldsymbol{\Gamma} := \lambda^{\varepsilon} \rho^{-1} \mathbf{T} + (\eta - \lambda^{\varepsilon} \varepsilon) \mathbf{I} = \boldsymbol{\Gamma}^T, \quad (70)$$

$$s := -l_n^{\nu}, \quad (71)$$

$$\mathbf{s} := s\mathbf{v}_n + \rho_n \boldsymbol{\Gamma} \mathbf{u}_n, \quad (72)$$

as well as the so-called *extra entropy flux vector*

$$\mathbf{k} := \boldsymbol{\phi}^{\rho\eta} + \lambda^\varepsilon \mathbf{q} - \sum \bar{\mathbf{T}}_\alpha \lambda_\alpha^v. \quad (73)$$

If in the inequality (64) all indicated differentiations are performed with due account of the chain rule of differentiation in the constitutive quantities, then (64) can be expressed as the statement

$$\mathbf{X}(\mathbf{Y}) \cdot \dot{\mathbf{Y}} + \pi_R^{\rho\eta} \geq 0, \quad \forall \dot{\mathbf{Y}} \in \mathbb{R}^K \quad (74)$$

where K is the dimension of the vector space, in which the vectors $\dot{\mathbf{Y}}$ live (see (66), (67)). $\mathbf{X}(\mathbf{Y})$ and $\pi_R^{\rho\eta}(\mathbf{Y})$ do not depend on $\dot{\mathbf{Y}}$, so (74) is linear in $\dot{\mathbf{Y}}$. Of necessity then

$$\mathbf{X}(\mathbf{Y}) \cdot \dot{\mathbf{Y}} = 0, \quad \forall \dot{\mathbf{Y}}, \quad \pi_R^{\rho\eta} \geq 0. \quad (75)$$

Sometimes (75)₁ is referred to as Liu identities and (75)₂ is the *residual entropy inequality*.

5.1 Inferences implied by the Liu identities

Explicit statements of implications of the Liu identities could only be found by introducing a number of ad hoc assumption. Apart from a few technical ones, which all are explicitly stated in *Schneider and Hutter* [35], we request:

Postulate 1 The Lagrange multiplier of the energy balance law, λ^ε , is a function of the empirical temperature and its total time derivative

$$\lambda^\varepsilon = \hat{\lambda}^\varepsilon(\theta, \dot{\theta}). \quad (76)$$

The function $\hat{\lambda}^\varepsilon(\cdot)$ is called the *coldness function*. □

In the course of computations, we were able to prove that $\hat{\lambda}^\varepsilon(\cdot)$ is a function of at most the independent constitutive variables. The above reduced functional form is motivated by many earlier results by Müller [30] and many others for which (76) has been a proven statement. Therefore, there is some confidence that (76) is reasonable. If $\dot{\theta}$ is not an independent constitutive variable, then $\lambda = \hat{\lambda}^\varepsilon(\theta)$ may be identified with $1/T$, where T is the Kelvin temperature.

With the postulate of the existence of the coldness function, some of the Liu identities imply the following statements:

$$\begin{aligned} - \left(\rho\varepsilon_I - \frac{1}{\lambda^\varepsilon} \rho\eta \right)_{,\theta} &= \frac{1}{\lambda^\varepsilon} \mathcal{P}_\theta - \frac{1}{(\lambda^\varepsilon)^2} \rho\eta \lambda^{\varepsilon, \theta}, \\ - \left(\rho\varepsilon_I - \frac{1}{\lambda^\varepsilon} \rho\eta \right)_{,\dot{\theta}} &= - \frac{1}{(\lambda^\varepsilon)^2} \rho\eta \lambda^{\varepsilon, \dot{\theta}}, \\ - \left(\rho\varepsilon_I - \frac{1}{\lambda^\varepsilon} \rho\eta \right)_{,\nabla\theta} &= \frac{1}{\lambda^\varepsilon} \mathcal{P}_{\nabla\theta}, \\ - \left(\rho\varepsilon_I - \frac{1}{\lambda^\varepsilon} \rho\eta \right)_{,\rho_\alpha} &= \frac{1}{\lambda^\varepsilon} \bar{l}_{\alpha 1}^\rho, \quad \alpha = 1, \dots, m, \\ - \left(\rho\varepsilon_I - \frac{1}{\lambda^\varepsilon} \rho\eta \right)_{,\nu_\alpha} &= \frac{1}{\lambda^\varepsilon} (l_{\alpha 1}^v + s), \quad \alpha = 1, \dots, n-1, \\ - \left(\rho\varepsilon_I - \frac{1}{\lambda^\varepsilon} \rho\eta \right)_{,\mathbf{v}_\alpha} &= \frac{1}{\lambda^\varepsilon} \bar{\rho}_\alpha (\lambda_\alpha^v + \lambda^\varepsilon \mathbf{u}_\alpha), \quad \alpha = 1, \dots, n, \\ - \left(\rho\varepsilon_I - \frac{1}{\lambda^\varepsilon} \rho\eta \right)_{,\mathbf{B}_\alpha} &= \frac{1}{\lambda^\varepsilon} \mathcal{P}_{\mathbf{B}_\alpha}, \quad \alpha = 1, \dots, n, \\ - \left(\rho\varepsilon_I - \frac{1}{\lambda^\varepsilon} \rho\eta \right)_{,\bar{\mathbf{Z}}_\alpha} &= \frac{1}{\lambda^\varepsilon} \lambda_\alpha^Z, \quad \alpha = 1, \dots, n, \end{aligned} \quad (77)$$

with

$$\bar{\xi}_\alpha = \frac{\bar{\rho}_\alpha}{\rho}, \quad l_{\alpha I}^\rho := l_\alpha^\rho + \frac{1}{2}\lambda^\varepsilon(\mathbf{u}_\alpha \cdot \mathbf{u}_\alpha), \quad (78)$$

$$\varepsilon_I = \sum \bar{\xi}_\alpha \varepsilon_\alpha, \quad l_{\alpha I}^v := l_\alpha^v + \frac{1}{2}\lambda^\varepsilon \rho_\alpha(\mathbf{u}_\alpha \cdot \mathbf{u}_\alpha) - \mathbf{k}, \quad (79)$$

$$\varepsilon_D = \frac{1}{2} \sum \bar{\xi}_\alpha \mathbf{u}_\alpha \cdot \mathbf{u}_\alpha, \quad \mathbf{k} := \frac{1}{2}\lambda^\varepsilon \rho_n(\mathbf{u}_n \cdot \mathbf{u}_n) \quad (80)$$

From these relations, we observe that the Lagrange multipliers for the momenta λ_α^v ($\alpha = 1, \dots, n$), those for the masses λ_α^ρ ($\alpha = 1, \dots, m$) and volume fractions λ_α^v ($\alpha = 1, \dots, n-1$), hidden in the definitions of $\bar{l}_{1\alpha}^\rho$ and $l_{1\alpha}^v$, see (68), (69), depend on the constitutive variables, because they are determined by the ‘inner’ part of a Helmholtz free energy-like quantity, defined as

$$\begin{aligned} \Psi^G &:= \varepsilon - (\lambda^\varepsilon)^{-1}\eta = \Psi_I^G + \Psi_D^G, \\ \Psi_I^G &:= \varepsilon_I - (\lambda^\varepsilon)^{-1}\eta, \quad \Psi_D^G := \varepsilon_D. \end{aligned} \quad (81)$$

Moreover, in view of (77)₅, (78) and (69), λ_α^v ($\alpha = 1, \dots, n-1$) also depend on the constraint variable, s , due to saturation. It is also not correct to call Ψ^G the Helmholtz free energy because we have not made the assumption $\lambda^\varepsilon = (\theta)^{-1}$. This is the reason for us to use the superscript G as the identifier of this distinction. On the other hand, we can regard Ψ_I^G as a *potential* because in (77), λ^ε is at our disposal to ascertain that $d(\rho\varepsilon_I - \frac{1}{\lambda^\varepsilon}\rho\eta)$ is the *total derivative* of a well defined function. In this way, we can regard λ^ε as an *integrating denominator*.

Relation (77)₆ motivates

Postulate 2 The Lagrange multiplier of the linear momentum of constituent α is selected as

$$\lambda_\alpha^v = -\lambda^\varepsilon \mathbf{u}_\alpha, \quad (82)$$

in which \mathbf{u}_α is the diffusion velocity. \square

In simpler mixture formulations (82) could be proved or is suggested by the Liu identities, see Svendsen and Hutter [36] and Kirchner [22].

Next, we introduce the following

Definition 1 1. The (*true*) *partial thermodynamic pressures*

$$\bar{p}_\alpha^G := \rho \rho_\alpha (\Psi_I^G)_{,\rho_\alpha}, \quad \alpha = 1, \dots, m, \quad (83)$$

2. *the configuration pressures*

$$\beta_\alpha^G := \rho (\Psi_I^G)_{,v_\alpha}, \quad \alpha = 1, \dots, n-1, \quad (84)$$

3. *the saturation pressure*

$$\mathcal{S} := \frac{s}{\lambda^\varepsilon} \stackrel{(71)}{=} - \frac{l_n^v}{\lambda^\varepsilon} \stackrel{(68)}{=} \rho_n \mathbf{u}_n \cdot \mathbf{v}_n - \frac{1}{\lambda^\varepsilon} (\rho_n \lambda_n^\rho + \lambda_n^v). \quad (85)$$

4. *the inner part of the constituent Gibbs free energies (chemical potentials, free enthalpies)*

$$\mu_{1\alpha}^G := \Psi_I^G + (\rho_\alpha)^{-1} p_\alpha^G. \quad (86)$$

\square

Incidentally, with the above definitions, it may be shown that the Gibbs free energies can be written as

$$\bar{\rho}_\alpha \mu_{1\alpha}^G = \begin{cases} \rho_\alpha (\rho \Psi_I^G)_{,\rho_\alpha} = v_\alpha \{ (\rho \Psi_I^G)_{,v_\alpha} + \iota_\alpha + \mathcal{S}_I \}, & \alpha = 1, \dots, m, \\ v_\alpha \{ (\rho \Psi_I^G)_{,v_\alpha} + \iota_\alpha + \mathcal{S}_I \}, & \alpha = m+1, \dots, n-1, \\ v_\alpha (\iota_\alpha + \mathcal{S}_I), & \alpha = n, \end{cases} \quad (87)$$

where the abbreviations

$$\iota_\alpha := (\lambda^\varepsilon)^{-1} \lambda_\alpha^v \quad (88)$$

and

$$\varsigma_I := \varsigma - \frac{1}{2} \rho_n (\mathbf{u}_n \cdot \mathbf{u}_n) \quad (89)$$

have been used. Whilst ι_α depends on the Lagrange multipliers λ^ε and λ_α^v , ς_I also has a dependence on the diffusive kinetic energy of constituent K_n . With the above formulae (77–89), the Postulates 1 and 2, and the technical assumptions stated in Schneider and Hutter [35], a great number of inferences can be drawn, which we state in the following propositions.

Proposition 1 (i) *The internal energy ε , entropy η and Helmholtz-like free energy Ψ_I^G cannot depend on $\vec{\nabla}\rho$, $\vec{\nabla}\mathbf{v}$, $\vec{\mathbf{D}}$ and $\vec{\mathbf{W}}$ and are thus only functions of $\mathbb{S}_R = \{\theta, \dot{\theta}, \nabla\theta, \vec{\rho}, \vec{v}, \vec{v}, \vec{\mathbf{B}}, \vec{\mathbf{Z}}\}$. Of these thermodynamic potentials, Ψ^G is particularly significant since Postulate 2, in conjunction with (77)₆, also rules out a dependence of Ψ_I^G on any \mathbf{v}_α : $\Psi_I^G = \Psi_I^G(\mathbb{S}_R \setminus \{\vec{\mathbf{v}}\})$.*

If $\dot{\theta} \notin \mathbb{S}$, then $\lambda^\varepsilon = \hat{\lambda}^\varepsilon(\theta) = 1/T$, where T is the Kelvin temperature.⁹ Moreover, $\varepsilon = \varepsilon(\mathbb{S}_{RR})$ and $\eta = \eta(\mathbb{S}_{RR})$, whilst $\Psi_I^G = \Psi_I^G(\mathbb{S}_{RR} \setminus \vec{\mathbf{v}})$, with $\mathbb{S}_{RR} = \mathbb{S}_R \setminus \{\dot{\theta}, \nabla\theta\}$.

- (ii) Since the constituent thermodynamic pressures, \bar{p}_α^G , constituent configuration pressures, β_α^G and the inner parts of the constituent Gibbs free energies, μ_α^G are all density weighted derivatives of the inner part of the Helmholtz-like free energy Ψ_I^G , see (83), (84), (86), they are, hence, equally functions of $\mathbb{S}_R \setminus \{\vec{\mathbf{v}}\}$.
- (iii) All Lagrange parameters except λ_n^v can be expressed in terms of thermodynamic quantities. Specifically,

$$\begin{aligned} \lambda_\alpha^\rho &= \lambda^\varepsilon \left(\mathbf{u}_\alpha \cdot \mathbf{v}_\alpha - \Psi_I^G - \rho_\alpha^{-1} p_\alpha^G + \frac{1}{2} \mathbf{u}_\alpha \cdot \mathbf{u}_\alpha \right), \\ &\quad (\alpha = 1, \dots, m), \\ \lambda_\alpha^v &= (-\rho_\alpha l_\alpha^\rho) \mathbf{H}(m - \alpha) - \lambda^\varepsilon \left(\varsigma + (\rho_\alpha - \rho_n) \Psi_I^G + \beta_\alpha \right. \\ &\quad \left. + \frac{1}{2} (\rho_\alpha \mathbf{u}_\alpha \cdot \mathbf{u}_\alpha - \rho_n \mathbf{u}_n \cdot \mathbf{u}_n) \right) \\ &= \lambda^\varepsilon \iota_\alpha, \quad (\alpha = 1, \dots, n-1), \end{aligned} \quad (90)$$

where \mathbf{H} is the Heaviside step function. It is seen (compare also (98) below) that all Lagrange multipliers, except λ_n^v , are determined as functions of the universal coldness function $\hat{\lambda}^\varepsilon(\theta, \dot{\theta})$, the Helmholtz-like free energy Ψ_I^G , the densities ρ_α , and diffusion velocities \mathbf{u}_α .

- (iv) The only undetermined field is a quantity proportional to $-\lambda_n^v$, defined in (71) as $s = -l_n^v$, or in (85) as $\varsigma = s/\lambda^\varepsilon$ and referred to as saturation pressure, see e.g. (91). This scalar variable replaces as a new free field the n -th volume fraction, that is lost as an independent field through the saturation condition.
- (v) Inner parts of the constituent Gibbs-like free energies, have their analogue, $\iota_\alpha := \lambda_\alpha^v/\lambda^\varepsilon$ ($\alpha \leq n-1$), and later will be shown to occur together only with the specific mass and volume fraction production rate densities, respectively. Thus, they play only a role when chemical reactions or fragmentations or internal phase changes occur and non-trivial volume fraction production rates arise. Therefore, in processes where these are absent, they are ‘dormant’ variables.
- (vi) The entropy is given by the formula

$$\eta = -\frac{1}{(1/\lambda^\varepsilon)_{,\theta}} \left\{ \Psi_{I,\theta}^G + \frac{\mathcal{P}_\theta}{\rho \lambda^\varepsilon} \right\}, \quad (92)$$

which reduces to the classical relation when $\dot{\theta}$ is not among the independent constitutive variables,

$$\eta = -\Psi_{I,\theta}^G \quad \text{if } \dot{\theta} \notin \mathbb{S}, \quad (93)$$

since in this case $\mathcal{P}_\theta = 0$ and θ may be identified with the absolute temperature T . Else \mathcal{P}_θ must be determined.

⁹ We shall henceforth in these cases simply write θ for T .

(vii) It is straightforward to derive from (77)_{2,3,7,8}, definition (81) and (92) as well as the formulae

$$\eta = -\frac{1}{(1/\lambda^\varepsilon)_{,\dot{\theta}}} \Psi_{I,\dot{\theta}}^G, \tag{94}$$

$$\mathcal{P}_\theta = -\rho \lambda^\varepsilon \left\{ (1/\lambda^\varepsilon)_{,\theta} \eta + \Psi_{I,\theta}^G \right\}, \tag{95}$$

$$\mathcal{P}_{\nabla\theta} = -\rho \lambda^\varepsilon \Psi_{I,\nabla\theta}^G, \tag{96}$$

$$\mathcal{P}_{\mathbf{B}_\alpha} = \begin{cases} -\rho \lambda^\varepsilon \Psi_{I,\mathbf{B}_\alpha}^G - \lambda^\varepsilon \Psi_I^G \nu_\alpha \frac{\partial \rho_\alpha}{\partial \mathbf{B}_\alpha}, & \text{if } \alpha = 1, \dots, m, \\ -\rho \lambda^\varepsilon \Psi_{I,\mathbf{B}_\alpha}^G, & \text{if } \alpha = m + 1, \dots, n, \end{cases} \tag{97}$$

$$\mathcal{P}_{\bar{\mathbf{z}}_\alpha} = \lambda_\alpha^Z = -\rho \lambda^\varepsilon \Psi_{I,\bar{\mathbf{z}}_\alpha}^G, \quad \alpha = 1, \dots, n, \tag{98}$$

provided $\dot{\theta}$ is an independent constitutive variable. □

The above formulae complete the exploitation of the integrability conditions (77). They are interesting because: *first*, they show that non-equilibrium entropy and $\mathcal{P}_\theta, \mathcal{P}_{\nabla\theta}, \mathcal{P}_{\mathbf{B}_\alpha}$ and $\lambda_\alpha^Z (\alpha = 1, \dots, n)$ are all derivable from the Helmholtz-like free energy, Ψ_I^G . *Second*, combining (92) with (94) yields an expression for \mathcal{P}_θ , namely

$$\mathcal{P}_\theta = \rho \lambda^\varepsilon (1/\lambda^\varepsilon)_{,\theta} \left\{ \frac{\Psi_{I,\dot{\theta}}^G}{(1/\lambda^\varepsilon)_{,\dot{\theta}}} - \frac{\Psi_{I,\theta}^G}{(1/\lambda^\varepsilon)_{,\theta}} \right\}. \tag{99}$$

Third, if Ψ_I^G does not depend on $\dot{\theta}$, then $\mathcal{P}_\theta = 0$, and the entropy follows from (92). Moreover, in this case the Liu identities imply $\mathcal{F}_{\dot{\theta}} = \mathcal{P}_{\nabla\theta} = \mathbf{0}$, and the Helmholtz-like free energy is independent of $\nabla\theta$.

All these results show a structure which a posteriori support expectations that one might have wished to guess but which are nevertheless surprising. Totally new and surprising is perhaps only (99).

The above results pertain to the Liu identities primarily involving the scalar one-form \mathcal{P} . Analogous statements can also be derived with the use of the vectorial one-form \mathcal{F} . We state results for these in

Proposition 2 (i) *The extra entropy flux vector possesses the representation*

$$\mathbf{k} = -\frac{1}{2} \lambda^\varepsilon \sum_\alpha \mathbf{K}_\alpha(\mathbb{S}) \mathbf{u}_\alpha, \tag{100}$$

with

$$\mathbf{K}_\alpha = \{ \bar{\mathbf{T}}_\alpha - \text{tr}(\bar{\mathbf{T}}_\alpha) \mathbf{I} \} + (\lambda^\varepsilon)^{-1} \{ \mathcal{F}_{\nu_\alpha} - \text{tr}(\mathcal{F}_{\nu_\alpha}) \mathbf{I} \}. \tag{101}$$

(ii) *It follows from the definition (73) and the above results that the entropy flux vector is given by*

$$\phi^{\rho\eta} = \begin{cases} -\lambda^\varepsilon \{ \mathbf{q} + \sum \{ (\bar{\mathbf{T}}_\alpha - \frac{1}{3} \text{tr}(\bar{\mathbf{T}}_\alpha) \mathbf{I}) + \frac{1}{3} \text{tr}(\bar{\mathbf{T}}_\alpha) \mathbf{I} \} \mathbf{u}_\alpha \}, & \text{if } \mathbf{k} = \mathbf{0}, \\ -\lambda^\varepsilon \mathbf{q} - \lambda^\varepsilon \sum \{ \frac{3}{2} \{ \bar{\mathbf{T}}_\alpha - \frac{1}{3} \text{tr}(\bar{\mathbf{T}}_\alpha) \mathbf{I} \} \mathbf{u}_\alpha \\ + \frac{1}{2} (\lambda^\varepsilon)^{-1} \{ \mathcal{F}_{\nu_\alpha} - \text{tr}(\mathcal{F}_{\nu_\alpha}) \mathbf{I} \} \mathbf{u}_\alpha \}, & \text{if } \mathbf{k} \neq \mathbf{0}. \end{cases} \tag{102}$$

(iii) For $\mathcal{P}_{\nabla\theta}$ an alternative expression to (96) is given by

$$\begin{aligned} \mathcal{P}_{\nabla\theta} &= -\lambda_{,\dot{\theta}}^\varepsilon \mathbf{q} - \frac{3}{2} \lambda_{,\dot{\theta}}^\varepsilon \sum \left(\bar{\mathbf{T}}_\alpha - \frac{1}{3} \text{tr}(\bar{\mathbf{T}}_\alpha) \mathbf{I} \right) \mathbf{u}_\alpha \\ &\quad - \frac{1}{2} \lambda^\varepsilon \sum (\bar{\mathbf{T}}_\alpha - \text{tr}(\bar{\mathbf{T}}_\alpha) \mathbf{I})_{,\dot{\theta}} \mathbf{u}_\alpha \\ &\quad - \frac{1}{2} \sum (\mathcal{F}_{\nu_\alpha} - \text{tr}(\mathcal{F}_{\nu_\alpha}) \mathbf{I})_{,\dot{\theta}} \mathbf{u}_\alpha, \end{aligned} \tag{103}$$

which reduces to $\mathcal{P}_{\nabla\theta} = \mathbf{0}$ when $\dot{\theta} \notin \mathbb{S}$. □

Therefore, \mathbf{k} , $\phi^{\rho\eta}$ and $\mathcal{P}_{\nabla\theta}$ are given by combinations of the diffusion velocities with tensorial coefficients which are constitutive quantities. Moreover, the entropy flux vector is not collinear to the heat flux vector, not even when $\mathbf{k} = \mathbf{0}$. Interestingly also, in all relations of Proposition 2 the one-form \mathcal{F} enters only via $\mathcal{F}_{\mathbf{v}_\alpha}$ and its derivative $\mathcal{F}_{\mathbf{v}_\alpha\dot{\theta}}$. All other derivatives of \mathcal{F} are non-observable in this theory. In addition, $\mathcal{P}_{\nabla\theta}$ is also given by (96) in Proposition 1, so that explicit knowledge of $\mathcal{F}_{\mathbf{v}_\alpha\dot{\theta}}$ is not necessary. This is a big advantage of this mixture formulation.

5.2 Implications of the residual entropy inequality

Lengthy calculations, explicitly worked out by Schneider and Hutter [35], show that the residual entropy inequality is given as

$$\begin{aligned}
*\boldsymbol{\pi}^{\rho\eta}_R &= \mathcal{P}_\theta(\dot{\theta}) - \left\{ \mathbf{k}_{,\theta} - (\lambda^\varepsilon)_{,\theta} \left\{ \mathbf{q} + \sum \bar{\mathbf{T}}_\alpha \mathbf{u}_\alpha \right\} \right\} \cdot (\nabla\theta) \\
&\quad + \lambda^\varepsilon \sum_{\alpha=1}^m \left\{ v_\alpha \left(\Delta_D^{*\alpha} + \rho_\alpha^{-1} \rho_\alpha^G \mathbf{I} \right) \mathbf{u}_\alpha - (\lambda^\varepsilon)^{-1} \mathbf{k}_{,\rho_\alpha} \right. \\
&\quad \left. - v_\alpha (\rho \lambda^\varepsilon)^{-1} \text{skw}(\mathcal{P}_{\nabla\theta} \otimes \nabla\theta) \mathbf{u}_\alpha \right\} \cdot (\nabla \rho_\alpha) \\
&\quad + \lambda^\varepsilon \sum_{\alpha=1}^{n-1} \left\{ \left\{ \rho_\alpha \Delta_D^{*\alpha} + \zeta_\alpha \mathbf{I} - \frac{1}{2} \rho_n (\mathbf{u}_n \cdot \mathbf{u}_n) \mathbf{I} \right\} \mathbf{u}_\alpha - \mathbf{c} - (\lambda^\varepsilon)^{-1} \mathbf{k}_{,\mathbf{v}_\alpha} \right. \\
&\quad \left. - (\lambda^\varepsilon)^{-1} \text{skw}(\mathcal{P}_{\nabla\theta} \otimes \nabla\theta) (\xi_\alpha \mathbf{u}_\alpha - \xi_n \mathbf{u}_n) \right\} \cdot (\nabla v_\alpha) \\
&\quad + \lambda^\varepsilon \sum_{\alpha=1}^n \left\{ \bar{\rho}_\alpha \left(\Delta_D^{*\alpha} + \mathbf{u}_\alpha \otimes \mathbf{u}_\alpha \right) + \left(\bar{\zeta}_\alpha - \frac{1}{2} v_\alpha \rho_n (\mathbf{u}_n \cdot \mathbf{u}_n) \right) \mathbf{I} \right. \\
&\quad \left. - 2\rho \text{sym} \left((\Psi_I^G)_{,\mathbf{B}_\alpha} \right) \mathbf{B}_\alpha - (\lambda^\varepsilon)^{-1} \mathbf{k}_{,\mathbf{v}_\alpha} + \bar{\mathbf{T}}_\alpha \right\} \cdot (\mathbf{D}_\alpha) \\
&\quad - \lambda^\varepsilon \sum_{\alpha=1}^n \rho (\Psi_I^G)_{,\bar{\mathbf{z}}_\alpha} \cdot \bar{\boldsymbol{\Phi}}_\alpha \\
&\quad - \lambda^\varepsilon \sum_{\alpha=1}^n \left\{ \mathbf{u}_\alpha \cdot \bar{\mathbf{m}}_\alpha^i + \bar{\rho}_\alpha \left(\mu_\alpha^G \mathbf{I} + \frac{1}{2} \mathbf{u}_\alpha \cdot \mathbf{u}_\alpha \right) c_\alpha - \iota_\alpha \bar{n}_\alpha \right\} \\
&\geq 0,
\end{aligned} \tag{104}$$

in which the following definitions have been used:

$$\Delta_D^{*\alpha} := \rho^{-1} \left\{ \mathbf{T}_D - (\lambda^\varepsilon)^{-1} \text{sym}(\mathcal{P}_{\nabla\theta} \otimes \nabla\theta) \right\} - \Psi_D^G \mathbf{I} + \frac{1}{2} (\mathbf{u}_\alpha \cdot \mathbf{u}_\alpha) \mathbf{I}, \tag{105}$$

$$\zeta_\alpha := \begin{cases} \beta_\alpha^G - \rho_n \Psi_I^G + \varsigma, & \alpha = 1, \dots, n-1, \\ -\rho_n \Psi_I^G + \varsigma, & \alpha = n, \end{cases} \tag{106}$$

$$\mathbf{c} := (\rho_n \Delta_D^{*n} + \zeta_n \mathbf{I}) \mathbf{u}_n, \tag{107}$$

$$\mathbf{T}_D := - \sum_{\alpha} \bar{\rho}_\alpha \mathbf{u}_\alpha \otimes \mathbf{u}_\alpha. \tag{108}$$

The most important consequences implied by the residual entropy inequality are the equilibrium representations for the constitutive quantities and, in a second step, their non-equilibrium parameterizations.

Definition 2 A process is called a thermodynamic equilibrium, denoted by $(\cdot)|_E$, if

- the *non-equilibrium variables*, \mathbf{n} , vanish, i.e.

$$\mathbf{n} := \left\{ \dot{\theta}, \nabla\theta, \bar{\mathbf{v}}, \bar{\mathbf{D}}, \bar{\mathbf{W}} \right\} = \mathbf{0}, \tag{109}$$

- the constitutive quantities of the frictional production rate densities, $\bar{\Phi}_\alpha$ ($\alpha = 1, \dots, n$), are zero in thermodynamic equilibrium,

$$\lim_{n \rightarrow 0} \bar{\Phi}_\alpha =: \bar{\Phi}_\alpha|_E = \mathbf{0}, \quad \alpha = 1, \dots, n, \quad (110)$$

- the interaction rate densities for mass, c_α , and volume fraction, n_α ($\alpha = 1, \dots, n$), also vanish in thermodynamic equilibrium,

$$\lim_{n \rightarrow 0} c_\alpha =: c_\alpha|_E = 0, \quad \lim_{n \rightarrow 0} n_\alpha =: n_\alpha|_E = 0, \quad \alpha = 1, \dots, n. \quad (111)$$

□

The equilibrium requirements in this definition make the entropy production ${}^*\pi^{\rho\eta}_R$ vanish, and because of the non-negativity of it, a local minimum. So, we may say ${}^*\pi^{\rho\eta}_R \geq 0$ in general, but ${}^*\pi^{\rho\eta}_R = 0$ for $n = 0$. Thus, *necessary* conditions for ${}^*\pi^{\rho\eta}_R$ having a minimum at $n = 0$ are

$${}^*\pi^{\rho\eta}_{R, n_I}|_E = 0 \quad \forall \quad n_I \in n, \quad (112)$$

as well as

$$\left\{ {}^*\pi^{\rho\eta}_{R, n_I n_J}|_E \right\} \text{ is non-negative definite } \quad n_I, n_J \in n. \quad (113)$$

Evaluation of (112) by performing the indicated differentiations with respect to $n = \{\mathbf{v}_\beta, \dot{\theta}, \nabla\theta, \mathbf{D}_\beta\}$ leads to the results, collected in

Proposition 3 *The following equilibrium properties can be derived from (112):*

- If $n_I = \mathbf{v}_\beta$:

$$\begin{aligned} \bar{\mathbf{m}}_\beta|_E &= \sum_{\alpha=1}^m \left\{ (\delta_{\alpha\beta} - \bar{\xi}_\beta) \nu_\alpha (\rho_\alpha)^{-1} p_\alpha^G|_E \mathbf{I} - (\lambda^\varepsilon)^{-1}|_E \mathbf{k}_{, \rho_\alpha \mathbf{v}_\beta}|_E \right\} \nabla \rho_\alpha \\ &+ \sum_{\alpha=1}^{n-1} \left\{ (\delta_{\alpha\beta} - \bar{\xi}_\beta) \zeta_\alpha|_E \mathbf{I} - \mathbf{c}_{, \mathbf{v}_\beta}|_E - (\lambda^\varepsilon)^{-1}|_E \mathbf{k}_{, \nu_\alpha \mathbf{v}_\beta}|_E \right\} \nabla \nu_\alpha \\ &- \sum_{\alpha=1}^n \rho \left(\Psi_I^G \right)_{, \bar{\mathbf{z}}_\alpha}|_E \left(\bar{\Phi}_\alpha \right)_{, \mathbf{v}_\beta}|_E \\ &- \sum_{\alpha=1}^n \left\{ \bar{\rho}_\alpha \mu_{\alpha I}^G|_E (c_\alpha)_{, \mathbf{v}_\beta}|_E - \iota_\alpha|_E (\bar{n}_\alpha)_{, \mathbf{v}_\beta}|_E \right\}. \end{aligned} \quad (114)$$

- If $n_I = \dot{\theta}$:

$$\begin{aligned} \mathcal{P}_\theta|_E &= \lambda^\varepsilon|_E \sum_{\alpha=1}^n \rho \left(\Psi_I^G \right)_{, \bar{\mathbf{z}}_\alpha}|_E \cdot \left(\bar{\Phi}_\alpha \right)_{, \dot{\theta}}|_E \\ &+ \lambda^\varepsilon|_E \sum_{\alpha=1}^n \left\{ \bar{\rho}_\alpha \mu_{\alpha I}^G|_E (c_\alpha)_{, \dot{\theta}}|_E - \iota_\alpha|_E (\bar{n}_\alpha)_{, \dot{\theta}}|_E \right\}. \end{aligned} \quad (115)$$

- If $n_I = \nabla\theta$:

$$\begin{aligned} (\lambda^\varepsilon)_{, \theta}|_E \mathbf{q}|_E &= \lambda^\varepsilon|_E \sum_{\alpha=1}^n \rho \left(\Psi_I^G \right)_{, \bar{\mathbf{z}}_\alpha}|_E \cdot \left(\bar{\Phi}_\alpha \right)_{, \nabla\theta}|_E \\ &+ \lambda^\varepsilon|_E \sum_{\alpha=1}^n \left\{ \bar{\rho}_\alpha \mu_{\alpha I}^G|_E (c_\alpha)_{, \nabla\theta}|_E - \iota_\alpha|_E (\bar{n}_\alpha)_{, \nabla\theta}|_E \right\}. \end{aligned} \quad (116)$$

- If $n_I = \mathbf{D}_\beta$:

$$\begin{aligned}\bar{\mathbf{T}}_\beta|_E &= -\bar{\zeta}_\beta|_E \mathbf{I} + 2\rho \operatorname{sym} \left((\Psi_I^G),_{\mathbf{B}_\beta} \right) |_E \mathbf{B}_\beta + (\lambda^\varepsilon)^{-1} |_E \mathbf{k},_{\mathbf{v}_\beta} |_E \\ &+ \sum \rho \left(\Psi_I^G \right),_{\bar{\mathbf{z}}_\alpha} |_E (\bar{\Phi}_\alpha),_{\mathbf{D}_\beta} |_E \\ &+ \sum \left\{ \bar{\rho}_\alpha \mu_\alpha^G |_E (c_\alpha),_{\mathbf{D}_\beta} |_E - \iota_\alpha |_E (\bar{n}_\alpha),_{\mathbf{D}_\beta} |_E \right\}\end{aligned}\quad (117)$$

□

Let us discuss the results stated in this proposition in due order.

- (1) First, we observe that the frictional constitutive quantities $\bar{\Phi}_\alpha$ ($\alpha = 1, \dots, n$) influence the equilibrium quantities $\bar{\mathbf{m}}_\beta|_E$, $\mathcal{P}_\theta|_E$, $\mathbf{q}|_E$ and $\bar{\mathbf{T}}_\beta|_E$ directly via the terms involving $(\bar{\Phi}_\alpha),_{n_I} |_E$. Similarly, $\bar{\mathbf{m}}_\beta|_E$, $\mathcal{P}_\theta|_E$, $\mathbf{q}|_E$ and $\bar{\mathbf{T}}_\beta|_E$ may also be influenced by the mass and volume fraction production rate densities, if the respective derivatives $(c_\alpha),_{n_I}$ and $(\bar{n}_\alpha),_{n_I}$ have non-zero values. We shall discuss these properties in greater detail below. Beyond these dependences the equilibrium interaction forces exhibit also additional dependences on $\nabla \rho_\alpha$ ($\alpha = 1, \dots, m$) and ∇v_β ($\beta = 1, \dots, n-1$) with also possible dependences on the thermodynamic, configuration and saturation pressures via p_α^G ($\alpha = 1, \dots, m$), ζ_γ ($\gamma = 1, \dots, n$) and the extra entropy flux vector \mathbf{k} ; the dependence on the latter arises provided $\mathbf{k},_{\rho_\alpha v_\alpha}$ and $\mathbf{k},_{v_\alpha v_\alpha}$ are different from zero. If all constituents are density preserving and no volume fraction interaction rate densities are present, consideration of ∇v_α ($\alpha = 1, \dots, n-1$) is essential for the description of $\bar{\mathbf{m}}_\beta|_E$. However, if we would disregard all ∇v_α 's in the constitutive relations, $\bar{\mathbf{m}}_\beta|_E$ would still not be zero in that case, because the variable ζ_α contains the saturation pressure and the inner free energy Ψ_I^G , see (106).
- (2) Relation (115) is a revealing by-product of the thermodynamic analysis, since the general formula (92) in Proposition 1 for the entropy implies in thermostatic equilibrium

$$\begin{aligned}\eta|_E &= \frac{-1}{(1/\lambda^\varepsilon),_\theta |_E} \left\{ (\Psi_{I,\theta}^G)|_E + \frac{\mathcal{P}_\theta|_E}{\rho \lambda^\varepsilon|_E} \right\} \\ &= \frac{-1}{(1/\lambda^\varepsilon),_\theta |_E} \left\{ (\Psi_{I,\theta}^G)|_E + \sum_{\alpha=1}^n \left(\Psi_I^G \right),_{\bar{\mathbf{z}}_\alpha} |_E \cdot (\bar{\Phi}_\alpha),_{\dot{\theta}} |_E \right. \\ &\quad \left. + \sum_{\alpha=1}^n \frac{1}{\rho} \left\{ \bar{\rho}_\alpha \mu_\alpha^G |_E (c_\alpha),_{\dot{\theta}} |_E - \iota_\alpha |_E (\bar{n}_\alpha),_{\dot{\theta}} |_E \right\} \right\}.\end{aligned}\quad (118)$$

Moreover, we remark that when $\dot{\theta} \notin \mathbb{S}$, one has $\mathcal{P}_\theta = 0$, $\lambda^\varepsilon = \lambda^\varepsilon(\theta) = 1/\theta$, so that (118) implies the classical relation $\eta = -\Psi_{I,\theta}^G$. Alternatively, for $\dot{\theta} \in \mathbb{S}$ the right-hand side of (118) is known when the thermodynamic quantities Ψ_I^G , $\bar{\Phi}_\alpha$, μ_α^G and ι_α are prescribed.

- (3) We observe in (116) that the equilibrium heat flux may not vanish if the production rate density derivatives $(\bar{\Phi}_\alpha),_{\nabla\theta} |_E$, $(c_\alpha),_{\nabla\theta} |_E$ and $(\bar{n}_\alpha),_{\nabla\theta} |_E$ differ from zero. If these contributions do not vanish, then $\mathbf{q}|_E$ should be interpreted not as a heat flux but as a conductive flux of mechanical energy. Such an equilibrium energy flux is, however, unlikely. So, to have $\mathbf{q}|_E = \mathbf{0}$, it suffices to request that $\bar{\Phi}_\alpha$, c_α and \bar{n}_α do not depend on $\nabla\theta$.
- (4) As for the partial equilibrium stress tensor, equation (117) shows in its first line that beyond the generalized pressure $\zeta_\beta|_E$ and the contribution $\mathbf{k},_{\mathbf{v}_\beta} |_E$, an elastic contribution arises, which depends on the constituent left Cauchy Green deformation tensor \mathbf{B}_β . For mature debris flows it is known that elastic effects are far from being dominant, but elastic contributions are nevertheless often used to describe shear stresses in thermodynamic equilibrium ('heap problem'). However, these equilibrium shear stresses are less due to elastic and more to frictional effects which are thought to be describable by means of a plasticity theory, e.g. hypoplasticity. The fourth term of constitutive relation (117) is exclusively due to frictional effects and has already been introduced by Svendsen et al. [37].
- (5) It is worth emphasizing that the results stated in Proposition 3 are mathematical consequences of the second law of thermodynamics. This fact should be kept in mind, in particular, for the equilibrium expressions

(114) for $\bar{\mathbf{m}}_\beta|_E$ and (117) for $\bar{\mathbf{T}}_\beta|_E$, which have purely mechanical significance. There is no freedom of their choice.¹⁰

It is at this point worthwhile to pause and to summarize what has been attained. We have expressed the equilibrium interaction forces (114), the equilibrium entropy (118), the equilibrium energy flux (116) and the equilibrium partial stress tensors (117) in terms of clearly identifiable contributions, all of which were obtained from the exploitation of the entropy principle, in particular the so-called Liu identities and the inferences deduced from them. A first set of these is generally of direct thermodynamic origin and involves a thermodynamic potential, derivatives of it with respect to the true constituent densities and the volume fraction densities, the saturation pressure as well as certain derivatives of the extra entropy flux vector. In the expression for the interaction forces (114) these terms also depend explicitly on $\nabla\rho_\alpha$ and ∇v_α (first two lines in (114)). In the expression for the entropy (118) they only involve $\Psi_{I,\theta}^G|_E$, in the heat flux (116) they are not present at all, and in the expression for the equilibrium constituent stress tensors (117) they comprise the pressure like quantity ζ_α , the elastic contributions and the extra entropy flux, stated in the first line of (117). The remaining contributions to the above mentioned equilibrium quantities are equally of thermodynamic origin, but they only exist if the production rate densities of the frictional tensorial variable, $\bar{\Phi}_\alpha$ and the constituent mass, c_α and volume fractions, n_α do not vanish. They all appear as sums of products of derivatives of $\bar{\Phi}_\alpha$, c_α and n_α with prefactors which are the same in the expressions of $\bar{\mathbf{m}}_\beta^i|_E$, $\eta|_E$, $\mathbf{q}|_E$ and $\bar{\mathbf{T}}_\alpha|_E$. The prefactors are

$$\begin{aligned} \rho(\Psi_I^G), \bar{z}_\alpha|_E & \text{ for the friction term } \bar{\Phi}_\alpha \\ \bar{\rho}_\alpha \mu_\alpha^G|_E & \text{ for the mass production } c_\alpha \\ \iota_\alpha|_E & \text{ for the volume fraction production } n_\alpha. \end{aligned} \quad (119)$$

They are known once and for all when the inner Helmholtz-like free energy is known as a function of its variables, and the constituent free energies, see (87), and the parameters ι_α , see (91), are known. The above factors, in turn, are multiplied

$$\begin{aligned} \text{for } \bar{\mathbf{m}}_\beta^i|_E & \text{ with } (\bar{\Phi}_\alpha),_{v_\beta}|_E (c_\alpha),_{v_\beta}|_E, (\bar{n}_\alpha),_{v_\beta}|_E \\ \text{for } \eta|_E & \text{ with } (\bar{\Phi}_\alpha),_{\dot{\theta}}|_E (c_\alpha),_{\dot{\theta}}|_E, (\bar{n}_\alpha),_{\dot{\theta}}|_E \\ \text{for } \mathbf{q}|_E & \text{ with } (\bar{\Phi}_\alpha),_{\nabla\theta}|_E (c_\alpha),_{\nabla\theta}|_E, (\bar{n}_\alpha),_{\nabla\theta}|_E \\ \text{for } \bar{\mathbf{T}}_\alpha|_E & \text{ with } (\bar{\Phi}_\alpha),_{\mathbf{D}_\beta}|_E (c_\alpha),_{\mathbf{D}_\beta}|_E, (\bar{n}_\alpha),_{\mathbf{D}_\beta}|_E \end{aligned} \quad (120)$$

and subsequently summed to reveal the corresponding representations arising in (114), (118), (116) and (117). The two lists (119) and (120) disclose the thermodynamic structure of the various contributions to the equilibrium quantities $\bar{\mathbf{m}}_\beta^i|_E$, $\eta|_E$, $\mathbf{q}|_E$ and $\bar{\mathbf{T}}_\alpha|_E$ particularly clear. The constituent equilibrium interaction forces receive contributions exclusively via derivatives of $\bar{\Phi}_\alpha$, c_α and n_α with respect to the constituent velocities. Analogously, the equilibrium entropy is directly affected only by corresponding derivatives with respect to $\dot{\theta}$, the equilibrium heat flux vector by corresponding derivatives with respect to $\nabla\theta$ and the equilibrium constituent stresses by those with respect to \mathbf{D}_β . This demonstrates, on the one hand, that contributions to $\bar{\mathbf{m}}_\beta^i|_E$ and $\text{div}(\bar{\mathbf{T}}_\alpha|_E)$ are not likely interchangeable. On the other hand, the list (120) can serve as a help when explicitly parameterising constitutive relations for $\bar{\Phi}_\alpha$, c_α and n_α . For instance, we may have reason to assume that thermal effects are insignificant. Then, it may be justified to postulate that

$$(\bar{\Phi}_\alpha, c_\alpha, n_\alpha),_{\dot{\theta}} = 0, \quad (\bar{\Phi}_\alpha, c_\alpha, n_\alpha),_{\nabla\theta} = \mathbf{0}. \quad (121)$$

This would yield

$$\eta|_E = -\Psi_{I,\theta}^G \quad \text{and} \quad \mathbf{q}|_E = \mathbf{0}, \quad (122)$$

agreeing with the classical relations. Moreover, we may assume $\bar{\Phi}_{\alpha,v_\beta} = \mathbf{0}$; in this case the contribution of the frictional variable to the interaction force would vanish, whilst that to the constituent stresses would still be present via $(\bar{\Phi}_\alpha),_{\mathbf{D}_\beta}|_E$. We shall see that these terms, when properly parameterised, will give rise to the thermodynamic justification of hypo-plasticity. In any case, keeping the full generality of the constitutive dependences of $\bar{\Phi}_\alpha$, c_α and n_α brought, via (119) and (120), light into a deeper understanding of the structure of the formulae of the constitutive quantities as imposed by the entropy principle. It is now much easier to understand the role played by ad-hoc simplifications of certain constitutive relations for $\bar{\Phi}_\alpha$, c_α and n_α than it would have been if such simplifications had been introduced at the outset.

¹⁰ We emphasize that this is a consequence of the second law of thermodynamics. Purely mechanical reasoning, that is sometimes used to ‘derive’ expressions for the interaction force, must be regarded as a priori estimates. They must be complemented by an additional term whose structure follows from the second law of thermodynamics.

5.3 Non-equilibrium representations for \vec{c} , \vec{n} and \mathbf{k}

Let $\mathbb{S}\mathbf{y} = \mathbb{S}_n \oplus (\mathbb{S}_{\vec{\nabla}\rho} \cup \mathbb{S}_{\vec{\nabla}v})$ be the space of the elements

$$\mathcal{Y} := \left\{ \dot{\theta}, \nabla\theta, \vec{\nabla}\rho, \vec{\nabla}v, \vec{v}, \vec{\mathbf{D}}, \vec{\mathbf{W}} \right\}. \quad (123)$$

It consists of the non-equilibrium elements \mathbf{n} and $\vec{\nabla}\rho$ and $\vec{\nabla}v$. The state $\mathcal{Y} = \mathbf{0}$ is a subspace of the space describing mixture thermodynamic equilibrium, because $\vec{\nabla}\rho$ and $\vec{\nabla}v$ are also set to zero.

In this section, we collect some results obtained when performing an isotropic expansion of the non-equilibrium quantities \vec{c} , \vec{n} and \mathbf{k} in terms of the elements \mathcal{Y} . Such expansions are more restrictive than an expansion about a mixture thermodynamic equilibrium, due to the additional requirement that $\mathcal{Y} = \mathbf{0}$ implies also $\nabla\rho_\alpha$ ($\alpha = 1, \dots, m$) and ∇v_β ($\beta = 1, \dots, n-1$).

A linear representation of the scalars c_α and n_α in terms of \mathcal{Y} would only involve $\dot{\theta}$ and $\text{tr}(\mathbf{D}_\beta)$, which is too simple and likely unrealistic. Therefore, at least a quadratic expansion is necessary. A minimal form of an ‘isotropic’ expansion of c_α thus reads as follows

$$\begin{aligned} c_\alpha &= c_\alpha^\dot{\theta}(\dot{\theta}) + \left\{ \sum_{\beta=1}^m c_{\alpha\beta}^{\theta\rho}(\nabla\rho_\beta) + \sum_{\beta=1}^{n-1} c_{\alpha\beta}^{\theta v}(\nabla v_\beta) \right\} \cdot (\nabla\theta) \\ &+ \sum_{\beta=1}^n \left\{ \sum_{\gamma=1}^m c_{\alpha\beta\gamma}^{\nu\rho}(\nabla\rho_\gamma) + \sum_{\gamma=1}^{n-1} c_{\alpha\beta\gamma}^{\nu v}(\nabla v_\gamma) \right\} \cdot (\mathbf{v}_\beta) \\ &+ \sum_{\beta=1}^n \left\{ c_{\alpha\beta}^{\mathbf{D}} \mathbf{I} + \mathbf{C}_{\alpha\beta}^{\mathbf{D}} \right\} \cdot (\mathbf{D}_\beta) \\ &+ \sum_{\beta=1}^n \left\{ \mathbf{C}_{\alpha\beta}^{\mathbf{W}} \right\} \cdot (\mathbf{W}_\beta) \\ &+ c_\alpha^{\mathbf{N}}, \end{aligned} \quad (124)$$

where the term $c_\alpha^{\mathbf{N}}$ accounts for the remaining non-linear contributions and depends on all constitutive variables. It must vanish in thermodynamic equilibrium, i.e.

$$c_\alpha^{\mathbf{N}}|_{\mathbf{E}} = 0, \quad (125)$$

to be in accordance with (111)₁. The tensors $\mathbf{C}_{\alpha\beta}^{\mathbf{D}}$ and $\mathbf{C}_{\alpha\beta}^{\mathbf{W}}$ are defined as

$$\begin{aligned} \mathbf{C}_{\alpha\beta}^{\mathbf{D}} &:= \sum_{\delta=1}^m \left\{ \sum_{\gamma=1}^m c_{\alpha\beta\gamma\delta}^{\mathbf{D}\rho} \text{sym}(\nabla\rho_\delta \otimes \nabla\rho_\gamma) + \sum_{\gamma=1}^{n-1} c_{\alpha\beta\gamma\delta}^{\mathbf{D}v\rho} \text{sym}(\nabla\rho_\delta \otimes \nabla v_\gamma) \right\} \\ &+ \sum_{\delta=1}^{n-1} \left\{ \sum_{\gamma=1}^{n-1} c_{\alpha\beta\gamma\delta}^{\mathbf{D}v} \text{sym}(\nabla v_\delta \otimes \nabla v_\gamma) \right\}, \end{aligned} \quad (126)$$

and

$$\begin{aligned} \mathbf{C}_{\alpha\beta}^{\mathbf{W}} &:= \sum_{\delta=1}^m \left\{ \sum_{\gamma=1}^m c_{\alpha\beta\gamma\delta}^{\mathbf{W}\rho} \text{skw}(\nabla\rho_\delta \otimes \nabla\rho_\gamma) + \sum_{\gamma=1}^{n-1} c_{\alpha\beta\gamma\delta}^{\mathbf{W}v\rho} \text{skw}(\nabla\rho_\delta \otimes \nabla v_\gamma) \right\} \\ &+ \sum_{\delta=1}^{n-1} \left\{ \sum_{\gamma=1}^{n-1} c_{\alpha\beta\gamma\delta}^{\mathbf{W}v} \text{skw}(\nabla v_\delta \otimes \nabla v_\gamma) \right\}. \end{aligned} \quad (127)$$

Analogous representations also hold for n_α :

$$\begin{aligned}
 n_\alpha &= n_\alpha^{\dot{\theta}}(\dot{\theta}) + \left\{ \sum_{\beta=1}^m n_{\alpha\beta}^{\theta\rho}(\nabla\rho_\beta) + \sum_{\beta=1}^{n-1} n_{\alpha\beta}^{\theta v}(\nabla v_\beta) \right\} \cdot (\nabla\theta) \\
 &+ \sum_{\beta=1}^n \left\{ \sum_{\gamma=1}^m n_{\alpha\beta\gamma}^{v\rho}(\nabla\rho_\gamma) + \sum_{\gamma=1}^{n-1} n_{\alpha\beta\gamma}^{vv}(\nabla v_\gamma) \right\} \cdot (\mathbf{v}_\beta) \\
 &+ \sum_{\beta=1}^n \left\{ n_{\alpha\beta}^D \mathbf{I} + \mathbf{N}_{\alpha\beta}^D \right\} \cdot (\mathbf{D}_\beta) \\
 &+ \sum_{\beta=1}^n \left\{ \mathbf{N}_{\alpha\beta}^W \right\} \cdot (\mathbf{W}_\beta) \\
 &+ n_\alpha^N,
 \end{aligned} \tag{128}$$

where the term n_α^N accounts for the remaining non-linear contributions and depends on all constitutive variables. It must vanish in thermodynamic equilibrium, i.e.

$$n_\alpha^N|_E = 0, \tag{129}$$

to be in accordance with (111)₂. The tensors $\mathbf{N}_{\alpha\beta}^D$ and $\mathbf{N}_{\alpha\beta}^W$ are defined as

$$\begin{aligned}
 \mathbf{N}_{\alpha\beta}^D &:= \sum_{\delta=1}^m \left\{ \sum_{\gamma=1}^m n_{\alpha\beta\gamma\delta}^{D\rho} \text{sym}(\nabla\rho_\delta \otimes \nabla\rho_\gamma) + \sum_{\gamma=1}^{n-1} n_{\alpha\beta\gamma\delta}^{Dv\rho} \text{sym}(\nabla\rho_\delta \otimes \nabla v_\gamma) \right\} \\
 &+ \sum_{\delta=1}^{n-1} \left\{ \sum_{\gamma=1}^{n-1} n_{\alpha\beta\gamma\delta}^{Dv} \text{sym}(\nabla v_\delta \otimes \nabla v_\gamma) \right\},
 \end{aligned} \tag{130}$$

and

$$\begin{aligned}
 \mathbf{N}_{\alpha\beta}^W &:= \sum_{\delta=1}^m \left\{ \sum_{\gamma=1}^m n_{\alpha\beta\gamma\delta}^{W\rho} \text{skw}(\nabla\rho_\delta \otimes \nabla\rho_\gamma) + \sum_{\gamma=1}^{n-1} n_{\alpha\beta\gamma\delta}^{Wv\rho} \text{skw}(\nabla\rho_\delta \otimes \nabla v_\gamma) \right\} \\
 &+ \sum_{\delta=1}^{n-1} \left\{ \sum_{\gamma=1}^{n-1} n_{\alpha\beta\gamma\delta}^{Wv} \text{skw}(\nabla v_\delta \otimes \nabla v_\gamma) \right\}.
 \end{aligned} \tag{131}$$

The coefficients arising in (124)–(127) and (128)–(131) can, in general, be expressed as isotropic tensor functions of the variables

$$\{\theta, \bar{\rho}, \bar{v}, \bar{\mathbf{B}}, \bar{\mathbf{Z}}\}, \tag{132}$$

but are in practical cases best assumed to be constants. They must obey a number of constraints, which are explicitly derived and stated by Schneider and Hutter [35].

Extra entropy flux \mathbf{k} If we apply the same expansion to the extra entropy flux, \mathbf{k} , we know from (100) that \mathbf{k} is given by a vector combination of \mathbf{u}_α (or, equivalently of \mathbf{v}_α) so that

$$\mathbf{k} = \sum (k_\alpha^v) \mathbf{v}_\alpha + \mathbf{k}^N, \tag{133}$$

where the coefficients k_α^v are defined as

$$k_\alpha^v \mathbf{I} := \mathbf{k}_{, \mathbf{v}_\alpha} |_{\mathcal{Y}=0} = \hat{k}_\alpha^v(\theta, \bar{\rho}, \bar{v}, \bar{\mathbf{B}}, \bar{\mathbf{Z}}) \mathbf{I}, \quad \alpha = 1, \dots, n \tag{134}$$

and \mathbf{k}^N , again, subsumes all other contributions of the constitutive variables and, due to the principle of objectivity \mathbf{k} satisfies the sum relations (see Schneider and Hutter [35])

$$\sum \mathbf{k}_{,\mathbf{v}_\beta} = \mathbf{0} \quad \Rightarrow \quad \sum k_\beta^v = 0, \quad \sum (\mathbf{k}^N)_{,\mathbf{v}_\beta} = \mathbf{0}. \quad (135)$$

These restrict the independences of the parameters k_β^v , $(\mathbf{k}^N)_{,\mathbf{v}_\beta}$.

5.4 Final representations for $\bar{\mathbf{m}}_\alpha^i|_E$, $\mathbf{q}|_E$, $\bar{\mathbf{T}}_\alpha|_E$ and $\eta|_E$

The purpose of the above ‘isotropic’ expansion is to simplify the derivatives of \bar{c} , \bar{n} and \mathbf{k} arising in the constitutive relations for the equilibrium quantities $\bar{\mathbf{m}}_\alpha^i|_E$, $\mathbf{q}|_E$, $\bar{\mathbf{T}}_\alpha|_E$ and $\eta|_E$. The expressions for the derivatives are then substituted in (114), (116), (117) and (118). The results for the case when θ is an independent constitutive variable are presented in Schneider and Hutter [35]. Here, we limit attention to the case that $\theta \notin \mathbb{S}$. For this case, we have shown that $\mathcal{P}_\theta = 0$, $\mathcal{P}_{\nabla\theta} = \mathbf{0}$ and $(\Psi_I^G)_{,\nabla\theta} = \mathbf{0}$. The emerging formulae are collected in

Proposition 4 *If $\lambda^\varepsilon = \hat{\lambda}^\varepsilon(\theta)$, entropy, equilibrium energy flux, partial equilibrium stresses and interaction forces are given by*

$$\eta = -(\Psi_I^G)_{,\theta}, \quad (136)$$

$$\begin{aligned} \lambda_{,\theta}^\varepsilon|_E \mathbf{q}|_E &= -\theta^{-1} \sum_{\beta=1}^m \left\{ \sum_{\alpha=1}^n \bar{\rho}_\alpha \mu_{I\alpha}^G|_E c_{\alpha\beta}^{\theta\rho} - \sum_{\alpha=1}^n \iota_\alpha n_{\alpha\beta}^{\theta\rho} \right\} (\nabla\rho\beta) \\ &\quad -\theta^{-1} \sum_{\beta=1}^{n-1} \left\{ \sum_{\alpha=1}^n \bar{\rho}_\alpha \mu_{I\alpha}^G|_E c_{\alpha\beta}^{\theta v} - \sum_{\alpha=1}^n \iota_\alpha n_{\alpha\beta}^{\theta v} \right\} (\nabla v\beta) \\ &\quad -\theta^{-1} \sum_{\alpha=1}^n \rho \left(\Psi_I^G \right)_{,\bar{\mathbf{z}}_\alpha}|_E (\bar{\Phi}_\alpha)_{,\nabla\theta}|_E \\ &\quad + \mathbf{q}^N|_E, \end{aligned} \quad (137)$$

$$\begin{aligned} \bar{\mathbf{T}}_\beta|_E &= -\bar{\omega}_\beta \mathbf{I} + 2\rho \operatorname{sym} \left(\Psi_{I,\mathbf{B}_\beta}^G \right)|_E \mathbf{B}_\beta|_E + \sum \rho \left(\Psi_{I,\bar{\mathbf{z}}_\alpha}^G \right)|_E (\bar{\Phi}_\alpha)_{,\mathbf{D}_\beta}|_E \\ &\quad + \sum_{\alpha=1}^n \bar{\rho}_\alpha \mu_{I\alpha}^G|_E \mathbf{C}_{\alpha\beta}^D - \sum_{\alpha=1}^n \bar{t}_\alpha|_E \mathbf{N}_{\alpha\beta}^D + \bar{\mathbf{T}}_\beta^N|_E, \end{aligned} \quad (138)$$

$$\begin{aligned} \bar{\mathbf{m}}_\beta^i|_E &= \sum_{\alpha=1}^m \left\{ \rho_\alpha^{-1} \bar{p}_\alpha|_E (\delta_{\alpha\beta} - \bar{\xi}_\beta) \mathbf{I} - \theta (k_\beta^v)_{,\rho_\alpha} \mathbf{I} \right. \\ &\quad \left. - \sum_{\gamma=1}^n \bar{\rho}_\gamma \mu_{I\gamma}^G|_E c_{\gamma\beta\alpha}^{\nu\rho} + \sum_{\gamma=1}^n \bar{t}_\gamma|_E n_{\gamma\beta\alpha}^{\nu\rho} \right\} (\nabla\rho\alpha) \\ &\quad + \sum_{\alpha=1}^{n-1} \left\{ \zeta_\alpha|_E (\delta_{\alpha\beta} - \bar{\xi}_\beta) \mathbf{I} - \mathbf{c}_{,\mathbf{v}_\beta}|_E - \theta (k_\beta^v)_{,\mathbf{v}_\alpha} \mathbf{I} \right. \\ &\quad \left. - \sum_{\gamma=1}^n \bar{\rho}_\gamma \mu_{I\gamma}^G|_E c_{\gamma\beta\alpha}^{\nu v} + \sum_{\gamma=1}^n \bar{t}_\gamma|_E n_{\gamma\beta\alpha}^{\nu v} \right\} (\nabla v\alpha) \\ &\quad + \sum_{\alpha=1}^n \rho \left(\Psi_I^G \right)_{,\bar{\mathbf{z}}_\alpha}|_E (\bar{\Phi}_\alpha)_{,\mathbf{v}_\beta}|_E \\ &\quad + \bar{\mathbf{m}}_\beta^N|_E, \end{aligned} \quad (139)$$

with

$$\bar{\omega}_\beta := \bar{\zeta}_\beta|_E - \theta k_\beta^v - \sum_{\alpha=1} \bar{\rho}_\alpha \mu_\alpha^G|_E c_{\alpha\beta}^D + \sum_{\alpha=1}^n \bar{t}_\alpha|_E n_{\alpha\beta}^D. \quad (140)$$

□

A complete exploitation of the equilibrium conditions also requires the satisfaction of the minimum requirement (113). The exploitation of these is better done with specialized constitutive relations, see Part II of this article.

6 Discussion

It is worthwhile to discuss in some detail the results that have been reached up to now. We start with the properties of the constituent stresses and interaction forces in thermodynamic equilibrium. The main results are collected in the formulae of Proposition 4.

The equilibrium stress tensor (138) comprises six terms, a pressure, an elastic and a frictional contribution in the first line of (138), and two terms that trace back to non-vanishing interaction rate densities of mass and volume fractions as well as terms that are due to higher order non-linearities, the latter three in the second line of (138). We know of no formulation where this last term would have a non-zero value. The first term in the first line may be interpreted as ‘pressure’, but as shown by (140), it is itself composed of a number of terms of different origin,

- $\bar{\zeta}_\beta|_E$ which may be called ‘true constituent pressure’,
- θk_β^v of purely thermodynamic nature. Its origin is the extra entropy flux \mathbf{k} in (73) or (100), of which the isotropic representation is given in (133), (134). Nothing is known about this term and no obvious arguments can presently be given that θk_β^v should be different from zero. So, we shall later set $k_\beta^v = 0$ for all β , see Part II.
- The remaining members of (140) may only differ from zero, when mass and volume fraction interaction rate densities are different from zero.

Looking at the ‘true constituent pressure’ $\bar{\zeta}_\beta|_E$, it follows from its definition, see (106), that

$$\zeta_\alpha := \begin{cases} \beta_\alpha^G - \rho_n \Psi_I^G + \zeta, & \alpha = 1, \dots, n-1, \\ -\rho_n \Psi_I^G + \zeta, & \alpha = n, \end{cases} \quad (141)$$

which, for the first $n-1$ components, is given by the configuration pressure and for all constituents by the inner free energy and the saturation pressure. It is evident from the definition above that $\bar{\zeta}_\alpha$ has the form

$$\bar{\zeta}_\alpha = \nu_\alpha \zeta_n + \nu_\alpha \beta_\alpha^G, \quad (\alpha = 1, \dots, n-1), \quad \zeta_n = -\rho_n \Psi_I^G + \zeta. \quad (142)$$

Only the first term on the right-hand side has the structure ‘volume fraction times an internal pressure’ where this internal pressure is the saturation pressure plus a contribution due to the inner free energy. This part is reminiscent of what is known as ‘pressure equilibrium’, which, in Part II, will be discussed in connection with the assumption of pressure equilibrium that applies to all pressure terms not just to some parts of the constituent pressure. The last two members of the pressure term (140) are the contributions due to the inter-constituent mass and volume fraction interaction rate densities; they obviously resemble the structure of interaction terms. Only if these productions are not present and the inner free energy does not depend on the constituent volume fractions, and when $k_\beta^v = 0$, the equilibrium pressure is given by

$$\bar{\zeta}_\alpha|_E = \nu_\alpha \zeta_n \quad (\alpha = 1, \dots, n). \quad (143)$$

Let us look next at the remaining contributions to the constituent equilibrium stress tensors (138). They consist in the first line of elastic and frictional contributions and both will further be analysed in Part II. Here, it may suffice to mention that the fluid and solid constituents need separate attention. Moreover, compressible and density preserving constituents need to be treated separately. We shall not go into any depth discussing the

contributions on the second line of (138) due to constituent mass and volume fraction interaction rate densities except that the equilibrium stress of one constituent is affected by contributions from all other constituents with non-vanishing mass and volume fraction interaction rate densities. The coefficients are given by the inner parts of the constituent free enthalpies (chemical potentials, Gibbs free energies) defined in (87)–(89). Notice also that the coefficient ι_α defined in (88) and given by the Lagrange multipliers λ^ε and λ_α^v only arises in connection with the constituent volume fraction production rate densities.

Consider next the constituent interaction forces. Their equilibrium values are given in (139). Apart from the very last non-linear term they consist of contributions that are proportional to the density gradients and similar ones that are proportional to the volume fraction gradients. Contributions of the former are only present for compressible constituents. The coefficients of the density gradient $\nabla\rho_\alpha$ represent (i) a contribution due to the thermodynamic pressure (83), (ii) due to the extra entropy flux (133), (later to be set to zero), (iii) due to the constituent free enthalpies (87) and (iv) the Lagrange multipliers in λ_α^v , defined in (91). Alternatively, the coefficients of the volume fraction densities ∇v_α are (i) due to the true pressure (106), (ii) due to the extra entropy flux (133), (134) (later to be set to zero), (iii) due to the free enthalpies (87), and (iv), due to the Lagrange multipliers in (91). These terms are very similar to one another, and they also have their correspondences in the equilibrium stresses.

We note that, modulo our assumptions, the formulae revealing the equilibrium properties of the constituent Cauchy stress tensors and the constituent interaction forces are rational deductions from the Second Law of Thermodynamics. In fact, there is no flexibility in their choice. Thermodynamic arguments have resulted in their precise definition. We may now also give a partial answer to the question whether the formulae provide room for a different splitting of the divergence of the constituent stress tensor and the interaction force. In principle, the formulae (138) to (139) show how terms arising in the constituent stress tensors and interaction forces can be moved from one to the other. They must appear in the interaction forces as the divergence of a second order tensor or the gradient of a scalar. Or products of scalars with gradients can be complemented to such terms. For instance $a\nabla b$ is replaced by $\nabla(ab) - b\nabla a$. Of course, there is a multitude of such possibilities by way of the gradient operator of any pressure term or the divergence of any stress contribution. Such transformations may, however, destroy the property that the newly defined interaction force, summed over all constituents, must vanish. Moreover, the thermodynamic structure explained in connection with the properties (120) may be destroyed in this way. In addition, such transformations are always connected with differentiations which destroy the global structure and therefore possibly weak formulation of the balance laws. It is for these reasons that we do not recommend them unless, of course, one wishes to search for the equivalence or non-equivalence of seemingly different formulations.

In Part II of this article, we shall apply this theory to a density preserving binary mixture, in which (i) $\dot{\theta}$ is not an independent constitutive variable, (ii) the mass and volume fraction production rate densities are ignored, (iii) the frictional production rate density, Φ_{solid} , is postulated such that a hypo-plastic frictional stress contribution is generated, (iv) nonlinear viscous stress contributions are suggested to arrive at a model, which is capable to describe shear band formation under quasi-static processes and develop into slope instabilities and further to catastrophic rapid shearing in avalanching flows and eventually into a set-down in the deposition zone. We shall also scrutinize the assumption of ‘pressure equilibrium’, lay open its restriction and replace it by a thermodynamically motivated alternative assumption, which removes these restrictions.

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